Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 – 06:50 PM BST

PDB ID	:	3MUU
Title	:	Crystal structure of the Sindbis virus E2-E1 heterodimer at low pH
Authors	:	Li, L.; Jose, J.; Xiang, Y.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2010-05-03
Resolution	:	3.29 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

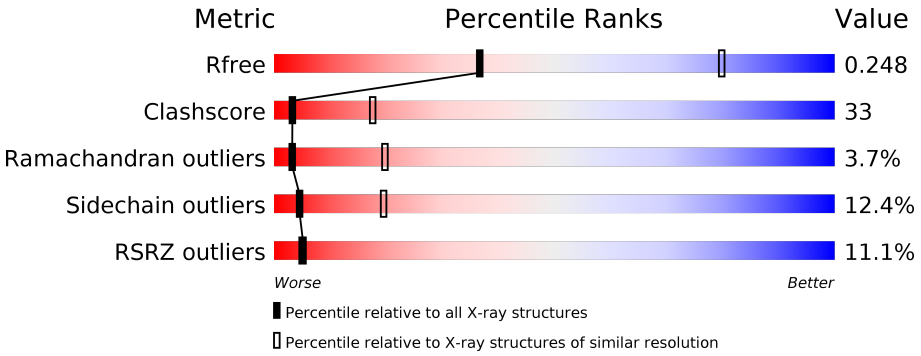
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.29 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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 <=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	750	8% 39% 36% 7% 17%
1	B	750	9% 37% 38% 7% 17%
1	C	750	8% 38% 37% 7% • 17%
1	D	750	11% 39% 36% 8% 17%
1	E	750	10% 40% 35% 7% 17%
1	F	750	9% 39% 36% 7% 18%

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Mol	Chain	Length	Quality of chain
2	G	4	25% 75%
2	I	4	100%
2	J	4	50% 50%
2	K	4	50% 50%
2	L	4	25% 75%
2	M	4	75% 25%
2	O	4	50% 50%
2	Q	4	100%
3	H	5	20% 80%
3	P	5	20% 40% 40%
3	R	5	20% 20% 60%
4	N	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	1	X	-	-	-
2	MAN	I	4	-	-	-	X
2	NAG	Q	1	X	-	-	-
3	MAN	H	4	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29159 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 Structural polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	Se	0	0	0
			4767	3015	808	910	24	10			
1	B	622	Total	C	N	O	S	Se	0	0	0
			4761	3013	808	906	24	10			
1	C	622	Total	C	N	O	S	Se	0	0	0
			4761	3012	807	908	24	10			
1	D	622	Total	C	N	O	S	Se	0	0	0
			4760	3009	807	910	24	10			
1	E	623	Total	C	N	O	S	Se	0	0	0
			4761	3012	808	907	24	10			
1	F	618	Total	C	N	O	S	Se	0	0	0
			4727	2990	801	902	24	10			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	GLY	-	linker	UNP P03316
A	346	GLY	-	linker	UNP P03316
A	347	GLY	-	linker	UNP P03316
A	348	SER	-	linker	UNP P03316
A	349	TRP	-	linker	UNP P03316
A	350	SER	-	linker	UNP P03316
A	351	HIS	-	linker	UNP P03316
A	352	PRO	-	linker	UNP P03316
A	353	GLN	-	linker	UNP P03316
A	354	PHE	-	linker	UNP P03316
A	355	GLU	-	linker	UNP P03316
A	356	LYS	-	linker	UNP P03316
A	357	GLY	-	linker	UNP P03316
A	358	GLY	-	linker	UNP P03316
A	359	GLY	-	linker	UNP P03316
A	360	GLY	-	linker	UNP P03316
A	435	GLY	ASP	engineered mutation	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	GLY	-	linker	UNP P03316
B	346	GLY	-	linker	UNP P03316
B	347	GLY	-	linker	UNP P03316
B	348	SER	-	linker	UNP P03316
B	349	TRP	-	linker	UNP P03316
B	350	SER	-	linker	UNP P03316
B	351	HIS	-	linker	UNP P03316
B	352	PRO	-	linker	UNP P03316
B	353	GLN	-	linker	UNP P03316
B	354	PHE	-	linker	UNP P03316
B	355	GLU	-	linker	UNP P03316
B	356	LYS	-	linker	UNP P03316
B	357	GLY	-	linker	UNP P03316
B	358	GLY	-	linker	UNP P03316
B	359	GLY	-	linker	UNP P03316
B	360	GLY	-	linker	UNP P03316
B	435	GLY	ASP	engineered mutation	UNP P03316
C	345	GLY	-	linker	UNP P03316
C	346	GLY	-	linker	UNP P03316
C	347	GLY	-	linker	UNP P03316
C	348	SER	-	linker	UNP P03316
C	349	TRP	-	linker	UNP P03316
C	350	SER	-	linker	UNP P03316
C	351	HIS	-	linker	UNP P03316
C	352	PRO	-	linker	UNP P03316
C	353	GLN	-	linker	UNP P03316
C	354	PHE	-	linker	UNP P03316
C	355	GLU	-	linker	UNP P03316
C	356	LYS	-	linker	UNP P03316
C	357	GLY	-	linker	UNP P03316
C	358	GLY	-	linker	UNP P03316
C	359	GLY	-	linker	UNP P03316
C	360	GLY	-	linker	UNP P03316
C	435	GLY	ASP	engineered mutation	UNP P03316
D	345	GLY	-	linker	UNP P03316
D	346	GLY	-	linker	UNP P03316
D	347	GLY	-	linker	UNP P03316
D	348	SER	-	linker	UNP P03316
D	349	TRP	-	linker	UNP P03316
D	350	SER	-	linker	UNP P03316
D	351	HIS	-	linker	UNP P03316
D	352	PRO	-	linker	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
D	353	GLN	-	linker	UNP P03316
D	354	PHE	-	linker	UNP P03316
D	355	GLU	-	linker	UNP P03316
D	356	LYS	-	linker	UNP P03316
D	357	GLY	-	linker	UNP P03316
D	358	GLY	-	linker	UNP P03316
D	359	GLY	-	linker	UNP P03316
D	360	GLY	-	linker	UNP P03316
D	435	GLY	ASP	engineered mutation	UNP P03316
E	345	GLY	-	linker	UNP P03316
E	346	GLY	-	linker	UNP P03316
E	347	GLY	-	linker	UNP P03316
E	348	SER	-	linker	UNP P03316
E	349	TRP	-	linker	UNP P03316
E	350	SER	-	linker	UNP P03316
E	351	HIS	-	linker	UNP P03316
E	352	PRO	-	linker	UNP P03316
E	353	GLN	-	linker	UNP P03316
E	354	PHE	-	linker	UNP P03316
E	355	GLU	-	linker	UNP P03316
E	356	LYS	-	linker	UNP P03316
E	357	GLY	-	linker	UNP P03316
E	358	GLY	-	linker	UNP P03316
E	359	GLY	-	linker	UNP P03316
E	360	GLY	-	linker	UNP P03316
E	435	GLY	ASP	engineered mutation	UNP P03316
F	345	GLY	-	linker	UNP P03316
F	346	GLY	-	linker	UNP P03316
F	347	GLY	-	linker	UNP P03316
F	348	SER	-	linker	UNP P03316
F	349	TRP	-	linker	UNP P03316
F	350	SER	-	linker	UNP P03316
F	351	HIS	-	linker	UNP P03316
F	352	PRO	-	linker	UNP P03316
F	353	GLN	-	linker	UNP P03316
F	354	PHE	-	linker	UNP P03316
F	355	GLU	-	linker	UNP P03316
F	356	LYS	-	linker	UNP P03316
F	357	GLY	-	linker	UNP P03316
F	358	GLY	-	linker	UNP P03316
F	359	GLY	-	linker	UNP P03316
F	360	GLY	-	linker	UNP P03316

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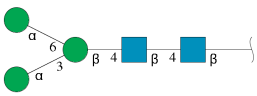
Chain	Residue	Modelled	Actual	Comment	Reference
F	435	GLY	ASP	engineered mutation	UNP P03316

- Molecule 2 is an oligosaccharide called 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
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	L	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	M	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called alpha-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
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

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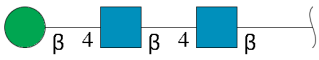
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



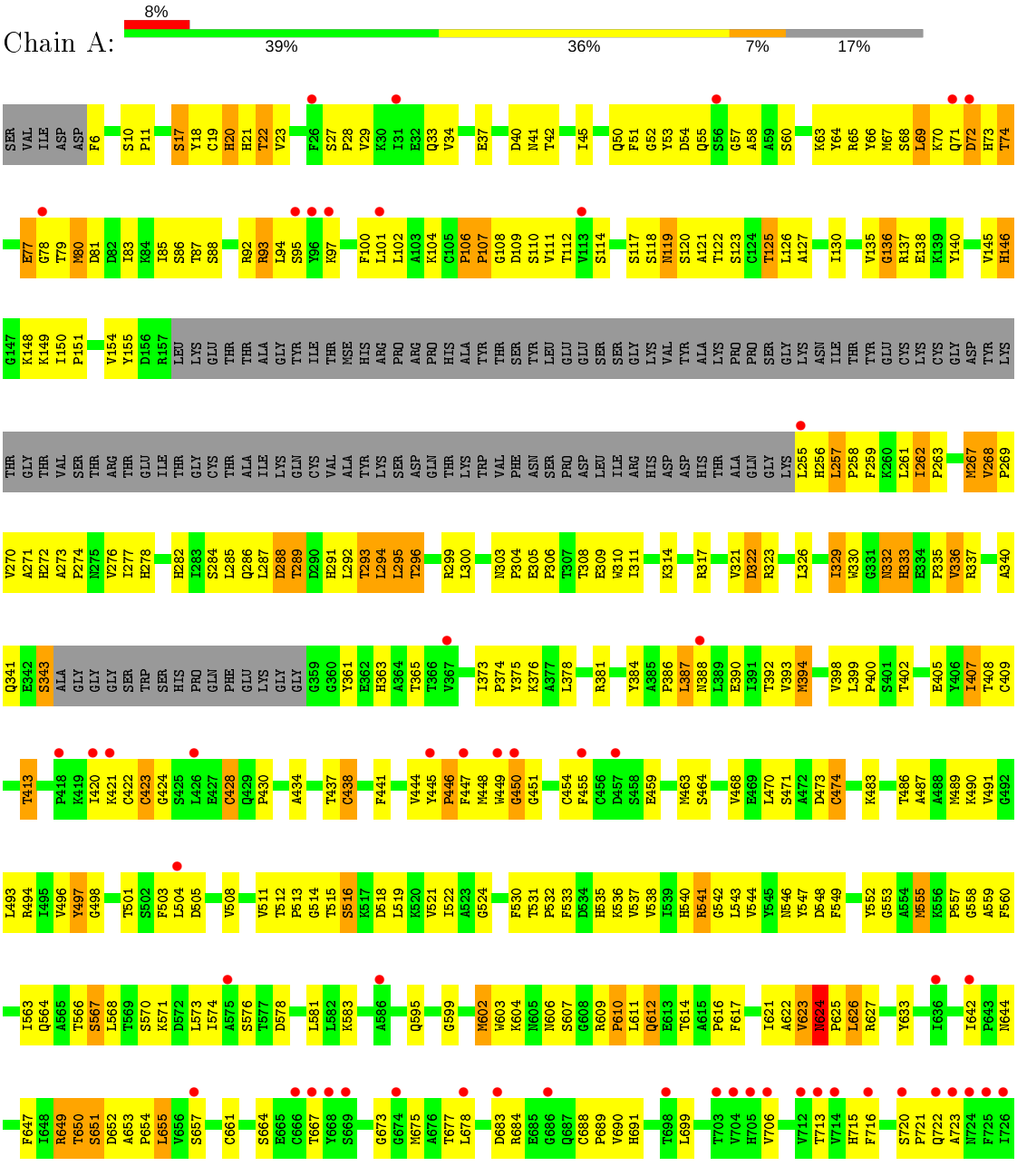
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

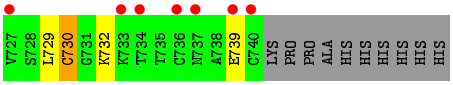
3 Residue-property plots (i)

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: Structural polyprotein

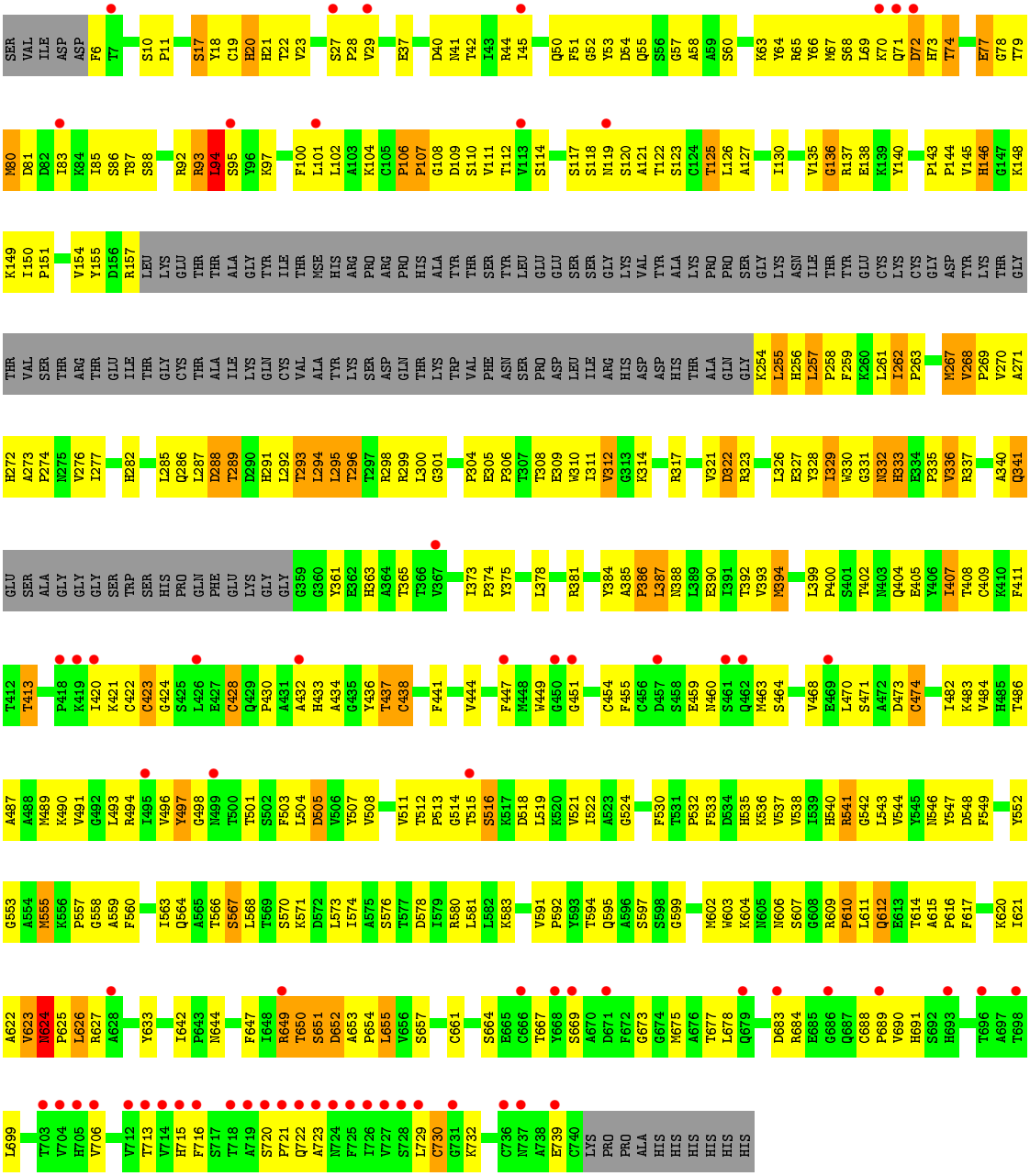
Chain A:





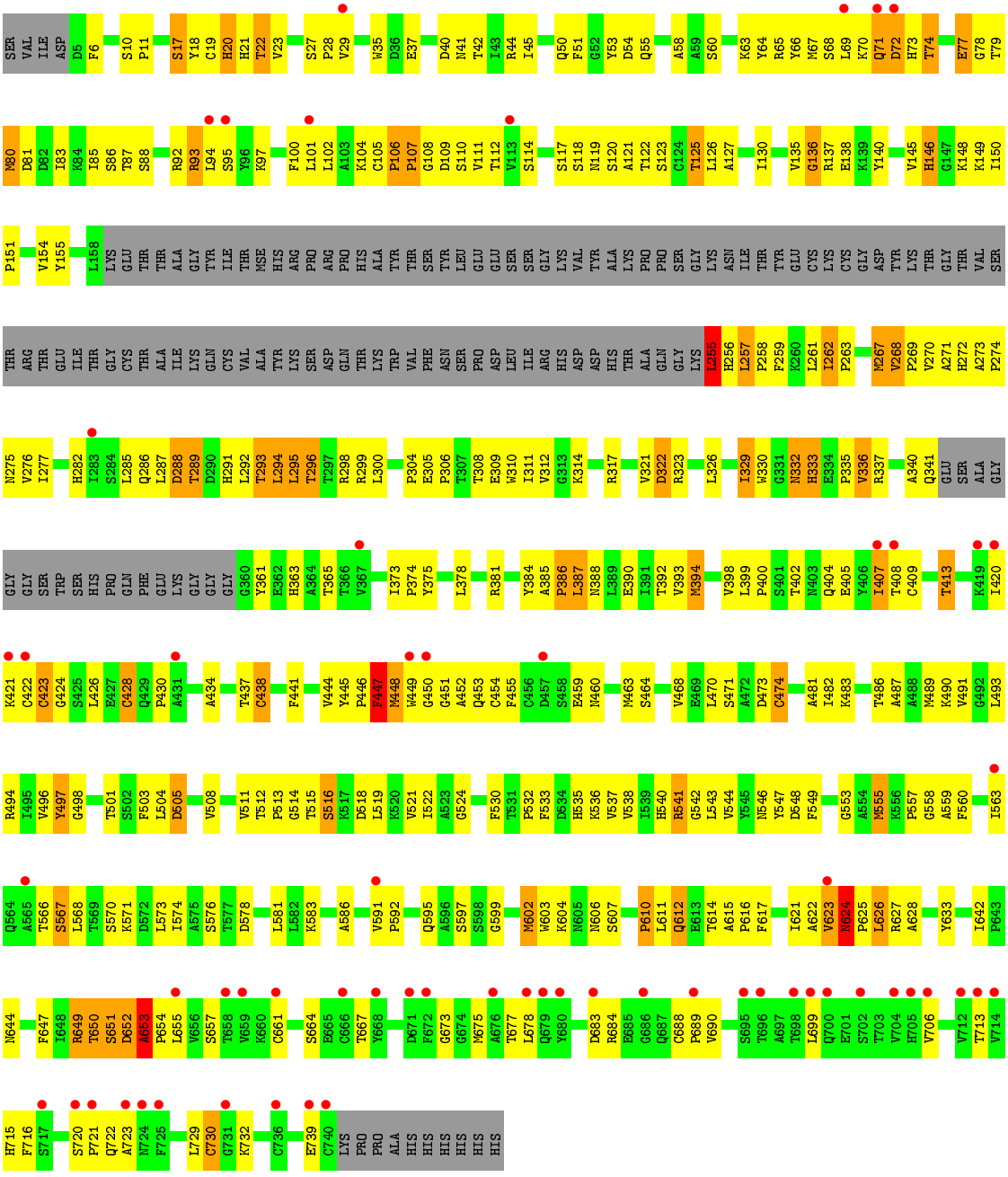
- Molecule 1: Structural polyprotein

Chain B:



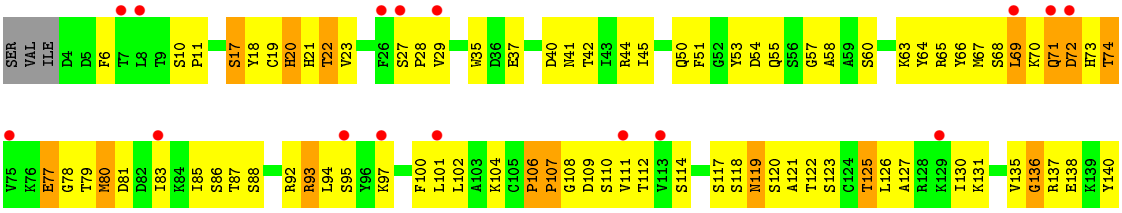
- Molecule 1: Structural polyprotein

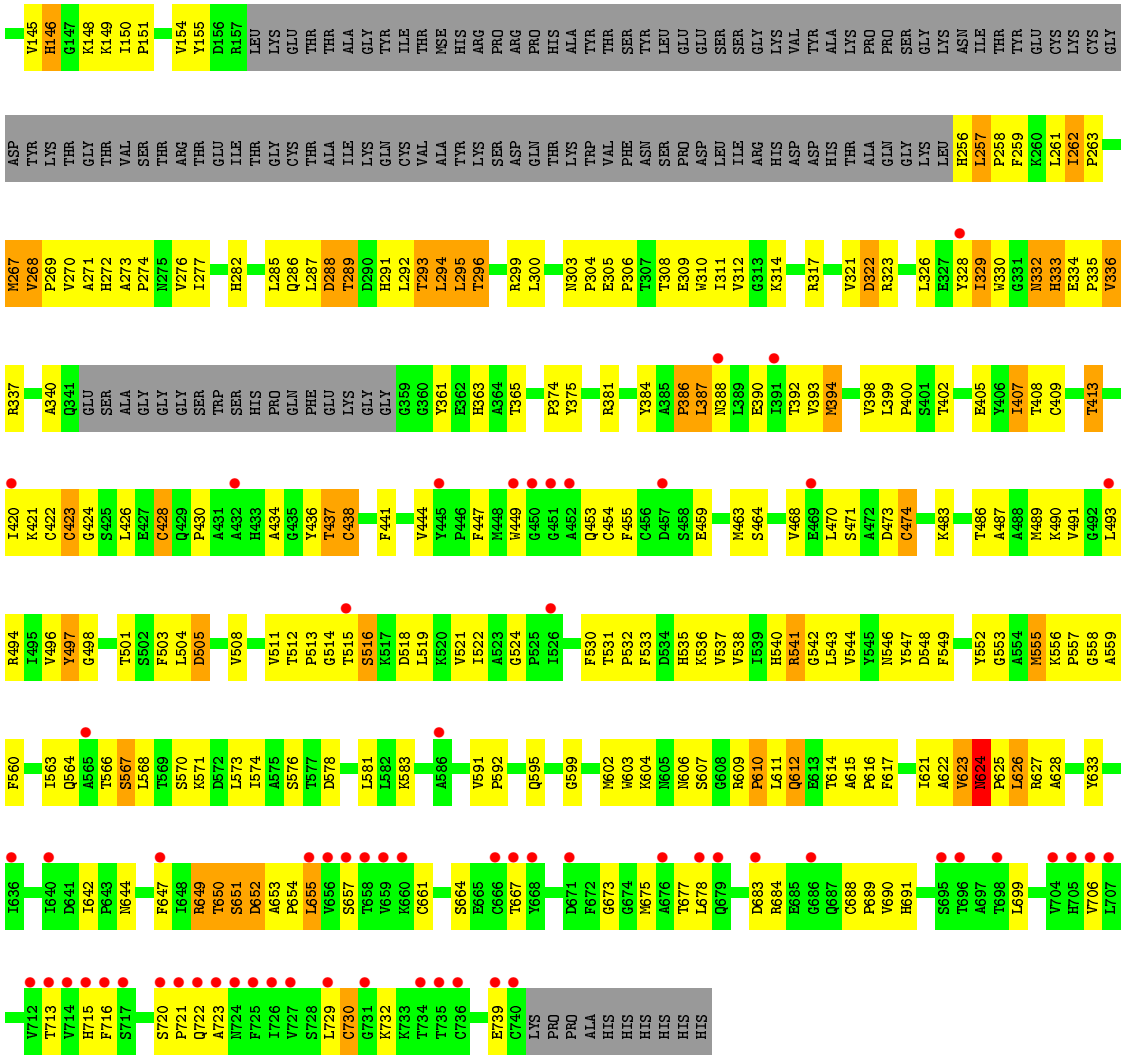
Chain C:



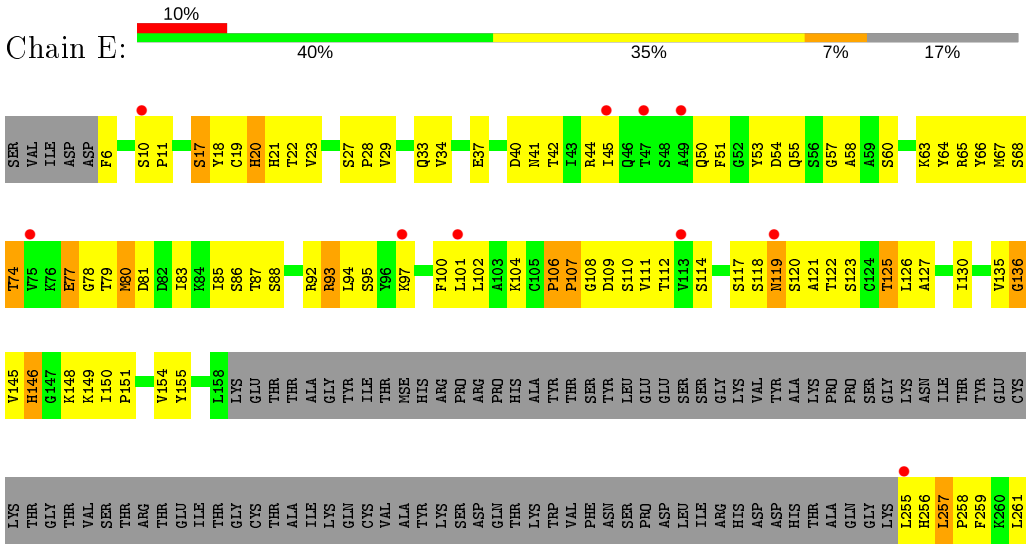
• Molecule 1: Structural polyprotein

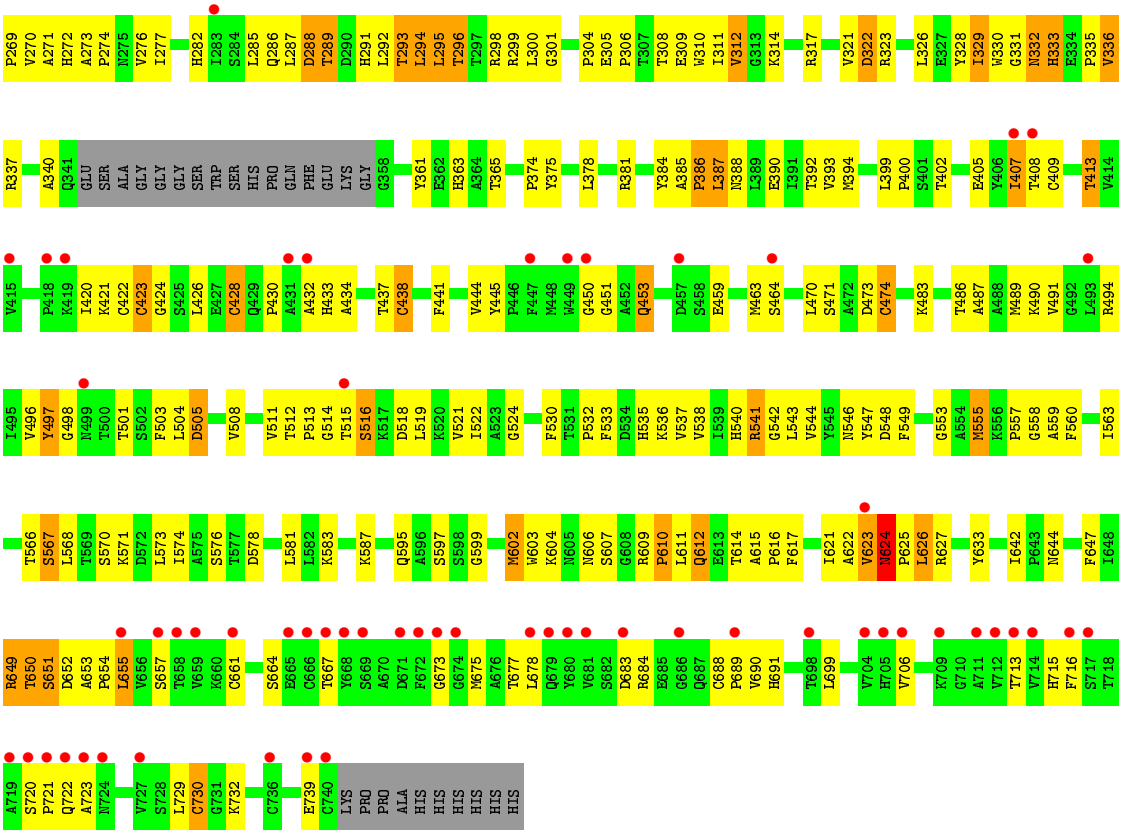
Chain D:





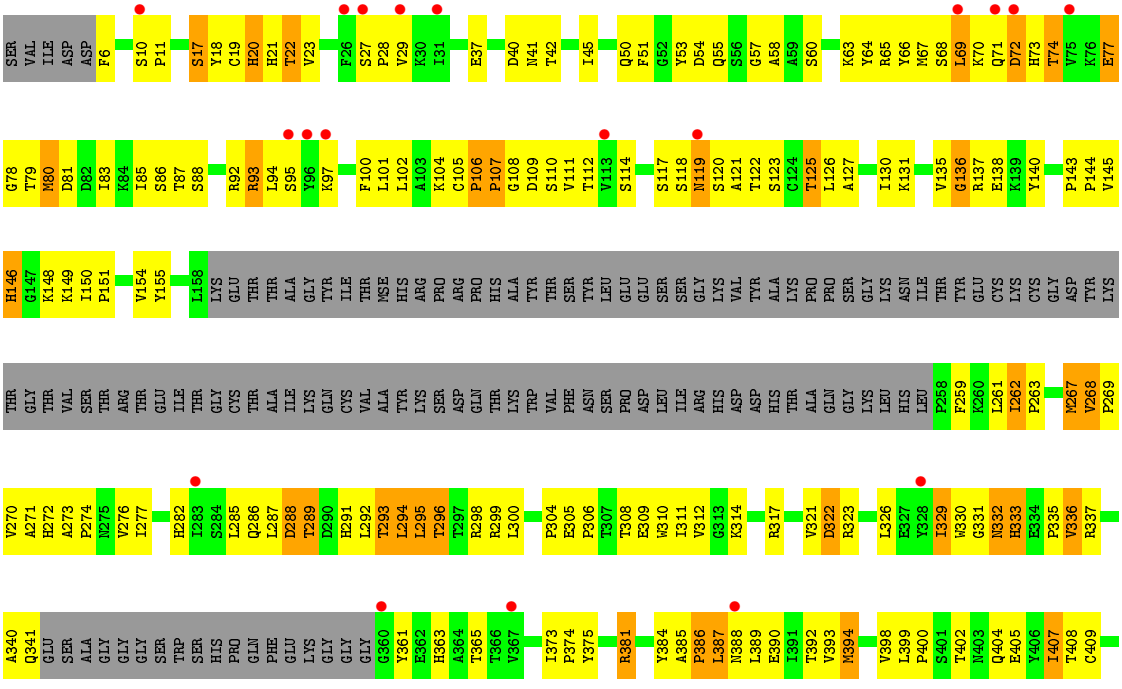
• Molecule 1: Structural polyprotein

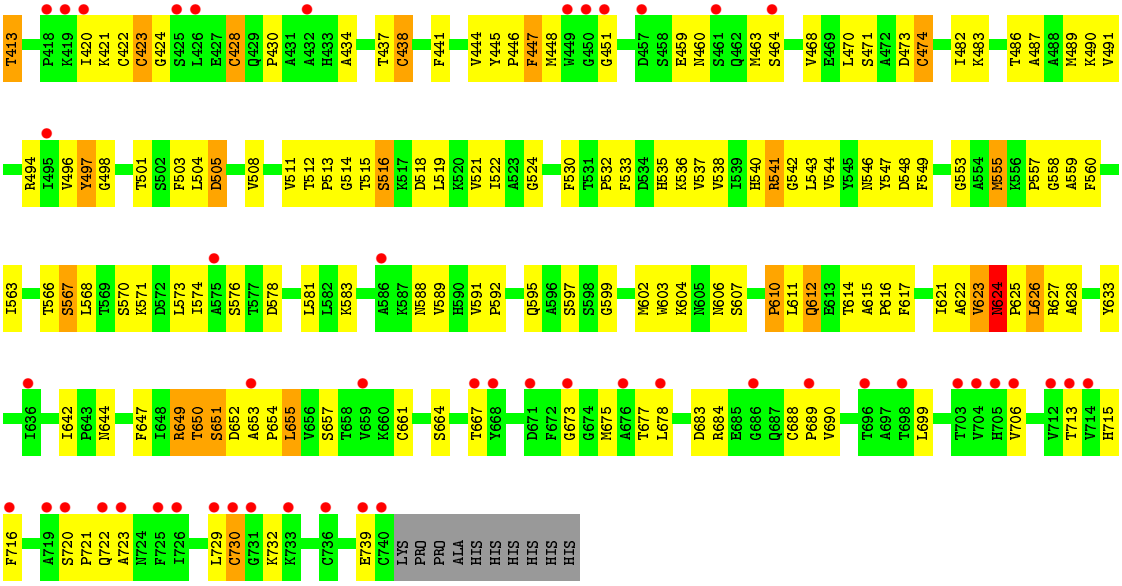




• Molecule 1: Structural polyprotein

Chain F:



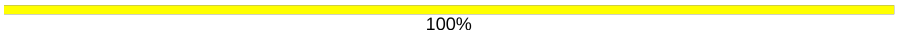


• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 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 I:



• Molecule 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 J:

• Molecule 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 K:

• Molecule 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:

• Molecule 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

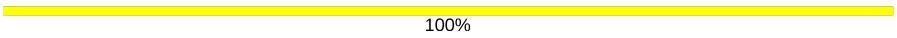
Chain M:

• Molecule 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 O:

• Molecule 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 Q:

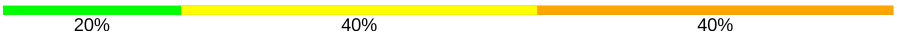


• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 3: alpha-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 P:



• Molecule 3: alpha-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 R:

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

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.48Å 158.43Å 160.68Å 60.42° 89.80° 89.65°	Depositor
Resolution (Å)	60.72 – 3.29 60.72 – 3.29	Depositor EDS
% Data completeness (in resolution range)	92.4 (60.72-3.29) 91.6 (60.72-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.239 , 0.252 0.237 , 0.248	Depositor DCC
R_{free} test set	4175 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	87.2	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 98.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,k-l,k 0.033 for h,l,-k+l 0.297 for h,-l,k-l 0.297 for h,-k+l,-k 0.037 for h,-k,-l 0.408 for -h,k,k-l 0.289 for -h,-l,-k 0.033 for -h,k-l,-l 0.309 for -h,-k+l,l 0.039 for -h,-k,-k+l 0.033 for -h,l,k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29159	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, MAN

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	0.35	0/4876	0.58	0/6624
1	B	0.35	0/4870	0.60	1/6615 (0.0%)
1	C	0.38	1/4870 (0.0%)	0.60	1/6617 (0.0%)
1	D	0.35	0/4869	0.58	0/6615
1	E	0.35	0/4870	0.58	0/6616
1	F	0.36	0/4835	0.67	3/6568 (0.0%)
All	All	0.36	1/29190 (0.0%)	0.60	5/39655 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	653	ALA	C-N	7.00	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	381	ARG	NE-CZ-NH1	-19.90	110.35	120.30
1	F	381	ARG	NE-CZ-NH2	17.34	128.97	120.30
1	B	94	LEU	CA-CB-CG	-7.54	97.95	115.30
1	F	381	ARG	CD-NE-CZ	7.40	133.97	123.60
1	C	255	LEU	CB-CG-CD2	5.25	119.92	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	VAL	Peptide
1	A	624	ASN	Peptide
1	B	254	LYS	Peptide
1	B	623	VAL	Peptide
1	B	624	ASN	Peptide
1	C	623	VAL	Peptide
1	C	624	ASN	Peptide
1	D	623	VAL	Peptide
1	D	624	ASN	Peptide
1	E	623	VAL	Peptide
1	E	624	ASN	Peptide
1	F	623	VAL	Peptide
1	F	624	ASN	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	4767	0	4659	316	0
1	B	4761	0	4661	335	0
1	C	4761	0	4651	329	0
1	D	4760	0	4645	320	0
1	E	4761	0	4653	311	0
1	F	4727	0	4619	304	0
2	G	50	0	42	2	0
2	I	50	0	43	0	0
2	J	50	0	43	2	0
2	K	50	0	42	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	50	0	43	2	0
2	M	50	0	42	1	0
2	O	50	0	42	0	0
2	Q	50	0	43	0	0
3	H	61	0	52	3	0
3	P	61	0	52	2	0
3	R	61	0	52	6	0
4	N	39	0	34	2	0
All	All	29159	0	28418	1903	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 33.

All (1903) 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:D:22:THR:HG21	1:E:104:LYS:HD2	1.29	1.14
1:D:88:SER:HB3	1:D:107:PRO:HG3	1.10	1.09
1:B:507:TYR:CE1	1:D:625:PRO:HG2	1.88	1.09
1:B:255:LEU:HG	1:B:256:HIS:H	1.14	1.08
1:B:88:SER:HB3	1:B:107:PRO:HG3	1.09	1.08
1:E:88:SER:HB3	1:E:107:PRO:HG3	1.09	1.06
1:C:88:SER:HB3	1:C:107:PRO:HG3	1.08	1.06
1:E:255:LEU:HG	1:E:256:HIS:H	1.14	1.05
1:B:311:ILE:HD11	1:B:330:TRP:HE1	1.20	1.05
1:A:255:LEU:HG	1:A:256:HIS:H	1.15	1.05
1:F:88:SER:HB3	1:F:107:PRO:HG3	1.08	1.05
1:A:145:VAL:HG22	1:C:17:SER:HB3	1.35	1.05
1:A:311:ILE:HD11	1:A:330:TRP:HE1	1.21	1.05
1:A:88:SER:HB3	1:A:107:PRO:HG3	1.09	1.05
1:B:22:THR:HG21	1:C:104:LYS:HD2	1.39	1.04
1:E:311:ILE:HD11	1:E:330:TRP:HE1	1.21	1.04
1:D:311:ILE:HD11	1:D:330:TRP:HE1	1.22	1.02
1:A:22:THR:HG21	1:B:104:LYS:HD2	1.38	1.02
1:F:311:ILE:HD11	1:F:330:TRP:HE1	1.20	1.02
1:B:93:ARG:HH11	1:B:93:ARG:H	1.06	1.01
1:B:304:PRO:HG3	1:B:616:PRO:HA	1.39	1.01
1:F:88:SER:HB3	1:F:107:PRO:CG	1.91	1.01
1:C:311:ILE:HD11	1:C:330:TRP:HE1	1.20	1.00
1:E:22:THR:HG21	1:F:104:LYS:HD2	1.41	1.00
1:E:88:SER:HB3	1:E:107:PRO:CG	1.92	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLY:HA3	1:B:268:VAL:HG21	1.44	1.00
1:C:88:SER:HB3	1:C:107:PRO:CG	1.91	1.00
1:F:93:ARG:H	1:F:93:ARG:HH11	1.08	1.00
1:A:88:SER:HB3	1:A:107:PRO:CG	1.92	0.99
1:B:257:LEU:H	1:B:258:PRO:HD3	1.27	0.99
1:C:93:ARG:H	1:C:93:ARG:HH11	1.09	0.99
1:D:88:SER:HB3	1:D:107:PRO:CG	1.93	0.99
1:B:88:SER:HB3	1:B:107:PRO:CG	1.92	0.99
1:D:93:ARG:HH11	1:D:93:ARG:H	1.07	0.98
1:A:257:LEU:H	1:A:258:PRO:HD3	1.27	0.98
1:F:136:GLY:HA3	1:F:268:VAL:HG21	1.45	0.98
1:A:93:ARG:H	1:A:93:ARG:HH11	1.10	0.97
1:B:289:THR:HG21	1:B:293:THR:HG21	1.47	0.97
1:C:289:THR:HG21	1:C:293:THR:HG21	1.45	0.97
1:A:289:THR:HG21	1:A:293:THR:HG21	1.45	0.97
1:C:136:GLY:HA3	1:C:268:VAL:HG21	1.44	0.97
1:C:257:LEU:H	1:C:258:PRO:HD3	1.27	0.97
1:E:257:LEU:H	1:E:258:PRO:HD3	1.27	0.97
1:D:104:LYS:HD2	1:F:22:THR:HG21	1.46	0.97
1:E:136:GLY:HA3	1:E:268:VAL:HG21	1.44	0.97
1:D:145:VAL:HG22	1:F:17:SER:HB3	1.43	0.96
1:D:257:LEU:H	1:D:258:PRO:HD3	1.28	0.96
1:A:136:GLY:HA3	1:A:268:VAL:HG21	1.46	0.96
1:D:136:GLY:HA3	1:D:268:VAL:HG21	1.45	0.96
1:A:104:LYS:HD2	1:C:22:THR:HG21	1.46	0.96
1:E:93:ARG:H	1:E:93:ARG:HH11	1.07	0.95
1:E:17:SER:HB3	1:F:145:VAL:HG22	1.47	0.95
1:E:304:PRO:HG3	1:E:616:PRO:HA	1.45	0.95
1:F:289:THR:HG21	1:F:293:THR:HG21	1.44	0.95
1:D:304:PRO:HG3	1:D:616:PRO:HA	1.49	0.95
1:D:289:THR:HG21	1:D:293:THR:HG21	1.46	0.95
1:E:289:THR:HG21	1:E:293:THR:HG21	1.46	0.94
1:B:17:SER:HB3	1:C:145:VAL:HG22	1.51	0.93
1:D:17:SER:HB3	1:E:145:VAL:HG22	1.53	0.90
1:C:428:CYS:HB2	1:C:463:MSE:SE	2.24	0.88
1:C:304:PRO:HG3	1:C:616:PRO:HA	1.54	0.87
1:E:428:CYS:HB2	1:E:463:MSE:SE	2.25	0.86
1:D:447:PHE:HD1	1:D:455:PHE:HA	1.40	0.85
1:A:255:LEU:HG	1:A:256:HIS:N	1.91	0.85
1:B:428:CYS:HB2	1:B:463:MSE:SE	2.26	0.85
1:A:17:SER:HB3	1:B:145:VAL:HG22	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:LEU:HG	1:E:256:HIS:N	1.90	0.84
1:A:304:PRO:HG3	1:A:616:PRO:HA	1.57	0.84
1:F:304:PRO:HG3	1:F:616:PRO:HA	1.57	0.84
1:B:507:TYR:HE1	1:D:625:PRO:HG2	1.43	0.84
1:B:255:LEU:HG	1:B:256:HIS:N	1.92	0.83
1:D:22:THR:HG21	1:E:104:LYS:CD	2.07	0.83
1:F:428:CYS:HB2	1:F:463:MSE:SE	2.29	0.83
1:C:677:THR:HG22	1:C:713:THR:HG22	1.60	0.83
1:E:677:THR:HG22	1:E:713:THR:HG22	1.61	0.83
1:F:677:THR:HG22	1:F:713:THR:HG22	1.61	0.82
1:B:677:THR:HG22	1:B:713:THR:HG22	1.61	0.82
1:A:677:THR:HG22	1:A:713:THR:HG22	1.60	0.82
1:D:677:THR:HG22	1:D:713:THR:HG22	1.60	0.82
1:A:428:CYS:HB2	1:A:463:MSE:SE	2.29	0.82
1:C:378:LEU:HD21	1:C:689:PRO:HB2	1.63	0.81
1:E:322:ASP:O	1:E:323:ARG:HB3	1.81	0.81
1:C:496:VAL:HG22	1:C:501:THR:HB	1.62	0.81
1:D:496:VAL:HG22	1:D:501:THR:HB	1.63	0.81
1:C:322:ASP:O	1:C:323:ARG:HB3	1.81	0.80
1:D:447:PHE:CD1	1:D:455:PHE:HA	2.17	0.80
1:A:496:VAL:HG22	1:A:501:THR:HB	1.64	0.80
1:C:257:LEU:N	1:C:258:PRO:HD3	1.95	0.80
1:D:322:ASP:O	1:D:323:ARG:HB3	1.81	0.80
1:C:445:TYR:HB3	1:C:451:GLY:HA3	1.62	0.80
1:D:428:CYS:HB2	1:D:463:MSE:SE	2.32	0.80
1:A:257:LEU:N	1:A:258:PRO:HD3	1.95	0.80
1:B:257:LEU:N	1:B:258:PRO:HD3	1.96	0.80
1:E:257:LEU:N	1:E:258:PRO:HD3	1.96	0.80
1:B:94:LEU:HD22	1:B:157:ARG:HD3	1.64	0.79
1:C:653:ALA:HB1	1:C:684:ARG:HH11	1.47	0.79
1:D:257:LEU:N	1:D:258:PRO:HD3	1.96	0.79
1:F:322:ASP:O	1:F:323:ARG:HB3	1.82	0.79
1:A:322:ASP:O	1:A:323:ARG:HB3	1.82	0.79
1:E:114:SER:HB3	1:E:123:SER:CB	2.13	0.79
1:F:114:SER:HB3	1:F:123:SER:CB	2.11	0.79
1:C:114:SER:HB3	1:C:123:SER:CB	2.13	0.79
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.66	0.79
1:A:255:LEU:CG	1:A:256:HIS:H	1.96	0.79
1:A:114:SER:HB3	1:A:123:SER:CB	2.13	0.78
1:D:137:ARG:NH2	1:D:329:ILE:HB	1.98	0.78
1:F:137:ARG:NH2	1:F:329:ILE:HB	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:SER:HB3	1:D:123:SER:CB	2.12	0.78
1:B:322:ASP:O	1:B:323:ARG:HB3	1.81	0.78
1:B:106:PRO:HB2	1:B:107:PRO:HD3	1.65	0.78
1:E:496:VAL:HG22	1:E:501:THR:HB	1.65	0.78
1:E:137:ARG:NH2	1:E:329:ILE:HB	1.98	0.78
1:F:88:SER:CB	1:F:107:PRO:HG3	2.04	0.78
1:B:114:SER:HB3	1:B:123:SER:CB	2.12	0.78
1:C:106:PRO:HB2	1:C:107:PRO:HD3	1.66	0.78
1:F:496:VAL:HG22	1:F:501:THR:HB	1.64	0.78
1:A:137:ARG:NH2	1:A:329:ILE:HB	1.98	0.78
1:C:675:MSE:HE2	1:C:715:HIS:HE1	1.49	0.78
1:D:329:ILE:HD13	1:D:335:PRO:HB3	1.66	0.78
1:E:255:LEU:CG	1:E:256:HIS:H	1.95	0.78
1:B:496:VAL:HG22	1:B:501:THR:HB	1.65	0.77
1:A:544:VAL:H	1:A:612:GLN:NE2	1.83	0.77
1:B:544:VAL:H	1:B:612:GLN:NE2	1.83	0.77
1:D:544:VAL:H	1:D:612:GLN:NE2	1.83	0.77
3:R:1:NAG:H61	3:R:2:NAG:O7	1.85	0.77
1:D:543:LEU:HA	1:D:612:GLN:NE2	2.00	0.77
1:F:675:MSE:HE2	1:F:715:HIS:HE1	1.50	0.77
1:C:655:LEU:H	1:C:683:ASP:HB2	1.49	0.77
1:D:106:PRO:HB2	1:D:107:PRO:HD3	1.66	0.77
1:D:675:MSE:HE2	1:D:715:HIS:HE1	1.50	0.77
1:A:88:SER:CB	1:A:107:PRO:HG3	2.05	0.76
1:F:114:SER:HB3	1:F:123:SER:HB2	1.68	0.76
3:P:3:BMA:H3	3:R:5:MAN:O3	1.85	0.76
1:A:329:ILE:HD13	1:A:335:PRO:HB3	1.67	0.76
1:C:137:ARG:NH2	1:C:329:ILE:HB	2.00	0.76
1:F:543:LEU:HA	1:F:612:GLN:NE2	2.00	0.76
3:R:2:NAG:H83	3:R:5:MAN:H61	1.66	0.76
1:E:106:PRO:HB2	1:E:107:PRO:HD3	1.66	0.76
3:H:4:MAN:O3	2:L:3:BMA:H5	1.85	0.76
1:B:137:ARG:NH2	1:B:329:ILE:HB	2.01	0.75
1:E:544:VAL:H	1:E:612:GLN:NE2	1.84	0.75
1:F:106:PRO:HB2	1:F:107:PRO:HD3	1.66	0.75
1:B:255:LEU:CG	1:B:256:HIS:H	1.92	0.75
1:F:544:VAL:H	1:F:612:GLN:NE2	1.85	0.75
1:B:675:MSE:HE2	1:B:715:HIS:HE1	1.51	0.75
1:C:114:SER:HB3	1:C:123:SER:HB2	1.68	0.75
1:F:610:PRO:HB2	1:F:612:GLN:HG2	1.69	0.75
1:A:675:MSE:HE2	1:A:715:HIS:HE1	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HG	1:A:310:TRP:CE2	2.22	0.75
1:B:22:THR:HG21	1:C:104:LYS:CD	2.15	0.75
1:E:22:THR:HG21	1:F:104:LYS:CD	2.16	0.75
1:A:610:PRO:HB2	1:A:612:GLN:HG2	1.69	0.74
1:A:543:LEU:HA	1:A:612:GLN:NE2	2.01	0.74
1:C:329:ILE:HD13	1:C:335:PRO:HB3	1.69	0.74
1:E:536:LYS:HG2	1:E:549:PHE:CZ	2.23	0.74
1:A:104:LYS:CD	1:C:22:THR:HG21	2.17	0.74
1:F:294:LEU:HG	1:F:310:TRP:CE2	2.21	0.74
1:C:150:ILE:HG23	1:C:151:PRO:HD2	1.68	0.74
1:E:150:ILE:HG23	1:E:151:PRO:HD2	1.69	0.74
1:F:655:LEU:H	1:F:683:ASP:HB2	1.53	0.74
1:E:675:MSE:HE2	1:E:715:HIS:HE1	1.50	0.74
1:B:543:LEU:HA	1:B:612:GLN:NE2	2.01	0.74
1:D:114:SER:HB3	1:D:123:SER:HB2	1.69	0.74
1:C:544:VAL:H	1:C:612:GLN:NE2	1.85	0.74
1:C:294:LEU:HG	1:C:310:TRP:CE2	2.23	0.73
1:D:88:SER:CB	1:D:107:PRO:HG3	2.05	0.73
1:E:610:PRO:HB2	1:E:612:GLN:HG2	1.70	0.73
1:E:543:LEU:HA	1:E:612:GLN:NE2	2.02	0.73
1:F:329:ILE:HD13	1:F:335:PRO:HB3	1.68	0.73
1:A:137:ARG:HH22	1:A:329:ILE:HB	1.54	0.73
1:B:114:SER:HB3	1:B:123:SER:HB2	1.69	0.73
1:B:447:PHE:CD1	1:B:455:PHE:HA	2.23	0.73
1:B:329:ILE:HD13	1:B:335:PRO:HB3	1.69	0.73
1:C:543:LEU:HA	1:C:612:GLN:NE2	2.02	0.73
1:A:447:PHE:CD1	1:A:455:PHE:HA	2.23	0.73
1:B:294:LEU:HG	1:B:310:TRP:CE2	2.24	0.73
1:D:150:ILE:HG23	1:D:151:PRO:HD2	1.70	0.73
1:E:114:SER:HB3	1:E:123:SER:HB2	1.69	0.73
1:F:361:TYR:HB2	1:F:381:ARG:NH2	2.03	0.73
1:C:610:PRO:HB2	1:C:612:GLN:HG2	1.70	0.73
1:D:610:PRO:HB2	1:D:612:GLN:HG2	1.69	0.73
1:B:655:LEU:H	1:B:683:ASP:HB2	1.53	0.73
1:D:536:LYS:HG2	1:D:549:PHE:CZ	2.24	0.73
1:B:11:PRO:HD3	1:B:50:GLN:HE21	1.54	0.72
1:C:536:LYS:HG2	1:C:549:PHE:CZ	2.24	0.72
2:K:1:NAG:H4	2:K:2:NAG:N2	2.02	0.72
1:A:114:SER:HB3	1:A:123:SER:HB2	1.69	0.72
1:B:150:ILE:HG23	1:B:151:PRO:HD2	1.70	0.72
1:C:11:PRO:HD3	1:C:50:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:TYR:CE1	1:F:22:THR:HG22	2.25	0.72
1:F:536:LYS:HG2	1:F:549:PHE:CZ	2.25	0.72
1:A:18:TYR:CE1	1:A:22:THR:HG22	2.24	0.72
1:C:11:PRO:HD3	1:C:50:GLN:NE2	2.04	0.72
1:D:655:LEU:H	1:D:683:ASP:HB2	1.53	0.72
1:D:11:PRO:HD3	1:D:50:GLN:HE21	1.55	0.72
1:D:538:VAL:HG23	1:D:547:TYR:HB3	1.70	0.72
1:E:270:VAL:HG22	1:E:333:HIS:CE1	2.25	0.72
1:E:329:ILE:HD13	1:E:335:PRO:HB3	1.71	0.72
1:A:95:SER:OG	1:A:259:PHE:CE1	2.41	0.72
1:E:655:LEU:H	1:E:683:ASP:HB2	1.53	0.72
1:A:85:ILE:HD11	1:A:101:LEU:HD13	1.71	0.72
1:B:538:VAL:HG23	1:B:547:TYR:HB3	1.71	0.71
1:C:85:ILE:HD11	1:C:101:LEU:HD13	1.72	0.71
1:F:11:PRO:HD3	1:F:50:GLN:HE21	1.53	0.71
1:A:655:LEU:H	1:A:683:ASP:HB2	1.54	0.71
1:D:18:TYR:CE1	1:D:22:THR:HG22	2.25	0.71
1:F:11:PRO:HD3	1:F:50:GLN:NE2	2.05	0.71
1:B:11:PRO:HD3	1:B:50:GLN:NE2	2.05	0.71
1:E:18:TYR:CE1	1:E:22:THR:HG22	2.25	0.71
1:F:150:ILE:HG23	1:F:151:PRO:HD2	1.71	0.71
1:A:11:PRO:HD3	1:A:50:GLN:HE21	1.55	0.71
1:C:18:TYR:CE1	1:C:22:THR:HG22	2.25	0.71
1:B:653:ALA:N	1:B:654:PRO:HD2	2.05	0.71
1:A:536:LYS:HG2	1:A:549:PHE:CZ	2.26	0.71
1:E:11:PRO:HD3	1:E:50:GLN:HE21	1.55	0.71
1:D:270:VAL:HG22	1:D:333:HIS:CE1	2.26	0.71
1:A:388:ASN:HB3	1:A:498:GLY:H	1.56	0.70
1:A:11:PRO:HD3	1:A:50:GLN:NE2	2.06	0.70
1:B:18:TYR:CE1	1:B:22:THR:HG22	2.25	0.70
1:B:287:LEU:HD22	1:B:330:TRP:NE1	2.07	0.70
1:E:294:LEU:HG	1:E:310:TRP:CE2	2.26	0.70
1:F:270:VAL:HG22	1:F:333:HIS:CE1	2.26	0.70
1:A:270:VAL:HG22	1:A:333:HIS:CE1	2.27	0.70
1:E:137:ARG:HH22	1:E:329:ILE:HB	1.54	0.70
1:D:11:PRO:HD3	1:D:50:GLN:NE2	2.05	0.70
1:A:150:ILE:HG23	1:A:151:PRO:HD2	1.73	0.70
1:A:22:THR:HG21	1:B:104:LYS:CD	2.19	0.70
1:A:538:VAL:HG23	1:A:547:TYR:HB3	1.72	0.70
1:A:79:THR:C	1:A:81:ASP:H	1.94	0.70
1:A:291:HIS:CD2	1:A:293:THR:HG22	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:HG23	1:A:512:THR:H	1.57	0.70
1:B:536:LYS:HG2	1:B:549:PHE:CZ	2.26	0.70
1:D:294:LEU:HG	1:D:310:TRP:CE2	2.27	0.70
1:D:79:THR:C	1:D:81:ASP:H	1.94	0.70
1:E:85:ILE:HD11	1:E:101:LEU:HD13	1.73	0.70
1:F:538:VAL:HG23	1:F:547:TYR:HB3	1.72	0.70
1:A:650:THR:HG22	1:A:650:THR:O	1.92	0.70
1:B:85:ILE:HD11	1:B:101:LEU:HD13	1.73	0.70
1:D:137:ARG:HH22	1:D:329:ILE:HB	1.54	0.70
1:A:299:ARG:HB2	1:A:304:PRO:HA	1.74	0.70
1:E:88:SER:CB	1:E:107:PRO:HG3	2.05	0.70
1:E:538:VAL:HG23	1:E:547:TYR:HB3	1.72	0.70
1:F:137:ARG:HH22	1:F:329:ILE:HB	1.54	0.70
1:A:447:PHE:HD1	1:A:454:CYS:O	1.75	0.70
1:A:446:PRO:HD2	1:A:450:GLY:O	1.90	0.70
1:E:11:PRO:HD3	1:E:50:GLN:NE2	2.06	0.70
1:F:511:VAL:HG23	1:F:512:THR:H	1.56	0.70
1:D:85:ILE:HD11	1:D:101:LEU:HD13	1.73	0.69
1:F:85:ILE:HD11	1:F:101:LEU:HD13	1.73	0.69
1:A:447:PHE:CE1	1:A:455:PHE:HD1	2.11	0.69
1:B:270:VAL:HG22	1:B:333:HIS:CE1	2.26	0.69
1:D:388:ASN:HB3	1:D:498:GLY:H	1.57	0.69
1:E:79:THR:C	1:E:81:ASP:H	1.95	0.69
1:C:88:SER:CB	1:C:107:PRO:HG3	2.04	0.69
1:D:653:ALA:N	1:D:654:PRO:HD2	2.08	0.69
1:D:291:HIS:CD2	1:D:293:THR:HG22	2.27	0.69
1:E:299:ARG:HB2	1:E:304:PRO:HA	1.73	0.69
1:E:287:LEU:HD22	1:E:330:TRP:NE1	2.06	0.69
1:C:95:SER:OG	1:C:259:PHE:CE1	2.42	0.69
1:B:610:PRO:HB2	1:B:612:GLN:HG2	1.72	0.69
1:C:538:VAL:HG23	1:C:547:TYR:HB3	1.73	0.69
1:D:108:GLY:HA3	1:D:130:ILE:HB	1.75	0.69
1:D:511:VAL:HG23	1:D:512:THR:H	1.57	0.69
1:D:650:THR:O	1:D:650:THR:HG22	1.93	0.69
1:B:624:ASN:HB3	1:B:625:PRO:CD	2.23	0.68
1:D:299:ARG:HB2	1:D:304:PRO:HA	1.73	0.68
1:F:299:ARG:HB2	1:F:304:PRO:HA	1.75	0.68
1:C:311:ILE:HD11	1:C:330:TRP:NE1	2.04	0.68
1:D:107:PRO:HG2	1:D:108:GLY:H	1.58	0.68
1:C:291:HIS:CD2	1:C:293:THR:HG22	2.28	0.68
1:C:650:THR:O	1:C:650:THR:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:HIS:CD2	1:E:293:THR:HG22	2.28	0.68
1:F:79:THR:C	1:F:81:ASP:H	1.95	0.68
1:A:287:LEU:HD22	1:A:330:TRP:NE1	2.08	0.68
1:B:511:VAL:HG23	1:B:512:THR:H	1.59	0.68
1:B:79:THR:C	1:B:81:ASP:H	1.96	0.68
1:C:270:VAL:HG22	1:C:333:HIS:CE1	2.28	0.68
1:B:88:SER:CB	1:B:107:PRO:HG3	2.05	0.68
1:C:299:ARG:HB2	1:C:304:PRO:HA	1.75	0.68
1:F:650:THR:O	1:F:650:THR:HG22	1.92	0.68
1:A:445:TYR:HB3	1:A:451:GLY:HA3	1.76	0.68
1:F:388:ASN:HB3	1:F:498:GLY:H	1.58	0.68
1:B:137:ARG:HH22	1:B:329:ILE:HB	1.59	0.68
1:B:386:PRO:HB2	1:B:689:PRO:HG2	1.76	0.68
1:C:79:THR:C	1:C:81:ASP:H	1.96	0.68
1:B:299:ARG:HB2	1:B:304:PRO:HA	1.75	0.67
1:C:108:GLY:HA3	1:C:130:ILE:HB	1.76	0.67
1:F:287:LEU:HD22	1:F:330:TRP:NE1	2.09	0.67
1:F:291:HIS:CD2	1:F:293:THR:HG22	2.29	0.67
1:C:107:PRO:HG2	1:C:108:GLY:H	1.59	0.67
1:E:95:SER:OG	1:E:259:PHE:CE1	2.42	0.67
1:C:287:LEU:HD22	1:C:330:TRP:NE1	2.10	0.67
1:D:530:PHE:HB3	1:D:633:TYR:CE1	2.29	0.67
1:C:511:VAL:HG23	1:C:512:THR:H	1.58	0.67
1:A:108:GLY:HA3	1:A:130:ILE:HB	1.76	0.67
1:B:291:HIS:CD2	1:B:293:THR:HG22	2.30	0.67
1:C:494:ARG:HB2	1:C:503:PHE:HD1	1.59	0.67
1:C:624:ASN:HB3	1:C:625:PRO:CD	2.25	0.67
1:C:388:ASN:HB3	1:C:498:GLY:H	1.59	0.67
1:E:108:GLY:HA3	1:E:130:ILE:HB	1.77	0.67
1:A:107:PRO:HG2	1:A:108:GLY:H	1.58	0.67
1:C:256:HIS:O	1:C:257:LEU:HD13	1.95	0.67
1:C:530:PHE:HB3	1:C:633:TYR:CE1	2.30	0.67
1:C:542:GLY:H	1:C:543:LEU:HD12	1.60	0.66
1:E:511:VAL:HG23	1:E:512:THR:H	1.59	0.66
1:F:108:GLY:HA3	1:F:130:ILE:HB	1.77	0.66
1:B:108:GLY:HA3	1:B:130:ILE:HB	1.76	0.66
1:B:256:HIS:O	1:B:257:LEU:HD13	1.95	0.66
1:E:388:ASN:HB3	1:E:498:GLY:H	1.60	0.66
1:B:388:ASN:HB3	1:B:498:GLY:H	1.59	0.66
1:F:624:ASN:HB3	1:F:625:PRO:CD	2.25	0.66
1:B:650:THR:HG22	1:B:650:THR:O	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:PRO:HG2	1:F:108:GLY:H	1.59	0.66
1:A:567:SER:HB2	1:A:571:LYS:HD2	1.78	0.66
1:B:107:PRO:HG2	1:B:108:GLY:H	1.60	0.66
1:B:97:LYS:HB2	1:B:259:PHE:CZ	2.31	0.66
1:B:494:ARG:HB2	1:B:503:PHE:HD1	1.61	0.66
1:D:494:ARG:HB2	1:D:503:PHE:HD1	1.61	0.66
1:E:107:PRO:HG2	1:E:108:GLY:H	1.59	0.66
1:C:136:GLY:HA3	1:C:268:VAL:CG2	2.25	0.66
1:F:299:ARG:HH12	1:F:305:GLU:CD	1.99	0.66
1:A:256:HIS:O	1:A:257:LEU:HD13	1.96	0.66
1:D:104:LYS:CD	1:F:22:THR:HG21	2.22	0.66
1:F:530:PHE:HB3	1:F:633:TYR:CE1	2.31	0.66
1:C:137:ARG:HH22	1:C:329:ILE:HB	1.59	0.66
1:D:542:GLY:H	1:D:543:LEU:HD12	1.61	0.66
1:E:299:ARG:HH12	1:E:305:GLU:CD	2.00	0.66
1:A:497:TYR:N	1:A:497:TYR:CD2	2.64	0.65
1:B:567:SER:HB2	1:B:571:LYS:HD2	1.78	0.65
1:E:624:ASN:HB3	1:E:625:PRO:CD	2.26	0.65
1:B:95:SER:OG	1:B:259:PHE:CE1	2.41	0.65
1:C:97:LYS:HB2	1:C:259:PHE:CZ	2.31	0.65
1:D:256:HIS:O	1:D:257:LEU:HD13	1.95	0.65
1:D:287:LEU:HD22	1:D:330:TRP:NE1	2.11	0.65
1:E:530:PHE:HB3	1:E:633:TYR:CE1	2.31	0.65
1:A:530:PHE:HB3	1:A:633:TYR:CE1	2.31	0.65
1:A:97:LYS:HB2	1:A:259:PHE:CZ	2.31	0.65
1:D:624:ASN:HB3	1:D:625:PRO:CD	2.27	0.65
1:A:299:ARG:HH12	1:A:305:GLU:CD	2.00	0.65
1:A:624:ASN:HB3	1:A:625:PRO:CD	2.26	0.65
1:B:299:ARG:HH12	1:B:305:GLU:CD	2.00	0.65
1:D:299:ARG:HH12	1:D:305:GLU:CD	2.00	0.65
1:E:536:LYS:HG2	1:E:549:PHE:CE2	2.32	0.65
1:A:106:PRO:HB2	1:A:107:PRO:CD	2.27	0.65
1:D:497:TYR:CD2	1:D:497:TYR:N	2.63	0.65
1:F:97:LYS:HB2	1:F:259:PHE:CZ	2.32	0.65
1:C:299:ARG:HH12	1:C:305:GLU:CD	1.99	0.65
1:E:256:HIS:O	1:E:257:LEU:HD13	1.96	0.65
1:F:494:ARG:HB2	1:F:503:PHE:HD1	1.62	0.65
1:A:494:ARG:HB2	1:A:503:PHE:HD1	1.62	0.64
1:B:37:GLU:OE1	1:B:473:ASP:OD2	2.15	0.64
1:D:108:GLY:HA2	1:D:130:ILE:HD12	1.79	0.64
1:D:384:TYR:HA	1:D:649:ARG:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLY:H	1:A:543:LEU:HD12	1.62	0.64
1:B:530:PHE:HB3	1:B:633:TYR:CE1	2.31	0.64
1:D:567:SER:HB2	1:D:571:LYS:HD2	1.77	0.64
1:E:19:CYS:HA	1:E:123:SER:O	1.98	0.64
1:F:19:CYS:HA	1:F:123:SER:O	1.97	0.64
1:F:542:GLY:H	1:F:543:LEU:HD12	1.60	0.64
1:B:289:THR:HG21	1:B:293:THR:CG2	2.26	0.64
1:E:97:LYS:HB2	1:E:259:PHE:CZ	2.32	0.64
1:E:494:ARG:HB2	1:E:503:PHE:HD1	1.61	0.64
1:E:650:THR:HG22	1:E:650:THR:O	1.97	0.64
1:D:558:GLY:O	1:D:599:GLY:HA2	1.97	0.64
1:C:567:SER:HB2	1:C:571:LYS:HD2	1.80	0.64
1:D:97:LYS:HB2	1:D:259:PHE:CZ	2.31	0.64
1:B:108:GLY:HA2	1:B:130:ILE:HD12	1.80	0.64
1:E:567:SER:HB2	1:E:571:LYS:HD2	1.79	0.64
1:C:19:CYS:HA	1:C:123:SER:O	1.98	0.64
1:E:106:PRO:HB2	1:E:107:PRO:CD	2.27	0.64
1:E:542:GLY:H	1:E:543:LEU:HD12	1.62	0.64
1:D:19:CYS:HA	1:D:123:SER:O	1.98	0.64
1:F:311:ILE:HD11	1:F:330:TRP:NE1	2.04	0.64
1:D:624:ASN:HB3	1:D:625:PRO:HD3	1.80	0.64
1:A:558:GLY:O	1:A:599:GLY:HA2	1.97	0.63
1:B:19:CYS:HA	1:B:123:SER:O	1.97	0.63
1:B:558:GLY:O	1:B:599:GLY:HA2	1.98	0.63
1:D:106:PRO:HB2	1:D:107:PRO:CD	2.27	0.63
1:F:108:GLY:HA2	1:F:130:ILE:HD12	1.79	0.63
1:A:19:CYS:HA	1:A:123:SER:O	1.98	0.63
1:B:653:ALA:HB1	1:B:684:ARG:HD2	1.79	0.63
1:C:289:THR:HG21	1:C:293:THR:CG2	2.25	0.63
1:E:384:TYR:HA	1:E:649:ARG:HA	1.80	0.63
1:A:543:LEU:HD23	1:A:610:PRO:HG3	1.81	0.63
1:B:388:ASN:O	1:B:497:TYR:HA	1.99	0.63
1:B:542:GLY:H	1:B:543:LEU:HD12	1.62	0.63
1:C:446:PRO:HG2	1:C:450:GLY:C	2.19	0.63
1:B:384:TYR:HA	1:B:649:ARG:HA	1.80	0.63
1:C:108:GLY:HA2	1:C:130:ILE:HD12	1.79	0.63
1:C:448:MSE:HG3	1:C:454:CYS:H	1.63	0.63
1:C:553:GLY:HA2	1:C:574:ILE:HD12	1.81	0.63
1:A:384:TYR:HA	1:A:649:ARG:HA	1.79	0.63
1:B:301:GLY:O	1:B:616:PRO:O	2.17	0.63
1:B:652:ASP:C	1:B:654:PRO:HD2	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:CG2	1:C:17:SER:HB3	2.21	0.63
1:E:108:GLY:HA2	1:E:130:ILE:HD12	1.80	0.63
1:A:108:GLY:HA2	1:A:130:ILE:HD12	1.79	0.63
1:E:497:TYR:N	1:E:497:TYR:CD2	2.66	0.63
1:F:413:THR:CG2	1:F:595:GLN:HE22	2.11	0.63
1:C:384:TYR:HA	1:C:649:ARG:HA	1.80	0.63
1:E:553:GLY:HA2	1:E:574:ILE:HD12	1.81	0.63
1:F:497:TYR:N	1:F:497:TYR:CD2	2.66	0.63
1:B:93:ARG:N	1:B:93:ARG:HH11	1.88	0.63
1:C:321:VAL:HG12	1:C:340:ALA:HB2	1.80	0.63
1:E:388:ASN:O	1:E:497:TYR:HA	1.99	0.63
1:F:558:GLY:O	1:F:599:GLY:HA2	1.99	0.63
1:B:106:PRO:HB2	1:B:107:PRO:CD	2.27	0.62
1:D:557:PRO:HB3	1:D:576:SER:O	1.98	0.62
1:B:624:ASN:HB3	1:B:625:PRO:HD3	1.80	0.62
1:C:388:ASN:O	1:C:497:TYR:HA	1.99	0.62
1:E:653:ALA:N	1:E:654:PRO:HD2	2.14	0.62
1:C:497:TYR:CD2	1:C:497:TYR:N	2.67	0.62
1:D:553:GLY:HA2	1:D:574:ILE:HD12	1.81	0.62
1:D:413:THR:CG2	1:D:595:GLN:HE22	2.11	0.62
1:E:413:THR:CG2	1:E:595:GLN:HE22	2.13	0.62
1:F:388:ASN:O	1:F:497:TYR:HA	1.99	0.62
1:F:567:SER:HB2	1:F:571:LYS:HD2	1.79	0.62
1:A:511:VAL:HG23	1:A:512:THR:N	2.14	0.62
1:C:624:ASN:HB3	1:C:625:PRO:HD3	1.81	0.62
1:B:553:GLY:HA2	1:B:574:ILE:HD12	1.82	0.62
1:B:413:THR:CG2	1:B:595:GLN:HE22	2.12	0.62
1:C:255:LEU:HD22	1:C:256:HIS:H	1.64	0.62
1:C:447:PHE:CE1	1:C:455:PHE:HA	2.34	0.62
1:A:271:ALA:HB1	1:A:330:TRP:CH2	2.35	0.62
1:A:624:ASN:HB3	1:A:625:PRO:HD3	1.82	0.62
1:D:497:TYR:HD2	1:D:497:TYR:N	1.96	0.62
1:A:497:TYR:HD2	1:A:497:TYR:N	1.97	0.62
1:C:413:THR:CG2	1:C:595:GLN:HE22	2.12	0.62
1:D:289:THR:HG21	1:D:293:THR:CG2	2.27	0.62
1:F:289:THR:HG21	1:F:293:THR:CG2	2.24	0.62
1:F:11:PRO:HG3	1:F:50:GLN:HB2	1.82	0.62
1:F:384:TYR:HA	1:F:649:ARG:HA	1.80	0.62
1:D:311:ILE:HD11	1:D:330:TRP:NE1	2.05	0.62
1:E:136:GLY:HA3	1:E:268:VAL:CG2	2.26	0.62
1:A:388:ASN:O	1:A:497:TYR:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLY:HA3	1:B:268:VAL:CG2	2.26	0.62
1:E:543:LEU:HD23	1:E:610:PRO:HG3	1.81	0.61
1:B:11:PRO:HG3	1:B:50:GLN:HB2	1.81	0.61
1:C:149:LYS:C	1:C:150:ILE:HD12	2.19	0.61
1:D:543:LEU:HD23	1:D:610:PRO:HG3	1.80	0.61
1:E:271:ALA:HB1	1:E:330:TRP:CH2	2.35	0.61
1:F:271:ALA:HB1	1:F:330:TRP:CH2	2.36	0.61
1:B:543:LEU:HD23	1:B:610:PRO:HG3	1.82	0.61
1:B:271:ALA:HB1	1:B:330:TRP:CH2	2.35	0.61
1:D:536:LYS:HG2	1:D:549:PHE:CE2	2.36	0.61
1:E:624:ASN:HB3	1:E:625:PRO:HD3	1.81	0.61
1:F:553:GLY:HA2	1:F:574:ILE:HD12	1.83	0.61
1:C:537:VAL:HG22	1:C:546:ASN:HD22	1.66	0.61
1:D:388:ASN:O	1:D:497:TYR:HA	2.00	0.61
1:D:93:ARG:HH11	1:D:93:ARG:N	1.89	0.61
1:A:321:VAL:HG12	1:A:340:ALA:HB2	1.83	0.61
1:A:421:LYS:HE2	1:A:424:GLY:HA3	1.83	0.61
1:D:271:ALA:HB1	1:D:330:TRP:CH2	2.36	0.61
1:D:610:PRO:O	1:D:614:THR:HG23	2.01	0.61
1:E:289:THR:HG21	1:E:293:THR:CG2	2.25	0.61
1:F:497:TYR:N	1:F:497:TYR:HD2	1.99	0.61
1:F:511:VAL:HG23	1:F:512:THR:N	2.15	0.61
1:A:413:THR:CG2	1:A:595:GLN:HE22	2.14	0.61
1:B:497:TYR:CD2	1:B:497:TYR:N	2.67	0.61
1:C:257:LEU:N	1:C:258:PRO:CD	2.64	0.61
1:F:149:LYS:C	1:F:150:ILE:HD12	2.21	0.61
1:A:514:GLY:O	1:A:516:SER:N	2.31	0.61
1:C:536:LYS:HG2	1:C:549:PHE:CE2	2.36	0.61
1:D:421:LYS:HE2	1:D:424:GLY:HA3	1.83	0.61
1:D:511:VAL:HG23	1:D:512:THR:N	2.15	0.61
1:E:497:TYR:HD2	1:E:497:TYR:N	1.99	0.61
1:F:536:LYS:HG2	1:F:549:PHE:CE2	2.36	0.61
1:F:557:PRO:HB3	1:F:576:SER:O	2.01	0.61
1:A:553:GLY:HA2	1:A:574:ILE:HD12	1.82	0.60
1:C:274:PRO:HD3	1:C:330:TRP:CE3	2.36	0.60
1:A:257:LEU:N	1:A:258:PRO:CD	2.64	0.60
1:E:257:LEU:N	1:E:258:PRO:CD	2.64	0.60
1:E:93:ARG:N	1:E:93:ARG:HH11	1.89	0.60
1:C:11:PRO:HG3	1:C:50:GLN:HB2	1.83	0.60
1:A:378:LEU:HG	1:A:691:HIS:CD2	2.37	0.60
1:A:447:PHE:HD1	1:A:455:PHE:HA	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HD12	1:B:127:ALA:H	1.67	0.60
1:B:300:LEU:HG	1:B:326:LEU:HA	1.84	0.60
1:B:537:VAL:HG22	1:B:546:ASN:HD22	1.67	0.60
1:E:149:LYS:C	1:E:150:ILE:HD12	2.22	0.60
1:A:289:THR:HG21	1:A:293:THR:CG2	2.26	0.60
1:D:496:VAL:HG22	1:D:501:THR:CB	2.32	0.60
1:D:11:PRO:HG3	1:D:50:GLN:HB2	1.83	0.60
1:F:624:ASN:HB3	1:F:625:PRO:HD3	1.84	0.60
1:A:536:LYS:HG2	1:A:549:PHE:CE2	2.37	0.60
1:E:298:ARG:HH12	1:E:615:ALA:HB3	1.66	0.60
1:F:423:CYS:HA	1:F:459:GLU:O	2.02	0.60
1:D:566:THR:OG1	1:D:571:LYS:HB2	2.02	0.59
1:E:11:PRO:HG3	1:E:50:GLN:HB2	1.83	0.59
1:E:511:VAL:HG23	1:E:512:THR:N	2.17	0.59
1:E:537:VAL:HG22	1:E:546:ASN:HD22	1.67	0.59
1:C:557:PRO:HB3	1:C:576:SER:O	2.02	0.59
1:D:257:LEU:N	1:D:258:PRO:CD	2.64	0.59
1:E:566:THR:OG1	1:E:571:LYS:HB2	2.02	0.59
1:F:451:GLY:O	1:F:589:VAL:HG23	2.02	0.59
1:A:496:VAL:HG22	1:A:501:THR:CB	2.33	0.59
1:A:537:VAL:HG22	1:A:546:ASN:HD22	1.67	0.59
1:C:511:VAL:HG23	1:C:512:THR:N	2.17	0.59
1:D:50:GLN:HE22	1:D:65:ARG:NH2	2.01	0.59
1:B:149:LYS:C	1:B:150:ILE:HD12	2.22	0.59
1:B:321:VAL:HG12	1:B:340:ALA:HB2	1.85	0.59
1:C:271:ALA:HB1	1:C:330:TRP:CH2	2.38	0.59
1:F:106:PRO:HB2	1:F:107:PRO:CD	2.28	0.59
1:A:126:LEU:HD12	1:A:127:ALA:H	1.67	0.59
1:B:470:LEU:HB3	1:B:474:CYS:SG	2.42	0.59
1:E:470:LEU:HB3	1:E:474:CYS:SG	2.43	0.59
1:B:257:LEU:H	1:B:258:PRO:CD	2.10	0.59
1:B:311:ILE:HD11	1:B:330:TRP:NE1	2.04	0.59
1:C:257:LEU:H	1:C:258:PRO:CD	2.09	0.59
1:C:497:TYR:HD2	1:C:497:TYR:N	2.00	0.59
1:D:136:GLY:HA3	1:D:268:VAL:CG2	2.27	0.59
1:F:496:VAL:HG22	1:F:501:THR:CB	2.33	0.59
1:F:537:VAL:HG22	1:F:546:ASN:HD22	1.68	0.59
1:A:557:PRO:HB3	1:A:576:SER:O	2.03	0.59
1:C:423:CYS:HA	1:C:459:GLU:O	2.02	0.59
1:F:136:GLY:HA3	1:F:268:VAL:CG2	2.27	0.59
1:B:257:LEU:N	1:B:258:PRO:CD	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:THR:OG1	1:B:571:LYS:HB2	2.03	0.59
1:C:50:GLN:HE22	1:C:65:ARG:NH2	2.01	0.59
1:D:126:LEU:HD12	1:D:127:ALA:H	1.68	0.59
1:D:387:LEU:HD12	1:D:647:PHE:CE1	2.38	0.59
1:E:558:GLY:O	1:E:599:GLY:HA2	2.03	0.59
1:F:566:THR:OG1	1:F:571:LYS:HB2	2.02	0.59
1:C:514:GLY:O	1:C:516:SER:N	2.30	0.59
1:E:574:ILE:O	1:E:574:ILE:HG13	2.01	0.59
1:C:543:LEU:HD23	1:C:610:PRO:HG3	1.84	0.58
1:D:95:SER:OG	1:D:259:PHE:CE1	2.42	0.58
1:F:470:LEU:HB3	1:F:474:CYS:SG	2.43	0.58
1:A:18:TYR:HE1	1:A:22:THR:HG22	1.68	0.58
1:B:497:TYR:HD2	1:B:497:TYR:N	2.00	0.58
1:B:511:VAL:HG23	1:B:512:THR:N	2.17	0.58
1:F:321:VAL:HG12	1:F:340:ALA:HB2	1.86	0.58
1:B:361:TYR:HB2	1:B:381:ARG:NH2	2.18	0.58
1:C:106:PRO:HB2	1:C:107:PRO:CD	2.28	0.58
1:C:496:VAL:HG22	1:C:501:THR:CB	2.30	0.58
1:C:386:PRO:HB2	1:C:689:PRO:HG2	1.85	0.58
1:F:274:PRO:HD3	1:F:330:TRP:CE3	2.38	0.58
1:F:610:PRO:O	1:F:614:THR:HG23	2.03	0.58
2:L:1:NAG:H62	2:L:2:NAG:O7	2.03	0.58
3:R:1:NAG:H61	3:R:2:NAG:C7	2.32	0.58
1:A:566:THR:OG1	1:A:571:LYS:HB2	2.03	0.58
1:D:514:GLY:O	1:D:516:SER:N	2.31	0.58
1:C:300:LEU:HG	1:C:326:LEU:HA	1.85	0.58
1:E:421:LYS:HE2	1:E:424:GLY:HA3	1.85	0.58
1:A:447:PHE:CD1	1:A:448:MSE:N	2.69	0.58
1:A:610:PRO:O	1:A:614:THR:HG23	2.03	0.58
1:D:361:TYR:HB2	1:D:381:ARG:NH2	2.19	0.58
1:D:543:LEU:HA	1:D:612:GLN:HE22	1.69	0.58
1:E:423:CYS:HA	1:E:459:GLU:O	2.04	0.58
1:A:423:CYS:HA	1:A:459:GLU:O	2.04	0.58
1:B:19:CYS:C	1:B:21:HIS:H	2.07	0.58
1:D:149:LYS:C	1:D:150:ILE:HD12	2.22	0.58
1:E:675:MSE:HE2	1:E:715:HIS:CE1	2.36	0.58
1:F:50:GLN:HE22	1:F:65:ARG:NH2	2.02	0.58
1:A:729:LEU:O	1:A:730:CYS:C	2.41	0.58
1:B:653:ALA:N	1:B:654:PRO:CD	2.67	0.58
1:D:537:VAL:HG22	1:D:546:ASN:HD22	1.68	0.58
1:E:729:LEU:O	1:E:730:CYS:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HG3	1:A:50:GLN:HB2	1.84	0.58
1:A:50:GLN:HE22	1:A:65:ARG:NH2	2.02	0.58
1:B:421:LYS:HE2	1:B:424:GLY:HA3	1.85	0.58
1:C:566:THR:OG1	1:C:571:LYS:HB2	2.02	0.58
1:E:300:LEU:HG	1:E:326:LEU:HA	1.85	0.58
1:F:126:LEU:HD12	1:F:127:ALA:H	1.69	0.58
1:C:544:VAL:H	1:C:612:GLN:HE22	1.51	0.57
1:C:729:LEU:O	1:C:730:CYS:C	2.42	0.57
1:D:497:TYR:HD2	1:D:497:TYR:H	1.52	0.57
1:D:729:LEU:O	1:D:730:CYS:C	2.42	0.57
1:F:544:VAL:H	1:F:612:GLN:HE22	1.50	0.57
1:A:19:CYS:C	1:A:21:HIS:H	2.07	0.57
1:B:274:PRO:HD3	1:B:330:TRP:CE3	2.39	0.57
1:B:423:CYS:HA	1:B:459:GLU:O	2.03	0.57
1:D:321:VAL:HG12	1:D:340:ALA:HB2	1.85	0.57
1:E:450:GLY:HA3	1:E:587:LYS:HA	1.85	0.57
1:E:50:GLN:HE22	1:E:65:ARG:NH2	2.03	0.57
1:E:514:GLY:O	1:E:516:SER:N	2.31	0.57
1:A:387:LEU:HD12	1:A:647:PHE:CE1	2.38	0.57
1:B:390:GLU:HG2	1:B:496:VAL:HB	1.87	0.57
1:D:19:CYS:C	1:D:21:HIS:H	2.07	0.57
1:E:361:TYR:HB2	1:E:381:ARG:NH2	2.20	0.57
1:E:450:GLY:HA2	1:E:587:LYS:O	2.04	0.57
1:A:288:ASP:OD1	1:A:314:LYS:HB2	2.05	0.57
1:A:300:LEU:HG	1:A:326:LEU:HA	1.86	0.57
1:B:729:LEU:O	1:B:730:CYS:C	2.42	0.57
1:D:399:LEU:O	1:D:487:ALA:HB1	2.03	0.57
1:E:387:LEU:HD12	1:E:647:PHE:CE1	2.39	0.57
1:F:27:SER:HB2	1:F:28:PRO:HD2	1.87	0.57
1:F:675:MSE:HE2	1:F:715:HIS:CE1	2.37	0.57
1:A:399:LEU:O	1:A:487:ALA:HB1	2.04	0.57
1:B:536:LYS:HG2	1:B:549:PHE:CE2	2.39	0.57
1:C:361:TYR:HB2	1:C:381:ARG:NH2	2.18	0.57
1:C:667:THR:OG1	1:C:673:GLY:HA3	2.05	0.57
1:D:300:LEU:HG	1:D:326:LEU:HA	1.85	0.57
1:D:50:GLN:HE22	1:D:65:ARG:HH21	1.51	0.57
1:D:544:VAL:H	1:D:612:GLN:HE22	1.52	0.57
1:E:311:ILE:HD11	1:E:330:TRP:NE1	2.05	0.57
1:F:300:LEU:HG	1:F:326:LEU:HA	1.85	0.57
1:A:27:SER:HB2	1:A:28:PRO:HD2	1.87	0.57
1:B:544:VAL:H	1:B:612:GLN:HE22	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:MSE:HE2	1:B:715:HIS:CE1	2.38	0.57
1:C:690:VAL:HG12	1:C:699:LEU:HD13	1.87	0.57
1:E:19:CYS:C	1:E:21:HIS:H	2.07	0.57
1:F:18:TYR:HE1	1:F:22:THR:HG22	1.69	0.57
1:F:653:ALA:HB1	1:F:684:ARG:HD2	1.87	0.57
1:A:544:VAL:H	1:A:612:GLN:HE22	1.52	0.57
1:B:387:LEU:HD12	1:B:647:PHE:CE1	2.39	0.57
1:F:421:LYS:HE2	1:F:424:GLY:HA3	1.85	0.57
1:F:543:LEU:HD23	1:F:610:PRO:HG3	1.86	0.57
1:F:653:ALA:N	1:F:654:PRO:HD2	2.19	0.57
1:A:268:VAL:HG22	1:A:269:PRO:HD2	1.87	0.57
1:A:654:PRO:HB3	1:A:684:ARG:C	2.25	0.57
1:A:92:ARG:HA	1:A:93:ARG:NH1	2.20	0.57
1:C:399:LEU:O	1:C:487:ALA:HB1	2.05	0.57
1:C:558:GLY:O	1:C:599:GLY:HA2	2.04	0.57
1:C:654:PRO:HB3	1:C:684:ARG:C	2.25	0.57
1:F:514:GLY:O	1:F:516:SER:N	2.30	0.57
1:A:361:TYR:HB2	1:A:381:ARG:NH2	2.19	0.57
1:A:622:ALA:HB3	1:A:627:ARG:HG3	1.87	0.57
1:B:543:LEU:HA	1:B:612:GLN:HE22	1.70	0.57
1:D:274:PRO:HD3	1:D:330:TRP:CE3	2.40	0.57
1:D:423:CYS:HA	1:D:459:GLU:O	2.04	0.57
1:A:274:PRO:HD3	1:A:330:TRP:CE3	2.39	0.57
1:B:298:ARG:HH12	1:B:615:ALA:HB3	1.70	0.57
1:D:390:GLU:HG2	1:D:496:VAL:HB	1.87	0.57
1:E:557:PRO:HB3	1:E:576:SER:O	2.05	0.57
1:E:544:VAL:H	1:E:612:GLN:HE22	1.51	0.57
1:E:690:VAL:HG12	1:E:699:LEU:HD13	1.86	0.57
1:F:387:LEU:HD12	1:F:647:PHE:CE1	2.40	0.57
1:A:149:LYS:C	1:A:150:ILE:HD12	2.25	0.56
1:A:278:HIS:HB3	1:A:343:SER:HB3	1.87	0.56
1:B:496:VAL:HG22	1:B:501:THR:CB	2.33	0.56
1:C:93:ARG:HH11	1:C:93:ARG:N	1.91	0.56
1:D:454:CYS:SG	1:D:455:PHE:N	2.75	0.56
1:D:667:THR:OG1	1:D:673:GLY:HA3	2.05	0.56
1:E:390:GLU:HG2	1:E:496:VAL:HB	1.86	0.56
1:E:654:PRO:HB3	1:E:684:ARG:C	2.25	0.56
1:F:399:LEU:O	1:F:487:ALA:HB1	2.05	0.56
1:F:654:PRO:HB3	1:F:684:ARG:C	2.25	0.56
1:F:667:THR:OG1	1:F:673:GLY:HA3	2.05	0.56
1:F:729:LEU:O	1:F:730:CYS:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:PHE:CZ	1:B:617:PHE:HD1	2.23	0.56
1:C:19:CYS:C	1:C:21:HIS:H	2.07	0.56
1:C:288:ASP:OD1	1:C:314:LYS:HB2	2.04	0.56
1:D:654:PRO:HB3	1:D:684:ARG:C	2.25	0.56
1:B:557:PRO:HB3	1:B:576:SER:O	2.05	0.56
1:C:27:SER:HB2	1:C:28:PRO:HD2	1.87	0.56
1:D:470:LEU:HB3	1:D:474:CYS:SG	2.46	0.56
1:E:18:TYR:HE1	1:E:22:THR:HG22	1.69	0.56
1:B:690:VAL:HG12	1:B:699:LEU:HD13	1.86	0.56
1:D:118:SER:O	1:D:119:ASN:HB2	2.05	0.56
1:D:622:ALA:HB3	1:D:627:ARG:HG3	1.87	0.56
1:A:390:GLU:HG2	1:A:496:VAL:HB	1.86	0.56
1:B:50:GLN:HE22	1:B:65:ARG:NH2	2.02	0.56
1:C:470:LEU:HB3	1:C:474:CYS:SG	2.46	0.56
1:E:37:GLU:OE1	1:E:473:ASP:OD2	2.24	0.56
1:E:441:PHE:CD1	1:E:583:LYS:HG2	2.41	0.56
1:C:421:LYS:HE2	1:C:424:GLY:HA3	1.87	0.56
1:E:622:ALA:HB3	1:E:627:ARG:HG3	1.87	0.56
1:A:138:GLU:OE2	1:A:271:ALA:HB2	2.05	0.56
1:B:374:PRO:HA	1:B:392:THR:HG22	1.88	0.56
1:B:574:ILE:HG13	1:B:574:ILE:O	2.06	0.56
1:C:51:PHE:HB3	1:C:80:MSE:SE	2.55	0.56
1:D:675:MSE:HE2	1:D:715:HIS:CE1	2.37	0.56
1:E:321:VAL:HG12	1:E:340:ALA:HB2	1.86	0.56
1:E:496:VAL:HG22	1:E:501:THR:CB	2.33	0.56
1:E:50:GLN:HE22	1:E:65:ARG:HH21	1.52	0.56
1:E:667:THR:OG1	1:E:673:GLY:HA3	2.05	0.56
2:J:3:BMA:C2	2:J:4:MAN:O5	2.53	0.56
1:A:470:LEU:HB3	1:A:474:CYS:SG	2.46	0.56
1:A:690:VAL:HG12	1:A:699:LEU:HD13	1.87	0.56
1:B:654:PRO:HB3	1:B:684:ARG:C	2.26	0.56
1:D:321:VAL:HG22	1:D:326:LEU:HD23	1.87	0.56
1:F:288:ASP:OD1	1:F:314:LYS:HB2	2.05	0.56
1:F:66:TYR:CD2	1:F:67:MSE:O	2.59	0.56
1:A:574:ILE:HG13	1:A:574:ILE:O	2.06	0.56
1:B:27:SER:HB2	1:B:28:PRO:HD2	1.86	0.56
1:C:66:TYR:CD2	1:C:67:MSE:O	2.59	0.56
1:D:257:LEU:H	1:D:258:PRO:CD	2.10	0.56
1:E:655:LEU:HB2	1:E:683:ASP:OD2	2.06	0.56
1:F:50:GLN:HE22	1:F:65:ARG:HH21	1.52	0.56
1:F:93:ARG:HH11	1:F:93:ARG:N	1.90	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:OG1	1:B:107:PRO:HD2	2.06	0.56
1:C:622:ALA:HB3	1:C:627:ARG:HG3	1.88	0.56
1:E:274:PRO:HD3	1:E:330:TRP:CE3	2.41	0.56
1:A:311:ILE:HD11	1:A:330:TRP:NE1	2.05	0.56
1:A:50:GLN:HE22	1:A:65:ARG:HH21	1.52	0.56
1:A:93:ARG:N	1:A:93:ARG:HH11	1.91	0.56
1:B:50:GLN:HE22	1:B:65:ARG:HH21	1.52	0.56
1:C:387:LEU:HD12	1:C:647:PHE:CE1	2.41	0.56
1:D:690:VAL:HG12	1:D:699:LEU:HD13	1.87	0.56
1:E:288:ASP:OD1	1:E:314:LYS:HB2	2.06	0.56
1:E:27:SER:HB2	1:E:28:PRO:HD2	1.88	0.56
1:A:87:THR:OG1	1:A:107:PRO:HD2	2.06	0.55
1:C:18:TYR:HE1	1:C:22:THR:HG22	1.68	0.55
1:E:87:THR:OG1	1:E:107:PRO:HD2	2.06	0.55
1:B:138:GLU:OE2	1:B:271:ALA:HB2	2.07	0.55
1:B:514:GLY:O	1:B:516:SER:N	2.31	0.55
1:C:441:PHE:CD1	1:C:583:LYS:HG2	2.42	0.55
1:C:50:GLN:HE22	1:C:65:ARG:HH21	1.52	0.55
1:F:135:VAL:HG12	1:F:140:TYR:OH	2.06	0.55
1:F:390:GLU:HG2	1:F:496:VAL:HB	1.86	0.55
1:C:126:LEU:HD12	1:C:127:ALA:H	1.71	0.55
1:D:393:VAL:HG23	1:D:491:VAL:HG13	1.89	0.55
1:E:126:LEU:HD12	1:E:127:ALA:H	1.71	0.55
1:A:135:VAL:HG12	1:A:140:TYR:OH	2.07	0.55
1:B:288:ASP:OD1	1:B:314:LYS:HB2	2.07	0.55
1:D:27:SER:HB2	1:D:28:PRO:HD2	1.88	0.55
1:D:574:ILE:HG13	1:D:574:ILE:O	2.06	0.55
1:F:19:CYS:C	1:F:21:HIS:H	2.08	0.55
1:F:451:GLY:HA2	1:F:588:ASN:HA	1.88	0.55
1:B:51:PHE:HB3	1:B:80:MSE:SE	2.55	0.55
1:B:667:THR:OG1	1:B:673:GLY:HA3	2.06	0.55
1:D:92:ARG:HA	1:D:93:ARG:NH1	2.21	0.55
1:E:374:PRO:HA	1:E:392:THR:HG22	1.88	0.55
1:F:441:PHE:CD1	1:F:583:LYS:HG2	2.42	0.55
1:A:114:SER:HB3	1:A:123:SER:HB3	1.88	0.55
1:A:292:LEU:HD22	1:A:310:TRP:HB3	1.88	0.55
1:C:655:LEU:HB2	1:C:683:ASP:OD2	2.06	0.55
1:E:530:PHE:CZ	1:E:617:PHE:HD1	2.25	0.55
1:B:610:PRO:O	1:B:614:THR:HG23	2.06	0.55
1:C:390:GLU:HG2	1:C:496:VAL:HB	1.87	0.55
1:C:675:MSE:HE2	1:C:715:HIS:CE1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:VAL:HG12	1:D:140:TYR:OH	2.07	0.55
1:D:288:ASP:OD1	1:D:314:LYS:HB2	2.05	0.55
1:D:655:LEU:HB2	1:D:683:ASP:OD2	2.06	0.55
1:F:51:PHE:HB3	1:F:80:MSE:SE	2.57	0.55
1:C:135:VAL:HG12	1:C:140:TYR:OH	2.06	0.55
1:D:87:THR:OG1	1:D:107:PRO:HD2	2.07	0.55
1:E:66:TYR:CD2	1:E:67:MSE:O	2.60	0.55
1:A:497:TYR:HD2	1:A:497:TYR:H	1.54	0.55
1:B:298:ARG:NH1	1:B:615:ALA:HB3	2.22	0.55
1:D:18:TYR:HE1	1:D:22:THR:HG22	1.70	0.55
1:D:268:VAL:HG22	1:D:269:PRO:HD2	1.88	0.55
1:F:655:LEU:HB2	1:F:683:ASP:OD2	2.07	0.55
1:B:114:SER:HB3	1:B:123:SER:HB3	1.88	0.55
1:F:118:SER:O	1:F:119:ASN:HB2	2.07	0.55
1:F:690:VAL:HG12	1:F:699:LEU:HD13	1.87	0.55
1:A:257:LEU:H	1:A:258:PRO:CD	2.09	0.54
1:A:667:THR:OG1	1:A:673:GLY:HA3	2.05	0.54
1:C:393:VAL:HG23	1:C:491:VAL:HG13	1.90	0.54
1:D:138:GLU:OE2	1:D:271:ALA:HB2	2.07	0.54
1:E:114:SER:HB3	1:E:123:SER:HB3	1.88	0.54
1:F:92:ARG:HA	1:F:93:ARG:NH1	2.22	0.54
1:A:118:SER:O	1:A:119:ASN:HB2	2.07	0.54
1:A:393:VAL:HG23	1:A:491:VAL:HG13	1.88	0.54
1:B:441:PHE:CD1	1:B:583:LYS:HG2	2.42	0.54
1:E:298:ARG:NH1	1:E:615:ALA:HB3	2.22	0.54
1:E:610:PRO:O	1:E:614:THR:HG23	2.06	0.54
1:A:79:THR:C	1:A:81:ASP:N	2.60	0.54
1:B:92:ARG:HA	1:B:93:ARG:NH1	2.22	0.54
1:C:610:PRO:O	1:C:614:THR:HG23	2.08	0.54
1:D:51:PHE:HB3	1:D:80:MSE:SE	2.58	0.54
1:E:292:LEU:HD22	1:E:310:TRP:HB3	1.88	0.54
1:B:655:LEU:HB2	1:B:683:ASP:OD2	2.06	0.54
1:B:79:THR:C	1:B:81:ASP:N	2.61	0.54
1:C:92:ARG:HA	1:C:93:ARG:NH1	2.22	0.54
1:D:622:ALA:HB3	1:D:627:ARG:CG	2.38	0.54
1:D:66:TYR:CD2	1:D:67:MSE:O	2.60	0.54
1:F:268:VAL:HG11	1:F:332:ASN:ND2	2.22	0.54
1:A:441:PHE:CD1	1:A:583:LYS:HG2	2.42	0.54
1:C:87:THR:OG1	1:C:107:PRO:HD2	2.07	0.54
1:D:374:PRO:HA	1:D:392:THR:HG22	1.89	0.54
1:D:79:THR:C	1:D:81:ASP:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:LEU:O	1:E:487:ALA:HB1	2.07	0.54
1:F:374:PRO:HA	1:F:392:THR:HG22	1.89	0.54
1:A:321:VAL:HG22	1:A:326:LEU:HD23	1.88	0.54
1:B:135:VAL:HG12	1:B:140:TYR:OH	2.07	0.54
1:B:399:LEU:O	1:B:487:ALA:HB1	2.07	0.54
1:C:114:SER:HB3	1:C:123:SER:HB3	1.90	0.54
1:F:295:LEU:HG	1:F:330:TRP:HD1	1.73	0.54
1:A:655:LEU:HB2	1:A:683:ASP:OD2	2.07	0.54
1:B:292:LEU:HD22	1:B:310:TRP:HB3	1.88	0.54
1:C:136:GLY:CA	1:C:268:VAL:HG21	2.29	0.54
1:C:374:PRO:HA	1:C:392:THR:HG22	1.90	0.54
1:C:445:TYR:CD2	1:C:452:ALA:HB3	2.43	0.54
1:C:574:ILE:O	1:C:574:ILE:HG13	2.07	0.54
1:E:268:VAL:HG22	1:E:269:PRO:HD2	1.90	0.54
1:E:295:LEU:HG	1:E:330:TRP:HD1	1.72	0.54
1:E:92:ARG:HA	1:E:93:ARG:NH1	2.22	0.54
1:F:87:THR:OG1	1:F:107:PRO:HD2	2.07	0.54
1:C:445:TYR:HB3	1:C:451:GLY:CA	2.33	0.54
1:D:79:THR:HG23	1:D:81:ASP:HB3	1.90	0.54
1:F:508:VAL:HG13	1:F:524:GLY:O	2.08	0.54
1:A:543:LEU:HA	1:A:612:GLN:HE22	1.72	0.54
1:E:20:HIS:NE2	1:E:121:ALA:HB1	2.23	0.54
1:E:138:GLU:OE2	1:E:271:ALA:HB2	2.07	0.54
1:F:114:SER:HB3	1:F:123:SER:HB3	1.87	0.54
1:E:622:ALA:HB3	1:E:627:ARG:CG	2.38	0.54
1:F:530:PHE:CZ	1:F:617:PHE:HD1	2.26	0.54
1:A:374:PRO:HA	1:A:392:THR:HG22	1.88	0.53
1:B:66:TYR:CD2	1:B:67:MSE:O	2.61	0.53
1:F:393:VAL:HG23	1:F:491:VAL:HG13	1.90	0.53
1:A:295:LEU:HG	1:A:330:TRP:HD1	1.73	0.53
1:C:445:TYR:HB3	1:C:452:ALA:N	2.23	0.53
1:D:114:SER:HB3	1:D:123:SER:HB3	1.88	0.53
1:E:257:LEU:H	1:E:258:PRO:CD	2.10	0.53
1:E:393:VAL:HG23	1:E:491:VAL:HG13	1.90	0.53
1:F:287:LEU:HD13	1:F:311:ILE:HD13	1.90	0.53
1:D:300:LEU:HD11	1:D:337:ARG:HD3	1.90	0.53
1:E:53:TYR:HD2	1:E:58:ALA:O	1.91	0.53
1:E:51:PHE:HB3	1:E:80:MSE:SE	2.58	0.53
1:F:543:LEU:HA	1:F:612:GLN:HE22	1.69	0.53
1:A:66:TYR:CD2	1:A:67:MSE:O	2.61	0.53
1:C:262:ILE:HG13	1:C:263:PRO:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:VAL:HG12	1:F:29:VAL:O	2.08	0.53
1:B:20:HIS:NE2	1:B:121:ALA:HB1	2.24	0.53
1:C:42:THR:HG22	1:C:104:LYS:HG3	1.91	0.53
1:C:454:CYS:SG	1:C:455:PHE:N	2.81	0.53
1:D:441:PHE:CD1	1:D:583:LYS:HG2	2.43	0.53
1:E:532:PRO:HD2	1:E:533:PHE:CD1	2.43	0.53
1:F:95:SER:OG	1:F:259:PHE:CE1	2.42	0.53
1:A:136:GLY:HA3	1:A:268:VAL:CG2	2.27	0.53
1:B:532:PRO:HD2	1:B:533:PHE:CD1	2.44	0.53
1:C:508:VAL:HG13	1:C:524:GLY:O	2.08	0.53
1:C:652:ASP:C	1:C:654:PRO:HD2	2.29	0.53
1:C:79:THR:C	1:C:81:ASP:N	2.61	0.53
1:D:532:PRO:HD2	1:D:533:PHE:CD1	2.44	0.53
1:C:497:TYR:HD2	1:C:497:TYR:H	1.57	0.53
1:D:508:VAL:HG13	1:D:524:GLY:O	2.09	0.53
1:E:118:SER:O	1:E:119:ASN:HB2	2.09	0.53
1:E:29:VAL:HG12	1:E:29:VAL:O	2.09	0.53
1:A:20:HIS:NE2	1:A:121:ALA:HB1	2.23	0.53
1:A:29:VAL:HG12	1:A:29:VAL:O	2.09	0.53
1:A:622:ALA:HB3	1:A:627:ARG:CG	2.38	0.53
1:D:292:LEU:HD22	1:D:310:TRP:HB3	1.90	0.53
1:D:447:PHE:HB2	1:D:455:PHE:O	2.09	0.53
1:E:301:GLY:O	1:E:616:PRO:O	2.27	0.53
1:B:18:TYR:HE1	1:B:22:THR:HG22	1.70	0.53
1:C:20:HIS:NE2	1:C:121:ALA:HB1	2.23	0.53
1:C:29:VAL:O	1:C:29:VAL:HG12	2.09	0.53
1:D:131:LYS:NZ	4:N:1:NAG:H81	2.24	0.53
1:B:29:VAL:O	1:B:29:VAL:HG12	2.09	0.53
1:B:93:ARG:H	1:B:93:ARG:NH1	1.90	0.53
1:C:292:LEU:HD22	1:C:310:TRP:HB3	1.90	0.53
1:C:85:ILE:HG22	1:C:86:SER:N	2.24	0.53
1:D:20:HIS:NE2	1:D:121:ALA:HB1	2.23	0.53
1:F:268:VAL:HG22	1:F:269:PRO:HD2	1.91	0.53
1:F:361:TYR:HB2	1:F:381:ARG:HH21	1.74	0.53
1:B:118:SER:O	1:B:119:ASN:HB2	2.10	0.52
1:B:295:LEU:HG	1:B:330:TRP:HD1	1.73	0.52
1:B:321:VAL:HG22	1:B:326:LEU:HD23	1.91	0.52
1:B:393:VAL:HG23	1:B:491:VAL:HG13	1.91	0.52
1:C:53:TYR:HD2	1:C:58:ALA:O	1.91	0.52
1:E:508:VAL:HG13	1:E:524:GLY:O	2.09	0.52
1:F:53:TYR:HD2	1:F:58:ALA:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:PHE:CZ	1:A:617:PHE:HD1	2.27	0.52
1:D:107:PRO:CG	1:D:108:GLY:H	2.22	0.52
1:E:135:VAL:HG12	1:E:140:TYR:OH	2.08	0.52
1:E:603:TRP:O	1:E:607:SER:N	2.43	0.52
1:F:497:TYR:H	1:F:497:TYR:HD2	1.55	0.52
1:B:137:ARG:NH1	1:B:296:THR:OG1	2.42	0.52
1:C:150:ILE:HG23	1:C:151:PRO:CD	2.39	0.52
1:C:447:PHE:HE1	1:C:455:PHE:HA	1.72	0.52
1:D:42:THR:HG22	1:D:104:LYS:HG3	1.91	0.52
1:F:138:GLU:OE2	1:F:271:ALA:HB2	2.10	0.52
1:A:287:LEU:HD13	1:A:311:ILE:HD13	1.92	0.52
1:C:530:PHE:CZ	1:C:617:PHE:HD1	2.27	0.52
1:D:295:LEU:HG	1:D:330:TRP:HD1	1.74	0.52
1:F:292:LEU:HD22	1:F:310:TRP:HB3	1.90	0.52
1:F:544:VAL:HG12	1:F:623:VAL:HG21	1.92	0.52
1:E:321:VAL:HG22	1:E:326:LEU:HD23	1.91	0.52
1:F:37:GLU:OE1	1:F:473:ASP:OD2	2.27	0.52
1:F:413:THR:HG23	1:F:595:GLN:HE22	1.75	0.52
1:F:532:PRO:HD2	1:F:533:PHE:CD1	2.44	0.52
1:A:483:LYS:HD3	1:A:535:HIS:NE2	2.25	0.52
1:A:51:PHE:HB3	1:A:80:MSE:SE	2.60	0.52
1:B:413:THR:HG23	1:B:595:GLN:HE22	1.75	0.52
1:B:438:CYS:HA	1:B:464:SER:O	2.10	0.52
1:B:622:ALA:HB3	1:B:627:ARG:HG3	1.91	0.52
1:D:438:CYS:HA	1:D:464:SER:O	2.09	0.52
1:D:93:ARG:NH1	1:D:93:ARG:H	1.91	0.52
1:F:20:HIS:NE2	1:F:121:ALA:HB1	2.23	0.52
1:F:79:THR:C	1:F:81:ASP:N	2.61	0.52
1:A:53:TYR:HD2	1:A:58:ALA:O	1.93	0.52
1:A:555:MSE:H	1:A:555:MSE:HE2	1.74	0.52
1:A:79:THR:HG23	1:A:81:ASP:HB3	1.91	0.52
1:B:268:VAL:HG22	1:B:269:PRO:HD2	1.92	0.52
1:B:85:ILE:HG22	1:B:86:SER:N	2.25	0.52
1:D:287:LEU:HD13	1:D:311:ILE:HD13	1.92	0.52
1:D:689:PRO:HD2	1:D:730:CYS:HA	1.92	0.52
1:E:112:THR:OG1	1:E:125:THR:HB	2.10	0.52
1:E:79:THR:HG23	1:E:81:ASP:HB3	1.91	0.52
1:F:321:VAL:HG22	1:F:326:LEU:HD23	1.91	0.52
1:A:112:THR:OG1	1:A:125:THR:HB	2.10	0.52
1:B:341:GLN:O	1:B:669:SER:O	2.27	0.52
1:C:294:LEU:HD23	1:C:309:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:VAL:HG12	1:D:29:VAL:O	2.09	0.52
1:D:72:ASP:HB2	1:D:74:THR:OG1	2.10	0.52
1:F:294:LEU:HG	1:F:310:TRP:NE1	2.25	0.52
1:F:438:CYS:HA	1:F:464:SER:O	2.10	0.52
1:A:137:ARG:NH1	1:A:296:THR:OG1	2.43	0.52
1:B:544:VAL:HG12	1:B:623:VAL:HG21	1.92	0.52
1:B:79:THR:HG23	1:B:81:ASP:HB3	1.92	0.52
1:C:295:LEU:HG	1:C:330:TRP:HD1	1.75	0.52
1:A:496:VAL:HG13	1:A:501:THR:HG22	1.92	0.52
1:B:496:VAL:HG13	1:B:501:THR:HG22	1.92	0.52
1:E:496:VAL:HG13	1:E:501:THR:HG22	1.92	0.52
1:A:508:VAL:HG13	1:A:524:GLY:O	2.10	0.51
1:C:438:CYS:HA	1:C:464:SER:O	2.10	0.51
1:E:85:ILE:HG22	1:E:86:SER:N	2.25	0.51
1:F:262:ILE:HG13	1:F:263:PRO:O	2.10	0.51
1:C:448:MSE:C	1:C:450:GLY:H	2.13	0.51
1:C:543:LEU:HA	1:C:612:GLN:HE22	1.71	0.51
1:E:45:ILE:HB	1:E:101:LEU:HB2	1.93	0.51
1:A:540:HIS:HD2	1:A:541:ARG:HB2	1.76	0.51
1:A:675:MSE:HE2	1:A:715:HIS:CE1	2.38	0.51
1:A:72:ASP:HB2	1:A:74:THR:OG1	2.10	0.51
1:A:79:THR:O	1:A:81:ASP:N	2.43	0.51
1:D:603:TRP:O	1:D:607:SER:N	2.44	0.51
1:D:79:THR:O	1:D:81:ASP:N	2.43	0.51
1:E:136:GLY:CA	1:E:268:VAL:HG21	2.30	0.51
1:F:276:VAL:HG22	1:F:285:LEU:HD23	1.91	0.51
1:F:79:THR:HG23	1:F:81:ASP:HB3	1.92	0.51
1:B:483:LYS:HD3	1:B:535:HIS:CE1	2.45	0.51
1:B:497:TYR:HD2	1:B:497:TYR:H	1.58	0.51
1:C:390:GLU:HG3	1:C:390:GLU:O	2.10	0.51
1:C:483:LYS:HD3	1:C:535:HIS:CE1	2.45	0.51
1:C:544:VAL:HG12	1:C:623:VAL:HG21	1.92	0.51
1:D:496:VAL:HG13	1:D:501:THR:HG22	1.92	0.51
1:E:483:LYS:HD3	1:E:535:HIS:CE1	2.44	0.51
1:E:544:VAL:HG12	1:E:623:VAL:HG21	1.91	0.51
1:F:483:LYS:HD3	1:F:535:HIS:CE1	2.45	0.51
1:A:689:PRO:HD2	1:A:730:CYS:HA	1.92	0.51
1:B:483:LYS:HD3	1:B:535:HIS:NE2	2.26	0.51
1:F:262:ILE:HG13	1:F:263:PRO:N	2.24	0.51
1:F:603:TRP:O	1:F:607:SER:N	2.44	0.51
1:A:438:CYS:HA	1:A:464:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:TYR:HD2	1:B:58:ALA:O	1.92	0.51
1:C:413:THR:HG23	1:C:595:GLN:HE22	1.76	0.51
1:C:496:VAL:HG13	1:C:501:THR:HG22	1.93	0.51
1:D:483:LYS:HD3	1:D:535:HIS:CE1	2.46	0.51
1:E:262:ILE:HG13	1:E:263:PRO:O	2.10	0.51
1:E:413:THR:HG23	1:E:595:GLN:HE22	1.75	0.51
1:F:622:ALA:HB3	1:F:627:ARG:CG	2.40	0.51
1:F:85:ILE:HG22	1:F:86:SER:N	2.26	0.51
1:A:42:THR:HG22	1:A:104:LYS:HG3	1.92	0.51
1:B:42:THR:HG22	1:B:104:LYS:HG3	1.93	0.51
1:B:508:VAL:HG13	1:B:524:GLY:O	2.10	0.51
1:B:540:HIS:HD2	1:B:541:ARG:HB2	1.76	0.51
1:B:689:PRO:HD2	1:B:730:CYS:HA	1.92	0.51
1:D:544:VAL:HG12	1:D:623:VAL:HG21	1.93	0.51
1:D:530:PHE:CZ	1:D:617:PHE:HD1	2.27	0.51
1:D:85:ILE:HG22	1:D:86:SER:N	2.25	0.51
1:E:137:ARG:NH1	1:E:296:THR:OG1	2.43	0.51
1:F:483:LYS:HD3	1:F:535:HIS:NE2	2.26	0.51
1:A:390:GLU:O	1:A:390:GLU:HG3	2.10	0.51
1:C:287:LEU:HD13	1:C:311:ILE:HD13	1.93	0.51
1:C:603:TRP:O	1:C:607:SER:N	2.44	0.51
1:C:649:ARG:O	1:C:651:SER:N	2.44	0.51
1:B:603:TRP:O	1:B:607:SER:N	2.43	0.51
1:B:94:LEU:HD22	1:B:157:ARG:CD	2.38	0.51
1:C:274:PRO:HD3	1:C:330:TRP:CZ3	2.46	0.51
1:C:483:LYS:HD3	1:C:535:HIS:NE2	2.26	0.51
1:C:581:LEU:HD22	1:C:581:LEU:N	2.26	0.51
1:D:483:LYS:HD3	1:D:535:HIS:NE2	2.25	0.51
1:D:540:HIS:HD2	1:D:541:ARG:HB2	1.76	0.51
1:E:287:LEU:HD13	1:E:311:ILE:HD13	1.93	0.51
1:E:294:LEU:HD23	1:E:309:GLU:O	2.11	0.51
1:E:555:MSE:H	1:E:555:MSE:HE2	1.75	0.51
1:E:689:PRO:HD2	1:E:730:CYS:HA	1.92	0.51
1:F:649:ARG:O	1:F:651:SER:N	2.44	0.51
1:B:287:LEU:HD13	1:B:311:ILE:HD13	1.93	0.51
1:B:45:ILE:HB	1:B:101:LEU:HB2	1.93	0.51
1:C:137:ARG:NH1	1:C:296:THR:OG1	2.42	0.51
1:E:42:THR:HG22	1:E:104:LYS:HG3	1.92	0.51
1:F:390:GLU:O	1:F:390:GLU:HG3	2.10	0.51
1:F:622:ALA:HB3	1:F:627:ARG:HG3	1.92	0.51
1:A:447:PHE:CZ	1:A:448:MSE:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ILE:HG13	1:B:263:PRO:O	2.11	0.50
1:C:118:SER:O	1:C:119:ASN:HB2	2.10	0.50
1:C:268:VAL:HG22	1:C:269:PRO:HD2	1.92	0.50
1:E:107:PRO:CG	1:E:108:GLY:H	2.23	0.50
1:E:438:CYS:HA	1:E:464:SER:O	2.11	0.50
1:E:483:LYS:HD3	1:E:535:HIS:NE2	2.26	0.50
1:F:496:VAL:HG13	1:F:501:THR:HG22	1.93	0.50
1:A:504:LEU:HD21	1:A:521:VAL:HB	1.93	0.50
1:B:94:LEU:CD2	1:B:157:ARG:HD3	2.38	0.50
1:C:321:VAL:HG22	1:C:326:LEU:HD23	1.94	0.50
1:C:653:ALA:O	1:C:684:ARG:HD2	2.11	0.50
1:D:413:THR:HG23	1:D:595:GLN:HE22	1.75	0.50
1:E:79:THR:C	1:E:81:ASP:N	2.61	0.50
1:E:79:THR:O	1:E:81:ASP:N	2.44	0.50
1:A:400:PRO:CA	1:A:487:ALA:HB2	2.41	0.50
1:A:85:ILE:HG22	1:A:86:SER:N	2.27	0.50
1:D:262:ILE:HG13	1:D:263:PRO:N	2.25	0.50
1:D:390:GLU:HG3	1:D:390:GLU:O	2.11	0.50
1:E:80:MSE:HE3	1:E:80:MSE:CA	2.41	0.50
1:A:262:ILE:HG13	1:A:263:PRO:N	2.25	0.50
1:A:262:ILE:HG13	1:A:263:PRO:O	2.11	0.50
1:C:689:PRO:HD2	1:C:730:CYS:HA	1.92	0.50
1:C:79:THR:HG23	1:C:81:ASP:HB3	1.92	0.50
1:D:262:ILE:HG13	1:D:263:PRO:O	2.11	0.50
1:E:504:LEU:HD21	1:E:521:VAL:HB	1.94	0.50
1:F:79:THR:O	1:F:81:ASP:N	2.44	0.50
1:A:447:PHE:CD1	1:A:454:CYS:O	2.61	0.50
1:A:278:HIS:CB	1:A:343:SER:HB3	2.41	0.50
1:A:400:PRO:HD2	1:A:626:LEU:O	2.12	0.50
1:C:138:GLU:OE2	1:C:271:ALA:HB2	2.12	0.50
1:C:622:ALA:HB3	1:C:627:ARG:CG	2.42	0.50
1:D:581:LEU:HD22	1:D:581:LEU:N	2.26	0.50
1:F:42:THR:HG22	1:F:104:LYS:HG3	1.92	0.50
1:F:80:MSE:HA	1:F:80:MSE:HE3	1.94	0.50
1:A:483:LYS:HD3	1:A:535:HIS:CE1	2.47	0.50
1:A:544:VAL:HG12	1:A:623:VAL:HG21	1.93	0.50
1:B:294:LEU:HG	1:B:310:TRP:NE1	2.26	0.50
1:B:722:GLN:HG2	1:B:739:GLU:HG2	1.94	0.50
1:C:262:ILE:HG13	1:C:263:PRO:O	2.11	0.50
1:C:277:ILE:HD12	1:C:286:GLN:NE2	2.27	0.50
1:C:420:ILE:O	1:C:420:ILE:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:689:PRO:HD2	1:F:730:CYS:HA	1.92	0.50
1:A:276:VAL:HG12	1:A:277:ILE:N	2.26	0.50
1:A:300:LEU:HD11	1:A:337:ARG:HD3	1.93	0.50
1:A:581:LEU:N	1:A:581:LEU:HD22	2.26	0.50
1:A:690:VAL:HG12	1:A:699:LEU:CD1	2.42	0.50
1:B:374:PRO:CA	1:B:392:THR:HG22	2.42	0.50
1:B:622:ALA:HB3	1:B:627:ARG:CG	2.41	0.50
1:B:690:VAL:HG12	1:B:699:LEU:CD1	2.42	0.50
1:C:532:PRO:HD2	1:C:533:PHE:CD1	2.47	0.50
1:D:400:PRO:HD2	1:D:626:LEU:O	2.12	0.50
1:E:276:VAL:HG22	1:E:285:LEU:HD23	1.94	0.50
1:E:400:PRO:HD2	1:E:626:LEU:O	2.12	0.50
1:F:112:THR:OG1	1:F:125:THR:HB	2.12	0.50
1:A:45:ILE:HB	1:A:101:LEU:HB2	1.94	0.50
1:D:504:LEU:HD21	1:D:521:VAL:HB	1.94	0.50
1:E:540:HIS:HD2	1:E:541:ARG:HB2	1.77	0.50
1:F:555:MSE:HE2	1:F:555:MSE:H	1.76	0.50
1:A:722:GLN:HG2	1:A:739:GLU:HG2	1.94	0.49
1:C:112:THR:OG1	1:C:125:THR:HB	2.11	0.49
1:C:722:GLN:HG2	1:C:739:GLU:HG2	1.94	0.49
1:F:106:PRO:CB	1:F:107:PRO:HD3	2.41	0.49
1:F:45:ILE:HB	1:F:101:LEU:HB2	1.93	0.49
1:A:603:TRP:O	1:A:607:SER:N	2.45	0.49
1:A:80:MSE:CA	1:A:80:MSE:HE3	2.42	0.49
1:C:255:LEU:HD22	1:C:256:HIS:CD2	2.47	0.49
1:C:45:ILE:HB	1:C:101:LEU:HB2	1.93	0.49
1:C:652:ASP:HB3	1:C:654:PRO:HD2	1.95	0.49
1:D:654:PRO:HB3	1:D:684:ARG:O	2.12	0.49
1:E:262:ILE:HG13	1:E:263:PRO:N	2.25	0.49
1:E:497:TYR:HD2	1:E:497:TYR:H	1.56	0.49
1:F:574:ILE:HG13	1:F:574:ILE:O	2.11	0.49
1:B:504:LEU:HD21	1:B:521:VAL:HB	1.94	0.49
1:B:79:THR:O	1:B:81:ASP:N	2.45	0.49
1:D:649:ARG:O	1:D:651:SER:N	2.45	0.49
1:F:581:LEU:HD22	1:F:581:LEU:N	2.27	0.49
1:A:532:PRO:HD2	1:A:533:PHE:CD1	2.48	0.49
1:B:262:ILE:HG13	1:B:263:PRO:N	2.27	0.49
1:B:138:GLU:OE2	1:B:271:ALA:N	2.46	0.49
1:A:154:VAL:HG22	1:A:155:TYR:N	2.28	0.49
1:B:255:LEU:CG	1:B:256:HIS:N	2.65	0.49
1:C:276:VAL:HG22	1:C:285:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASP:HB2	1:C:74:THR:OG1	2.12	0.49
1:C:79:THR:O	1:C:81:ASP:N	2.45	0.49
1:D:112:THR:OG1	1:D:125:THR:HB	2.12	0.49
1:D:374:PRO:CA	1:D:392:THR:HG22	2.42	0.49
1:D:63:LYS:C	1:D:80:MSE:HG2	2.33	0.49
1:E:374:PRO:CA	1:E:392:THR:HG22	2.42	0.49
1:E:63:LYS:C	1:E:80:MSE:HG2	2.32	0.49
1:E:690:VAL:HG12	1:E:699:LEU:CD1	2.42	0.49
1:E:72:ASP:HB2	1:E:74:THR:OG1	2.13	0.49
1:A:276:VAL:HG22	1:A:285:LEU:HD23	1.94	0.49
1:A:336:VAL:CG2	1:A:337:ARG:N	2.76	0.49
1:A:374:PRO:CA	1:A:392:THR:HG22	2.42	0.49
1:C:400:PRO:HD2	1:C:626:LEU:O	2.13	0.49
1:C:63:LYS:C	1:C:80:MSE:HG2	2.33	0.49
1:C:644:ASN:HA	1:C:647:PHE:CD2	2.48	0.49
1:D:45:ILE:HB	1:D:101:LEU:HB2	1.94	0.49
1:D:625:PRO:HD2	1:D:627:ARG:HH12	1.78	0.49
1:E:654:PRO:HB3	1:E:684:ARG:O	2.12	0.49
1:A:294:LEU:HG	1:A:310:TRP:NE1	2.26	0.49
1:A:400:PRO:HA	1:A:487:ALA:CB	2.43	0.49
1:B:649:ARG:O	1:B:651:SER:N	2.45	0.49
1:B:654:PRO:HB3	1:B:684:ARG:O	2.13	0.49
1:D:268:VAL:HG11	1:D:332:ASN:ND2	2.27	0.49
1:D:80:MSE:HA	1:D:80:MSE:HE3	1.94	0.49
1:E:276:VAL:HG12	1:E:277:ILE:N	2.28	0.49
1:E:543:LEU:HA	1:E:612:GLN:HE22	1.72	0.49
1:F:504:LEU:HD21	1:F:521:VAL:HB	1.95	0.49
1:F:63:LYS:C	1:F:80:MSE:HG2	2.33	0.49
1:B:112:THR:OG1	1:B:125:THR:HB	2.12	0.49
1:C:504:LEU:HD21	1:C:521:VAL:HB	1.95	0.49
1:C:508:VAL:HG12	1:C:508:VAL:O	2.13	0.49
1:A:63:LYS:C	1:A:80:MSE:HG2	2.33	0.49
1:C:80:MSE:HE3	1:C:80:MSE:HA	1.95	0.49
1:E:138:GLU:OE2	1:E:271:ALA:N	2.46	0.49
1:E:300:LEU:HD11	1:E:337:ARG:HD3	1.95	0.49
1:E:649:ARG:O	1:E:651:SER:N	2.46	0.49
1:E:722:GLN:HG2	1:E:739:GLU:HG2	1.94	0.49
1:F:276:VAL:HG12	1:F:277:ILE:N	2.28	0.49
1:B:390:GLU:O	1:B:390:GLU:HG3	2.13	0.49
1:B:555:MSE:HE2	1:B:555:MSE:H	1.77	0.49
1:C:80:MSE:HE3	1:C:80:MSE:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:VAL:HG22	1:D:285:LEU:HD23	1.95	0.49
1:D:400:PRO:CA	1:D:487:ALA:HB2	2.42	0.49
1:E:77:GLU:HG2	1:E:78:GLY:N	2.28	0.49
1:F:508:VAL:HG12	1:F:508:VAL:O	2.12	0.49
1:F:407:ILE:HG21	1:F:568:LEU:HD13	1.95	0.49
1:D:137:ARG:NH1	1:D:296:THR:OG1	2.46	0.48
1:D:653:ALA:N	1:D:654:PRO:CD	2.74	0.48
1:D:722:GLN:HG2	1:D:739:GLU:HG2	1.94	0.48
1:F:722:GLN:HG2	1:F:739:GLU:HG2	1.94	0.48
1:B:268:VAL:HG11	1:B:332:ASN:ND2	2.28	0.48
1:B:72:ASP:HB2	1:B:74:THR:OG1	2.12	0.48
1:B:92:ARG:HA	1:B:93:ARG:HH12	1.79	0.48
1:C:77:GLU:HG2	1:C:78:GLY:N	2.28	0.48
1:E:644:ASN:HA	1:E:647:PHE:CD2	2.49	0.48
1:F:644:ASN:HA	1:F:647:PHE:CD2	2.48	0.48
1:F:77:GLU:HG2	1:F:78:GLY:N	2.28	0.48
1:F:93:ARG:H	1:F:93:ARG:NH1	1.92	0.48
1:B:136:GLY:CA	1:B:268:VAL:HG21	2.30	0.48
1:B:688:CYS:SG	1:B:706:VAL:HG21	2.53	0.48
1:E:688:CYS:SG	1:E:706:VAL:HG21	2.53	0.48
1:F:446:PRO:O	1:F:447:PHE:CB	2.61	0.48
1:F:80:MSE:CA	1:F:80:MSE:HE3	2.43	0.48
1:A:649:ARG:O	1:A:651:SER:N	2.45	0.48
1:A:653:ALA:N	1:A:654:PRO:HD2	2.28	0.48
1:C:690:VAL:HG12	1:C:699:LEU:CD1	2.42	0.48
1:D:154:VAL:HG22	1:D:155:TYR:N	2.28	0.48
1:D:644:ASN:HA	1:D:647:PHE:CD2	2.48	0.48
1:D:80:MSE:HE3	1:D:80:MSE:CA	2.43	0.48
1:E:537:VAL:HG22	1:E:546:ASN:ND2	2.28	0.48
1:F:274:PRO:HD3	1:F:330:TRP:CZ3	2.48	0.48
1:F:690:VAL:HG12	1:F:699:LEU:CD1	2.43	0.48
1:A:272:HIS:O	1:A:273:ALA:C	2.51	0.48
1:B:399:LEU:HD12	1:B:399:LEU:N	2.28	0.48
1:B:420:ILE:HD12	1:B:420:ILE:O	2.14	0.48
1:C:321:VAL:CG1	1:C:340:ALA:HB2	2.44	0.48
1:D:92:ARG:HA	1:D:93:ARG:HH12	1.78	0.48
1:F:420:ILE:HD12	1:F:420:ILE:O	2.13	0.48
1:F:688:CYS:SG	1:F:706:VAL:HG21	2.54	0.48
1:A:644:ASN:HA	1:A:647:PHE:CD2	2.48	0.48
1:A:64:TYR:CG	1:A:83:ILE:HD11	2.49	0.48
1:B:644:ASN:HA	1:B:647:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:VAL:HG22	1:C:546:ASN:ND2	2.27	0.48
1:D:276:VAL:HG12	1:D:277:ILE:N	2.27	0.48
1:D:277:ILE:HD12	1:D:286:GLN:NE2	2.28	0.48
1:D:53:TYR:HD2	1:D:58:ALA:O	1.97	0.48
1:F:150:ILE:HG23	1:F:151:PRO:CD	2.42	0.48
1:F:92:ARG:HA	1:F:93:ARG:HH12	1.79	0.48
1:A:106:PRO:CB	1:A:107:PRO:HD3	2.40	0.48
1:A:537:VAL:HG22	1:A:546:ASN:ND2	2.28	0.48
1:C:336:VAL:CG2	1:C:337:ARG:N	2.76	0.48
1:D:400:PRO:HA	1:D:487:ALA:CB	2.44	0.48
1:D:652:ASP:C	1:D:654:PRO:HD2	2.34	0.48
1:E:420:ILE:O	1:E:420:ILE:HD12	2.13	0.48
1:E:92:ARG:HA	1:E:93:ARG:HH12	1.79	0.48
1:F:154:VAL:HG22	1:F:155:TYR:N	2.28	0.48
1:F:336:VAL:CG2	1:F:337:ARG:N	2.77	0.48
1:F:400:PRO:HD2	1:F:626:LEU:O	2.13	0.48
1:F:72:ASP:HB2	1:F:74:THR:OG1	2.13	0.48
1:A:107:PRO:CG	1:A:108:GLY:H	2.22	0.48
1:A:413:THR:HG23	1:A:595:GLN:HE22	1.77	0.48
1:B:594:THR:HG21	1:C:272:HIS:HA	1.95	0.48
1:C:445:TYR:CB	1:C:451:GLY:HA3	2.37	0.48
1:E:400:PRO:CA	1:E:487:ALA:HB2	2.44	0.48
1:F:374:PRO:CA	1:F:392:THR:HG22	2.44	0.48
1:A:262:ILE:HD12	1:A:263:PRO:HD2	1.96	0.48
1:B:274:PRO:HD3	1:B:330:TRP:CZ3	2.49	0.48
1:E:504:LEU:O	1:E:504:LEU:HD12	2.14	0.48
1:A:449:TRP:O	1:A:451:GLY:N	2.46	0.48
1:B:394:MSE:HE2	1:B:394:MSE:HB3	1.91	0.48
1:C:688:CYS:SG	1:C:706:VAL:HG21	2.53	0.48
1:D:106:PRO:CB	1:D:107:PRO:HD3	2.40	0.48
1:D:555:MSE:HE2	1:D:555:MSE:H	1.78	0.48
1:E:329:ILE:HG12	1:E:329:ILE:H	1.49	0.48
1:E:80:MSE:HE3	1:E:80:MSE:HA	1.94	0.48
1:E:93:ARG:NH1	1:E:93:ARG:H	1.91	0.48
1:F:137:ARG:NH1	1:F:296:THR:OG1	2.45	0.48
1:F:400:PRO:CA	1:F:487:ALA:HB2	2.44	0.48
1:B:336:VAL:CG2	1:B:337:ARG:N	2.77	0.47
1:D:690:VAL:HG12	1:D:699:LEU:CD1	2.43	0.47
1:E:400:PRO:HA	1:E:487:ALA:CB	2.44	0.47
1:F:329:ILE:HG12	1:F:329:ILE:H	1.50	0.47
1:A:294:LEU:HD23	1:A:309:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:MSE:HA	1:A:80:MSE:HE3	1.95	0.47
1:B:537:VAL:HG22	1:B:546:ASN:ND2	2.28	0.47
1:C:300:LEU:HD11	1:C:337:ARG:HD3	1.95	0.47
1:C:374:PRO:CA	1:C:392:THR:HG22	2.43	0.47
1:C:92:ARG:HA	1:C:93:ARG:HH12	1.80	0.47
1:D:106:PRO:CB	1:D:107:PRO:CD	2.92	0.47
1:F:148:LYS:O	1:F:267:MSE:HA	2.15	0.47
1:F:138:GLU:OE2	1:F:271:ALA:N	2.47	0.47
1:F:64:TYR:CG	1:F:83:ILE:HD11	2.49	0.47
1:B:106:PRO:CB	1:B:107:PRO:CD	2.92	0.47
1:B:508:VAL:O	1:B:508:VAL:HG12	2.15	0.47
1:B:400:PRO:HD2	1:B:626:LEU:O	2.14	0.47
1:C:540:HIS:HD2	1:C:541:ARG:HB2	1.79	0.47
1:D:336:VAL:CG2	1:D:337:ARG:N	2.78	0.47
1:D:77:GLU:HG2	1:D:78:GLY:N	2.29	0.47
1:E:106:PRO:CB	1:E:107:PRO:CD	2.92	0.47
1:D:145:VAL:CG2	1:F:17:SER:HB3	2.30	0.47
1:F:277:ILE:HD12	1:F:286:GLN:NE2	2.30	0.47
1:F:540:HIS:HD2	1:F:541:ARG:HB2	1.79	0.47
1:F:654:PRO:HB3	1:F:684:ARG:O	2.14	0.47
1:B:106:PRO:CB	1:B:107:PRO:HD3	2.40	0.47
1:B:400:PRO:HA	1:B:487:ALA:CB	2.44	0.47
1:B:80:MSE:HA	1:B:80:MSE:HE3	1.95	0.47
1:C:294:LEU:HG	1:C:310:TRP:NE1	2.28	0.47
1:D:615:ALA:HA	1:D:616:PRO:HD3	1.55	0.47
1:D:661:CYS:HA	1:D:678:LEU:HD23	1.97	0.47
1:E:154:VAL:HG22	1:E:155:TYR:N	2.29	0.47
1:E:390:GLU:O	1:E:390:GLU:HG3	2.13	0.47
1:A:420:ILE:HD12	1:A:420:ILE:O	2.13	0.47
1:B:148:LYS:O	1:B:267:MSE:HA	2.14	0.47
1:B:276:VAL:HG22	1:B:285:LEU:HD23	1.95	0.47
1:E:137:ARG:H	1:E:332:ASN:HD22	1.63	0.47
1:F:400:PRO:HA	1:F:487:ALA:CB	2.45	0.47
1:B:294:LEU:HD23	1:B:309:GLU:O	2.14	0.47
1:B:80:MSE:CA	1:B:80:MSE:HE3	2.45	0.47
1:D:493:LEU:HD23	1:D:493:LEU:HA	1.61	0.47
1:E:148:LYS:O	1:E:267:MSE:HA	2.15	0.47
1:F:272:HIS:O	1:F:273:ALA:C	2.53	0.47
1:A:268:VAL:HG22	1:A:269:PRO:CD	2.44	0.47
1:B:63:LYS:C	1:B:80:MSE:HG2	2.35	0.47
1:C:375:TYR:O	1:C:390:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ILE:HD12	1:D:263:PRO:HD2	1.97	0.47
1:E:305:GLU:N	1:E:306:PRO:HD3	2.30	0.47
1:E:336:VAL:CG2	1:E:337:ARG:N	2.77	0.47
1:B:300:LEU:HD11	1:B:337:ARG:HD3	1.96	0.47
1:B:504:LEU:O	1:B:504:LEU:HD12	2.13	0.47
1:B:505:ASP:OD1	1:D:505:ASP:OD1	2.32	0.47
1:C:106:PRO:CB	1:C:107:PRO:CD	2.93	0.47
1:C:268:VAL:HG11	1:C:332:ASN:ND2	2.29	0.47
1:D:375:TYR:O	1:D:390:GLU:HA	2.15	0.47
1:D:508:VAL:HG12	1:D:508:VAL:O	2.15	0.47
1:E:378:LEU:HG	1:E:691:HIS:CG	2.49	0.47
1:F:375:TYR:O	1:F:390:GLU:HA	2.14	0.47
1:F:394:MSE:HB3	1:F:394:MSE:HE2	1.92	0.47
1:F:621:ILE:H	1:F:621:ILE:CD1	2.27	0.47
1:A:268:VAL:HG11	1:A:332:ASN:ND2	2.29	0.47
1:B:375:TYR:O	1:B:390:GLU:HA	2.15	0.47
1:B:661:CYS:HA	1:B:678:LEU:HD23	1.97	0.47
1:B:77:GLU:HG2	1:B:78:GLY:N	2.29	0.47
1:D:294:LEU:HD23	1:D:309:GLU:O	2.15	0.47
1:A:407:ILE:HG21	1:A:568:LEU:HD13	1.96	0.47
1:A:688:CYS:SG	1:A:706:VAL:HG21	2.55	0.47
1:B:154:VAL:HG22	1:B:155:TYR:N	2.29	0.47
1:B:400:PRO:CA	1:B:487:ALA:HB2	2.45	0.47
1:C:148:LYS:O	1:C:267:MSE:HA	2.14	0.47
1:C:720:SER:OG	1:C:723:ALA:HB2	2.15	0.47
1:D:537:VAL:HG22	1:D:546:ASN:ND2	2.29	0.47
1:D:688:CYS:SG	1:D:706:VAL:HG21	2.54	0.47
1:A:305:GLU:N	1:A:306:PRO:HD3	2.30	0.47
1:A:445:TYR:CG	1:A:451:GLY:HA3	2.51	0.47
1:A:504:LEU:HD21	1:A:521:VAL:CG2	2.45	0.47
1:A:60:SER:HB2	1:A:63:LYS:HB2	1.97	0.47
1:A:661:CYS:HA	1:A:678:LEU:HD23	1.97	0.47
1:B:305:GLU:N	1:B:306:PRO:HD3	2.30	0.47
1:C:154:VAL:HG22	1:C:155:TYR:N	2.30	0.47
1:C:272:HIS:O	1:C:273:ALA:C	2.53	0.47
1:C:400:PRO:CA	1:C:487:ALA:HB2	2.45	0.47
1:C:451:GLY:HA2	1:C:586:ALA:HB1	1.95	0.47
1:D:504:LEU:HD21	1:D:521:VAL:CG2	2.45	0.47
1:D:54:ASP:CG	1:D:55:GLN:H	2.18	0.47
1:F:262:ILE:HD12	1:F:263:PRO:HD2	1.96	0.47
1:A:277:ILE:HD12	1:A:286:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:TYR:O	1:A:390:GLU:HA	2.15	0.46
1:D:449:TRP:HD1	1:D:453:GLN:HG3	1.80	0.46
1:E:375:TYR:O	1:E:390:GLU:HA	2.15	0.46
1:F:504:LEU:HD21	1:F:521:VAL:CG2	2.45	0.46
1:F:720:SER:OG	1:F:723:ALA:HB2	2.15	0.46
1:A:97:LYS:HB3	1:A:100:PHE:HB2	1.97	0.46
1:A:145:VAL:HG22	1:C:17:SER:CB	2.25	0.46
1:A:321:VAL:CG1	1:A:340:ALA:HB2	2.45	0.46
1:A:621:ILE:CD1	1:A:621:ILE:H	2.28	0.46
1:B:150:ILE:HG23	1:B:151:PRO:CD	2.41	0.46
1:C:107:PRO:CG	1:C:108:GLY:H	2.23	0.46
1:C:621:ILE:CD1	1:C:621:ILE:H	2.28	0.46
1:C:64:TYR:CG	1:C:83:ILE:HD11	2.50	0.46
1:D:399:LEU:N	1:D:399:LEU:HD12	2.30	0.46
1:E:294:LEU:HG	1:E:310:TRP:NE1	2.30	0.46
1:C:262:ILE:HD12	1:C:263:PRO:HD2	1.97	0.46
1:C:305:GLU:N	1:C:306:PRO:HD3	2.30	0.46
1:D:407:ILE:HG21	1:D:568:LEU:HD13	1.96	0.46
1:D:422:CYS:SG	1:D:455:PHE:N	2.88	0.46
1:F:294:LEU:HD23	1:F:309:GLU:O	2.16	0.46
1:A:274:PRO:HD3	1:A:330:TRP:CZ3	2.51	0.46
1:A:399:LEU:N	1:A:399:LEU:HD12	2.30	0.46
1:A:77:GLU:HG2	1:A:78:GLY:N	2.28	0.46
1:D:400:PRO:HA	1:D:487:ALA:HB2	1.98	0.46
1:D:64:TYR:CG	1:D:83:ILE:HD11	2.51	0.46
1:E:268:VAL:HG11	1:E:332:ASN:ND2	2.30	0.46
1:E:378:LEU:HG	1:E:691:HIS:CD2	2.51	0.46
1:E:60:SER:HB2	1:E:63:LYS:HB2	1.98	0.46
1:E:64:TYR:CG	1:E:83:ILE:HD11	2.50	0.46
1:F:106:PRO:CB	1:F:107:PRO:CD	2.93	0.46
1:F:655:LEU:N	1:F:683:ASP:HB2	2.27	0.46
1:A:400:PRO:HA	1:A:487:ALA:HB2	1.97	0.46
1:B:486:THR:HG22	1:B:487:ALA:H	1.81	0.46
1:C:37:GLU:OE1	1:C:473:ASP:OD2	2.33	0.46
1:D:720:SER:OG	1:D:723:ALA:HB2	2.15	0.46
1:D:97:LYS:HB3	1:D:100:PHE:HB2	1.98	0.46
1:E:399:LEU:N	1:E:399:LEU:HD12	2.31	0.46
1:A:148:LYS:O	1:A:267:MSE:HA	2.16	0.46
1:A:399:LEU:C	1:A:487:ALA:HB1	2.36	0.46
1:A:489:MSE:HG3	1:A:508:VAL:HB	1.98	0.46
1:F:504:LEU:O	1:F:504:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:661:CYS:HA	1:F:678:LEU:HD23	1.97	0.46
2:K:1:NAG:C4	2:K:2:NAG:N2	2.74	0.46
1:A:363:HIS:NE2	1:A:365:THR:HG23	2.30	0.46
1:B:146:HIS:H	1:B:146:HIS:CD2	2.34	0.46
1:B:276:VAL:HG12	1:B:277:ILE:N	2.29	0.46
1:B:449:TRP:C	1:B:451:GLY:H	2.19	0.46
1:B:64:TYR:CG	1:B:83:ILE:HD11	2.50	0.46
1:B:97:LYS:HB3	1:B:100:PHE:HB2	1.98	0.46
1:C:106:PRO:CB	1:C:107:PRO:HD3	2.41	0.46
1:C:555:MSE:HB2	1:C:555:MSE:HE3	1.70	0.46
1:C:407:ILE:HG21	1:C:568:LEU:HD13	1.95	0.46
1:C:661:CYS:HA	1:C:678:LEU:HD23	1.97	0.46
1:D:150:ILE:HG23	1:D:151:PRO:CD	2.41	0.46
1:D:268:VAL:HG22	1:D:269:PRO:CD	2.45	0.46
1:E:494:ARG:HB2	1:E:503:PHE:CD1	2.47	0.46
1:E:555:MSE:HE3	1:E:555:MSE:HB2	1.75	0.46
1:E:720:SER:OG	1:E:723:ALA:HB2	2.16	0.46
1:F:513:PRO:HA	1:F:522:ILE:HG12	1.98	0.46
1:A:295:LEU:HG	1:A:330:TRP:CD1	2.51	0.46
1:C:40:ASP:OD1	1:C:41:ASN:N	2.48	0.46
1:C:504:LEU:HD21	1:C:521:VAL:CG2	2.46	0.46
1:F:559:ALA:O	1:F:599:GLY:HA3	2.16	0.46
1:A:654:PRO:HB3	1:A:684:ARG:O	2.16	0.46
1:B:277:ILE:HD12	1:B:286:GLN:NE2	2.31	0.46
1:B:60:SER:HB2	1:B:63:LYS:HB2	1.98	0.46
1:B:720:SER:OG	1:B:723:ALA:HB2	2.16	0.46
1:C:53:TYR:CD2	1:C:58:ALA:O	2.69	0.46
1:E:150:ILE:HG23	1:E:151:PRO:CD	2.40	0.46
1:F:54:ASP:CG	1:F:55:GLN:H	2.19	0.46
1:F:581:LEU:HD22	1:F:581:LEU:H	1.81	0.46
1:A:54:ASP:CG	1:A:55:GLN:H	2.19	0.46
1:C:400:PRO:HA	1:C:487:ALA:CB	2.46	0.46
1:C:494:ARG:HB2	1:C:503:PHE:CD1	2.45	0.46
1:D:295:LEU:HG	1:D:330:TRP:CD1	2.51	0.46
1:E:54:ASP:CG	1:E:55:GLN:H	2.19	0.46
1:E:97:LYS:HB3	1:E:100:PHE:HB2	1.98	0.46
1:F:494:ARG:HB2	1:F:503:PHE:CD1	2.47	0.46
1:A:146:HIS:H	1:A:146:HIS:CD2	2.34	0.45
1:A:37:GLU:OE1	1:A:473:ASP:OD2	2.33	0.45
1:C:63:LYS:HD3	1:C:79:THR:HA	1.98	0.45
1:E:262:ILE:HD12	1:E:263:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:HIS:NE2	1:E:365:THR:HG23	2.32	0.45
1:E:655:LEU:N	1:E:683:ASP:HB2	2.27	0.45
1:F:413:THR:HG21	1:F:595:GLN:NE2	2.31	0.45
1:A:138:GLU:OE2	1:A:271:ALA:N	2.48	0.45
1:A:650:THR:CG2	1:A:650:THR:O	2.64	0.45
1:A:92:ARG:HA	1:A:93:ARG:HH12	1.79	0.45
1:B:262:ILE:HD12	1:B:263:PRO:HD2	1.97	0.45
1:B:268:VAL:HG22	1:B:269:PRO:CD	2.46	0.45
1:C:10:SER:HA	1:C:50:GLN:NE2	2.32	0.45
3:R:1:NAG:H61	3:R:2:NAG:N2	2.30	0.45
1:A:40:ASP:OD1	1:A:41:ASN:N	2.50	0.45
1:A:508:VAL:O	1:A:508:VAL:HG12	2.15	0.45
1:B:63:LYS:HD3	1:B:79:THR:HA	1.98	0.45
1:C:446:PRO:O	1:C:447:PHE:O	2.34	0.45
1:C:45:ILE:HD12	1:C:85:ILE:HD13	1.99	0.45
1:C:497:TYR:CD1	1:C:642:ILE:HG23	2.51	0.45
1:C:60:SER:HB2	1:C:63:LYS:HB2	1.99	0.45
1:E:106:PRO:CB	1:E:107:PRO:HD3	2.41	0.45
1:A:110:SER:HB2	1:A:126:LEU:O	2.16	0.45
1:A:581:LEU:H	1:A:581:LEU:HD22	1.81	0.45
1:C:399:LEU:N	1:C:399:LEU:HD12	2.32	0.45
1:C:413:THR:HG21	1:C:595:GLN:NE2	2.32	0.45
1:C:97:LYS:HB3	1:C:100:PHE:HB2	1.98	0.45
1:D:363:HIS:NE2	1:D:365:THR:HG23	2.31	0.45
1:D:45:ILE:HD12	1:D:85:ILE:HD13	1.99	0.45
1:D:581:LEU:HD22	1:D:581:LEU:H	1.80	0.45
1:E:268:VAL:HG22	1:E:269:PRO:CD	2.46	0.45
1:E:508:VAL:HG12	1:E:508:VAL:O	2.15	0.45
1:E:581:LEU:HD22	1:E:581:LEU:N	2.31	0.45
1:E:604:LYS:C	1:E:606:ASN:H	2.20	0.45
1:F:537:VAL:HG22	1:F:546:ASN:ND2	2.29	0.45
1:F:621:ILE:N	1:F:621:ILE:HD12	2.31	0.45
1:F:653:ALA:N	1:F:654:PRO:CD	2.79	0.45
1:A:497:TYR:CD1	1:A:642:ILE:HG23	2.51	0.45
1:C:504:LEU:O	1:C:504:LEU:HD12	2.17	0.45
1:D:136:GLY:CA	1:D:268:VAL:HG21	2.33	0.45
1:D:399:LEU:C	1:D:487:ALA:HB1	2.37	0.45
1:E:277:ILE:HD12	1:E:286:GLN:NE2	2.31	0.45
1:E:274:PRO:HD3	1:E:330:TRP:CZ3	2.52	0.45
1:F:40:ASP:OD1	1:F:41:ASN:N	2.50	0.45
1:B:497:TYR:CD1	1:B:642:ILE:HG23	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:LYS:C	1:B:606:ASN:H	2.19	0.45
1:C:137:ARG:H	1:C:332:ASN:HD22	1.64	0.45
1:D:110:SER:HB2	1:D:126:LEU:O	2.17	0.45
1:D:321:VAL:HG12	1:D:321:VAL:O	2.16	0.45
1:D:413:THR:HG21	1:D:595:GLN:NE2	2.31	0.45
1:F:97:LYS:HB3	1:F:100:PHE:HB2	1.99	0.45
1:F:400:PRO:HA	1:F:487:ALA:HB2	1.99	0.45
1:A:625:PRO:HD2	1:A:627:ARG:HH12	1.81	0.45
1:A:720:SER:OG	1:A:723:ALA:HB2	2.16	0.45
1:B:110:SER:HB2	1:B:126:LEU:O	2.17	0.45
1:B:272:HIS:O	1:B:273:ALA:C	2.55	0.45
1:B:45:ILE:HD12	1:B:85:ILE:HD13	1.98	0.45
1:B:581:LEU:HD22	1:B:581:LEU:N	2.32	0.45
1:C:321:VAL:HG12	1:C:321:VAL:O	2.16	0.45
1:C:363:HIS:NE2	1:C:365:THR:HG23	2.32	0.45
1:C:513:PRO:HA	1:C:522:ILE:HG12	1.99	0.45
1:C:591:VAL:HA	1:C:592:PRO:HD3	1.79	0.45
1:D:148:LYS:O	1:D:267:MSE:HA	2.16	0.45
1:D:274:PRO:HD3	1:D:330:TRP:CZ3	2.51	0.45
1:D:292:LEU:HD23	1:D:312:VAL:HG22	1.99	0.45
1:D:486:THR:HG22	1:D:487:ALA:H	1.81	0.45
1:F:107:PRO:CG	1:F:108:GLY:H	2.23	0.45
1:F:305:GLU:N	1:F:306:PRO:HD3	2.32	0.45
1:F:363:HIS:NE2	1:F:365:THR:HG23	2.32	0.45
1:B:295:LEU:HG	1:B:330:TRP:CD1	2.52	0.45
1:B:321:VAL:O	1:B:321:VAL:HG12	2.16	0.45
1:B:407:ILE:HG21	1:B:568:LEU:HD13	1.97	0.45
1:B:642:ILE:HB	1:B:647:PHE:HZ	1.82	0.45
1:C:604:LYS:C	1:C:606:ASN:H	2.20	0.45
1:C:655:LEU:N	1:C:683:ASP:HB2	2.25	0.45
1:D:138:GLU:OE2	1:D:271:ALA:N	2.50	0.45
1:D:294:LEU:HG	1:D:310:TRP:NE1	2.32	0.45
1:E:321:VAL:HG12	1:E:321:VAL:O	2.17	0.45
1:E:661:CYS:HA	1:E:678:LEU:HD23	1.97	0.45
1:F:321:VAL:HG12	1:F:321:VAL:O	2.17	0.45
1:F:497:TYR:CD1	1:F:642:ILE:HG23	2.52	0.45
1:A:445:TYR:CB	1:A:451:GLY:HA3	2.47	0.45
1:A:53:TYR:CD2	1:A:58:ALA:O	2.70	0.45
1:A:602:MSE:HE3	1:A:602:MSE:HB3	1.58	0.45
1:C:268:VAL:HG22	1:C:269:PRO:CD	2.47	0.45
1:C:568:LEU:C	1:C:570:SER:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:ILE:N	1:C:621:ILE:HD12	2.32	0.45
1:D:420:ILE:HD12	1:D:420:ILE:O	2.16	0.45
1:D:497:TYR:CD1	1:D:642:ILE:HG23	2.51	0.45
1:E:486:THR:HG22	1:E:487:ALA:H	1.82	0.45
1:E:53:TYR:CD2	1:E:58:ALA:O	2.69	0.45
1:E:63:LYS:HD3	1:E:79:THR:HA	1.98	0.45
1:A:150:ILE:HG23	1:A:151:PRO:CD	2.45	0.45
1:A:45:ILE:HD12	1:A:85:ILE:HD13	1.99	0.45
1:A:87:THR:OG1	1:A:106:PRO:HD2	2.17	0.45
1:B:642:ILE:HB	1:B:647:PHE:CZ	2.52	0.45
1:D:272:HIS:O	1:D:273:ALA:C	2.56	0.45
1:E:400:PRO:HA	1:E:487:ALA:HB2	1.99	0.45
1:E:45:ILE:HD12	1:E:85:ILE:HD13	1.98	0.45
1:E:504:LEU:HD21	1:E:521:VAL:CG2	2.47	0.45
1:A:284:SER:HB3	2:G:1:NAG:O5	2.17	0.44
1:A:63:LYS:HD3	1:A:79:THR:HA	1.99	0.44
1:B:559:ALA:O	1:B:599:GLY:HA3	2.17	0.44
1:B:621:ILE:H	1:B:621:ILE:CD1	2.30	0.44
1:B:580:ARG:NH2	1:C:275:ASN:HB2	2.32	0.44
1:C:399:LEU:C	1:C:487:ALA:HB1	2.37	0.44
1:C:54:ASP:CG	1:C:55:GLN:H	2.19	0.44
1:C:581:LEU:HD22	1:C:581:LEU:H	1.81	0.44
1:D:305:GLU:N	1:D:306:PRO:HD3	2.33	0.44
1:D:489:MSE:HG3	1:D:508:VAL:HB	1.99	0.44
1:D:494:ARG:HB2	1:D:503:PHE:CD1	2.47	0.44
1:D:63:LYS:HD3	1:D:79:THR:HA	1.99	0.44
1:E:497:TYR:CD1	1:E:642:ILE:HG23	2.52	0.44
1:F:110:SER:HB2	1:F:126:LEU:O	2.18	0.44
1:F:298:ARG:HH12	1:F:615:ALA:HB3	1.81	0.44
1:F:568:LEU:C	1:F:570:SER:H	2.20	0.44
1:A:321:VAL:O	1:A:321:VAL:HG12	2.16	0.44
1:A:486:THR:HG22	1:A:487:ALA:H	1.82	0.44
1:B:287:LEU:CD2	1:B:330:TRP:NE1	2.80	0.44
1:B:649:ARG:HG3	1:B:649:ARG:H	1.51	0.44
1:C:446:PRO:HG2	1:C:450:GLY:O	2.16	0.44
1:F:10:SER:HA	1:F:50:GLN:NE2	2.32	0.44
1:F:300:LEU:HD11	1:F:337:ARG:HD3	1.98	0.44
1:F:399:LEU:C	1:F:487:ALA:HB1	2.38	0.44
1:F:486:THR:HG22	1:F:487:ALA:H	1.82	0.44
1:F:53:TYR:CD2	1:F:58:ALA:O	2.70	0.44
1:A:642:ILE:HB	1:A:647:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:OE2	1:C:271:ALA:N	2.50	0.44
1:C:486:THR:HG22	1:C:487:ALA:H	1.81	0.44
1:C:93:ARG:H	1:C:93:ARG:NH1	1.93	0.44
1:E:407:ILE:HG22	1:E:408:THR:N	2.32	0.44
1:F:399:LEU:HD12	1:F:399:LEU:N	2.32	0.44
1:A:106:PRO:CB	1:A:107:PRO:CD	2.92	0.44
1:B:454:CYS:SG	1:B:460:ASN:OD1	2.76	0.44
1:B:504:LEU:HD21	1:B:521:VAL:CG2	2.46	0.44
1:C:276:VAL:HG12	1:C:277:ILE:N	2.33	0.44
1:D:40:ASP:OD1	1:D:41:ASN:N	2.49	0.44
1:D:642:ILE:HB	1:D:647:PHE:HZ	1.83	0.44
1:D:699:LEU:HD23	1:D:716:PHE:HB3	2.00	0.44
1:E:271:ALA:CB	1:E:330:TRP:CZ3	3.00	0.44
1:F:21:HIS:O	1:F:23:VAL:N	2.51	0.44
1:F:45:ILE:HD12	1:F:85:ILE:HD13	1.99	0.44
1:B:108:GLY:CA	1:B:130:ILE:HB	2.47	0.44
1:E:21:HIS:O	1:E:23:VAL:N	2.51	0.44
1:F:268:VAL:HG22	1:F:269:PRO:CD	2.47	0.44
1:F:295:LEU:HG	1:F:330:TRP:CD1	2.51	0.44
1:A:394:MSE:HE2	1:A:394:MSE:HB3	1.92	0.44
1:A:621:ILE:N	1:A:621:ILE:HD12	2.33	0.44
1:A:642:ILE:HB	1:A:647:PHE:CZ	2.52	0.44
1:B:54:ASP:CG	1:B:55:GLN:H	2.21	0.44
1:D:112:THR:HG23	1:D:125:THR:HG22	1.99	0.44
1:D:394:MSE:HB3	1:D:394:MSE:HE2	1.91	0.44
1:D:60:SER:HB2	1:D:63:LYS:HB2	2.00	0.44
1:D:642:ILE:HB	1:D:647:PHE:CZ	2.52	0.44
1:E:146:HIS:CD2	1:E:146:HIS:H	2.34	0.44
1:E:287:LEU:CD2	1:E:330:TRP:NE1	2.77	0.44
1:E:399:LEU:C	1:E:487:ALA:HB1	2.37	0.44
1:E:407:ILE:HG21	1:E:568:LEU:HD13	1.99	0.44
1:E:568:LEU:C	1:E:570:SER:H	2.21	0.44
1:E:642:ILE:HB	1:E:647:PHE:CZ	2.52	0.44
1:F:604:LYS:C	1:F:606:ASN:H	2.21	0.44
1:B:40:ASP:OD1	1:B:41:ASN:N	2.50	0.44
1:B:568:LEU:C	1:B:570:SER:H	2.21	0.44
1:E:270:VAL:HG22	1:E:333:HIS:HE1	1.80	0.44
1:E:40:ASP:OD1	1:E:41:ASN:N	2.49	0.44
1:F:385:ALA:HA	1:F:386:PRO:HD2	1.79	0.44
1:A:102:LEU:HD11	1:A:155:TYR:CB	2.48	0.44
1:A:112:THR:HG23	1:A:125:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ARG:HB2	1:A:503:PHE:CD1	2.47	0.44
1:B:363:HIS:NE2	1:B:365:THR:HG23	2.32	0.44
1:C:21:HIS:O	1:C:23:VAL:N	2.50	0.44
1:D:146:HIS:H	1:D:146:HIS:CD2	2.35	0.44
1:E:137:ARG:HH21	1:E:331:GLY:H	1.66	0.44
1:E:621:ILE:N	1:E:621:ILE:HD12	2.33	0.44
1:A:108:GLY:CA	1:A:130:ILE:HB	2.47	0.44
1:A:513:PRO:HA	1:A:522:ILE:HG12	2.00	0.44
1:A:72:ASP:O	1:A:73:HIS:HB2	2.17	0.44
1:B:513:PRO:HA	1:B:522:ILE:HG12	1.99	0.44
1:D:10:SER:HA	1:D:50:GLN:NE2	2.32	0.44
1:D:604:LYS:C	1:D:606:ASN:H	2.22	0.44
1:E:295:LEU:HG	1:E:330:TRP:CD1	2.51	0.44
1:E:559:ALA:O	1:E:599:GLY:HA3	2.18	0.44
1:F:131:LYS:NZ	3:R:1:NAG:H81	2.33	0.44
1:F:512:THR:HA	1:F:513:PRO:HD3	1.75	0.44
1:F:72:ASP:O	1:F:73:HIS:HB2	2.18	0.44
1:A:102:LEU:HD11	1:A:155:TYR:HB3	2.00	0.43
1:A:504:LEU:HD12	1:A:504:LEU:O	2.17	0.43
1:B:399:LEU:C	1:B:487:ALA:HB1	2.38	0.43
1:E:385:ALA:HA	1:E:386:PRO:HD2	1.78	0.43
1:E:407:ILE:CG2	1:E:408:THR:N	2.81	0.43
1:E:653:ALA:N	1:E:654:PRO:CD	2.79	0.43
1:E:386:PRO:HG3	1:E:730:CYS:O	2.18	0.43
1:F:63:LYS:HD3	1:F:79:THR:HA	1.99	0.43
1:F:87:THR:OG1	1:F:106:PRO:HD2	2.18	0.43
2:J:3:BMA:O2	2:J:4:MAN:O5	2.32	0.43
1:A:559:ALA:O	1:A:599:GLY:HA3	2.18	0.43
1:A:699:LEU:HD23	1:A:716:PHE:HB3	2.00	0.43
1:B:112:THR:HG23	1:B:125:THR:HG22	2.00	0.43
1:C:559:ALA:O	1:C:599:GLY:HA3	2.18	0.43
1:E:489:MSE:HG3	1:E:508:VAL:HB	2.00	0.43
1:F:112:THR:HG23	1:F:125:THR:HG22	2.01	0.43
1:F:60:SER:HB2	1:F:63:LYS:HB2	1.99	0.43
1:F:642:ILE:HB	1:F:647:PHE:CZ	2.53	0.43
1:F:649:ARG:O	1:F:650:THR:C	2.56	0.43
1:A:21:HIS:O	1:A:23:VAL:N	2.51	0.43
1:A:287:LEU:CD2	1:A:330:TRP:NE1	2.80	0.43
1:A:653:ALA:O	1:A:654:PRO:C	2.56	0.43
1:B:493:LEU:HD23	1:B:493:LEU:HA	1.60	0.43
1:B:530:PHE:CE2	1:B:617:PHE:HD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:LEU:O	1:D:504:LEU:HD12	2.17	0.43
1:E:625:PRO:HD2	1:E:627:ARG:HH12	1.82	0.43
1:E:642:ILE:HB	1:E:647:PHE:HZ	1.83	0.43
1:A:271:ALA:CB	1:A:330:TRP:CZ3	3.02	0.43
1:B:107:PRO:CG	1:B:108:GLY:H	2.23	0.43
1:B:400:PRO:HA	1:B:487:ALA:HB2	1.99	0.43
1:B:494:ARG:HB2	1:B:503:PHE:CD1	2.47	0.43
1:B:621:ILE:N	1:B:621:ILE:HD12	2.33	0.43
1:C:445:TYR:O	1:C:460:ASN:ND2	2.51	0.43
1:D:69:LEU:HA	1:D:69:LEU:HD22	1.84	0.43
1:D:87:THR:OG1	1:D:106:PRO:HD2	2.18	0.43
1:E:272:HIS:O	1:E:273:ALA:C	2.57	0.43
1:E:621:ILE:CD1	1:E:621:ILE:H	2.31	0.43
1:F:321:VAL:CG1	1:F:340:ALA:HB2	2.48	0.43
1:A:445:TYR:CD1	1:A:451:GLY:HA3	2.53	0.43
1:B:10:SER:HA	1:B:50:GLN:NE2	2.33	0.43
1:B:53:TYR:CD2	1:B:58:ALA:O	2.70	0.43
1:C:447:PHE:CD1	1:C:455:PHE:HA	2.53	0.43
1:C:664:SER:OG	1:C:675:MSE:HB3	2.19	0.43
1:E:19:CYS:C	1:E:21:HIS:N	2.72	0.43
1:E:292:LEU:HD23	1:E:312:VAL:HG22	2.00	0.43
1:E:6:PHE:HA	1:E:57:GLY:O	2.18	0.43
1:E:602:MSE:HB3	1:E:602:MSE:HE3	1.68	0.43
1:E:612:GLN:H	1:E:612:GLN:HG2	1.53	0.43
1:F:146:HIS:CD2	1:F:146:HIS:H	2.35	0.43
1:F:555:MSE:HB2	1:F:555:MSE:HE3	1.69	0.43
1:F:398:VAL:HB	1:F:628:ALA:HB3	1.99	0.43
1:A:447:PHE:CG	1:A:448:MSE:N	2.86	0.43
1:C:146:HIS:CD2	1:C:146:HIS:H	2.36	0.43
1:C:642:ILE:HB	1:C:647:PHE:CZ	2.53	0.43
1:D:102:LEU:HD11	1:D:155:TYR:HB3	2.01	0.43
1:D:21:HIS:O	1:D:23:VAL:N	2.52	0.43
1:D:568:LEU:C	1:D:570:SER:H	2.21	0.43
1:D:72:ASP:O	1:D:73:HIS:HB2	2.19	0.43
1:E:102:LEU:HD11	1:E:155:TYR:CB	2.49	0.43
1:E:615:ALA:HA	1:E:616:PRO:HD3	1.57	0.43
1:A:271:ALA:HB3	1:A:330:TRP:CZ3	2.54	0.43
1:A:449:TRP:HA	1:A:449:TRP:CE3	2.52	0.43
1:B:21:HIS:O	1:B:23:VAL:N	2.52	0.43
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.77	0.43
1:B:413:THR:HG21	1:B:595:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLY:N	1:B:63:LYS:O	2.51	0.43
1:C:102:LEU:HD11	1:C:155:TYR:CB	2.49	0.43
1:C:295:LEU:HG	1:C:330:TRP:CD1	2.53	0.43
1:C:298:ARG:HH12	1:C:615:ALA:HB3	1.83	0.43
1:C:394:MSE:HB3	1:C:394:MSE:HE2	1.90	0.43
1:D:513:PRO:HA	1:D:522:ILE:HG12	2.00	0.43
1:E:112:THR:HG23	1:E:125:THR:HG22	2.01	0.43
1:E:664:SER:OG	1:E:675:MSE:HB3	2.19	0.43
1:F:287:LEU:HD13	1:F:311:ILE:CD1	2.49	0.43
1:A:655:LEU:N	1:A:683:ASP:HB2	2.28	0.43
1:B:137:ARG:HH21	1:B:331:GLY:H	1.65	0.43
1:B:271:ALA:CB	1:B:330:TRP:CZ3	3.02	0.43
1:B:699:LEU:HD23	1:B:716:PHE:HB3	2.01	0.43
1:C:489:MSE:HB2	1:C:489:MSE:HE3	1.90	0.43
1:C:398:VAL:HB	1:C:628:ALA:HB3	2.00	0.43
1:E:17:SER:HB3	1:F:145:VAL:CG2	2.33	0.43
1:E:503:PHE:C	1:E:503:PHE:CD2	2.92	0.43
1:E:512:THR:HA	1:E:513:PRO:HD3	1.74	0.43
1:F:111:VAL:O	1:F:125:THR:HA	2.19	0.43
1:F:136:GLY:CA	1:F:268:VAL:HG21	2.31	0.43
1:F:690:VAL:HG22	1:F:729:LEU:HD23	2.01	0.43
1:A:104:LYS:HD2	1:C:22:THR:CG2	2.34	0.43
1:A:10:SER:HA	1:A:50:GLN:NE2	2.33	0.43
1:A:69:LEU:HA	1:A:69:LEU:HD22	1.84	0.43
1:B:340:ALA:C	1:B:341:GLN:HG2	2.39	0.43
1:B:547:TYR:OH	1:B:560:PHE:HB3	2.19	0.43
1:D:621:ILE:CD1	1:D:621:ILE:H	2.31	0.43
1:D:621:ILE:N	1:D:621:ILE:HD12	2.33	0.43
1:D:690:VAL:HG22	1:D:729:LEU:HD23	2.01	0.43
1:E:110:SER:HB2	1:E:126:LEU:O	2.18	0.43
1:E:657:SER:HA	1:E:732:LYS:HE3	2.01	0.43
1:F:699:LEU:HD23	1:F:716:PHE:HB3	2.00	0.43
1:A:136:GLY:CA	1:A:268:VAL:HG21	2.33	0.43
1:A:493:LEU:HA	1:A:493:LEU:HD23	1.60	0.43
1:A:568:LEU:C	1:A:570:SER:H	2.22	0.43
1:A:690:VAL:HG22	1:A:729:LEU:HD23	2.01	0.43
1:B:292:LEU:HD23	1:B:312:VAL:HG22	2.00	0.43
1:B:413:THR:HG23	1:B:468:VAL:HG12	2.01	0.43
1:C:102:LEU:HD11	1:C:155:TYR:HB3	2.01	0.43
1:C:112:THR:HG23	1:C:125:THR:HG22	2.00	0.43
1:C:699:LEU:HD23	1:C:716:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:ALA:O	1:D:599:GLY:HA3	2.18	0.43
1:D:664:SER:OG	1:D:675:MSE:HB3	2.19	0.43
1:E:699:LEU:HD23	1:E:716:PHE:HB3	2.01	0.43
1:F:664:SER:OG	1:F:675:MSE:HB3	2.19	0.43
1:B:102:LEU:HD11	1:B:155:TYR:CB	2.48	0.42
1:B:137:ARG:H	1:B:332:ASN:HD22	1.67	0.42
1:B:287:LEU:HD22	1:B:330:TRP:CE2	2.54	0.42
1:B:328:TYR:O	1:B:328:TYR:CD1	2.72	0.42
1:B:491:VAL:O	1:B:505:ASP:HA	2.19	0.42
1:C:110:SER:HB2	1:C:126:LEU:O	2.19	0.42
1:C:400:PRO:HA	1:C:487:ALA:HB2	2.01	0.42
1:C:642:ILE:HB	1:C:647:PHE:HZ	1.83	0.42
1:E:328:TYR:O	1:E:328:TYR:CD1	2.71	0.42
1:E:422:CYS:O	1:E:423:CYS:HB2	2.19	0.42
1:E:445:TYR:CG	1:E:451:GLY:HA3	2.53	0.42
1:F:445:TYR:O	1:F:460:ASN:ND2	2.52	0.42
1:B:471:SER:C	1:B:473:ASP:N	2.72	0.42
1:B:6:PHE:HA	1:B:57:GLY:O	2.19	0.42
1:C:108:GLY:CA	1:C:130:ILE:HB	2.47	0.42
1:D:303:ASN:HA	1:D:304:PRO:HD3	1.83	0.42
1:D:137:ARG:H	1:D:332:ASN:HD22	1.66	0.42
1:D:512:THR:HA	1:D:513:PRO:HD3	1.75	0.42
1:E:87:THR:OG1	1:E:106:PRO:HD2	2.19	0.42
1:E:10:SER:HA	1:E:50:GLN:NE2	2.33	0.42
1:F:292:LEU:HD23	1:F:312:VAL:HG22	2.01	0.42
1:F:503:PHE:CD2	1:F:503:PHE:C	2.91	0.42
1:F:642:ILE:HB	1:F:647:PHE:HZ	1.84	0.42
1:A:531:THR:HA	1:A:532:PRO:HD3	1.89	0.42
1:B:102:LEU:HD11	1:B:155:TYR:HB3	2.00	0.42
1:B:95:SER:OG	1:B:259:PHE:CZ	2.67	0.42
1:B:271:ALA:HB3	1:B:330:TRP:CZ3	2.55	0.42
1:B:404:GLN:HA	1:B:482:ILE:HG12	2.00	0.42
1:B:655:LEU:N	1:B:683:ASP:HB2	2.27	0.42
1:D:300:LEU:CD1	1:D:337:ARG:HD3	2.49	0.42
1:D:531:THR:HA	1:D:532:PRO:HD3	1.89	0.42
1:E:489:MSE:HE3	1:E:489:MSE:HB2	1.92	0.42
1:E:72:ASP:O	1:E:73:HIS:HB2	2.19	0.42
1:F:398:VAL:O	1:F:400:PRO:HD3	2.19	0.42
1:A:413:THR:HG21	1:A:595:GLN:NE2	2.34	0.42
1:B:385:ALA:HA	1:B:386:PRO:HD2	1.78	0.42
1:B:407:ILE:HG22	1:B:408:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:CYS:O	1:B:423:CYS:HB2	2.19	0.42
1:B:447:PHE:HA	1:B:454:CYS:O	2.20	0.42
1:C:407:ILE:HG22	1:C:408:THR:N	2.34	0.42
1:E:102:LEU:HD11	1:E:155:TYR:HB3	2.00	0.42
1:F:102:LEU:HD11	1:F:155:TYR:CB	2.49	0.42
1:A:19:CYS:C	1:A:21:HIS:N	2.72	0.42
1:A:664:SER:OG	1:A:675:MSE:HB3	2.19	0.42
1:C:385:ALA:HA	1:C:386:PRO:HD2	1.79	0.42
1:C:422:CYS:O	1:C:423:CYS:HB2	2.20	0.42
1:C:452:ALA:O	1:C:453:GLN:C	2.58	0.42
1:D:145:VAL:HG22	1:F:17:SER:CB	2.31	0.42
1:E:547:TYR:OH	1:E:560:PHE:HB3	2.20	0.42
1:E:649:ARG:H	1:E:649:ARG:HG3	1.52	0.42
1:F:389:LEU:HD12	1:F:389:LEU:HA	1.86	0.42
2:G:3:BMA:O3	2:G:4:MAN:C4	2.63	0.42
1:B:287:LEU:HD13	1:B:311:ILE:CD1	2.49	0.42
1:D:407:ILE:HG22	1:D:408:THR:N	2.34	0.42
1:F:471:SER:C	1:F:473:ASP:N	2.72	0.42
1:F:649:ARG:O	1:F:651:SER:HB2	2.20	0.42
3:H:3:BMA:H61	3:H:5:MAN:H2	1.32	0.42
1:B:555:MSE:HB2	1:B:555:MSE:HE3	1.65	0.42
1:B:625:PRO:HD2	1:B:627:ARG:HH12	1.84	0.42
1:B:72:ASP:O	1:B:73:HIS:HB2	2.19	0.42
1:C:111:VAL:O	1:C:125:THR:HA	2.20	0.42
1:C:287:LEU:HD13	1:C:311:ILE:CD1	2.50	0.42
1:C:404:GLN:HA	1:C:482:ILE:HG12	2.02	0.42
1:C:489:MSE:HG3	1:C:508:VAL:HB	2.00	0.42
1:C:690:VAL:HG22	1:C:729:LEU:HD23	2.01	0.42
1:C:72:ASP:O	1:C:73:HIS:HB2	2.18	0.42
1:D:591:VAL:HA	1:D:592:PRO:HD3	1.79	0.42
1:F:19:CYS:C	1:F:21:HIS:N	2.73	0.42
1:F:271:ALA:HB3	1:F:330:TRP:CZ3	2.54	0.42
1:F:657:SER:HA	1:F:732:LYS:HE3	2.01	0.42
1:A:413:THR:HG23	1:A:468:VAL:HG12	2.01	0.42
1:A:604:LYS:C	1:A:606:ASN:H	2.22	0.42
1:B:87:THR:OG1	1:B:106:PRO:HD2	2.20	0.42
1:B:471:SER:C	1:B:473:ASP:H	2.23	0.42
1:B:378:LEU:HG	1:B:691:HIS:CB	2.50	0.42
1:C:87:THR:OG1	1:C:106:PRO:HD2	2.19	0.42
1:C:413:THR:HG23	1:C:468:VAL:HG12	2.02	0.42
1:D:37:GLU:OE1	1:D:473:ASP:OD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:688:CYS:HA	1:D:689:PRO:HD3	1.93	0.42
1:E:271:ALA:HB3	1:E:330:TRP:CZ3	2.54	0.42
1:E:378:LEU:HD23	1:E:378:LEU:HA	1.77	0.42
1:E:413:THR:HG21	1:E:595:GLN:NE2	2.35	0.42
1:F:102:LEU:HD11	1:F:155:TYR:HB3	2.01	0.42
1:A:471:SER:C	1:A:473:ASP:N	2.72	0.42
1:A:503:PHE:CD2	1:A:503:PHE:C	2.93	0.42
1:B:436:TYR:O	1:B:437:THR:HG23	2.20	0.42
1:D:329:ILE:HG12	1:D:329:ILE:H	1.53	0.42
1:D:422:CYS:O	1:D:423:CYS:HB2	2.20	0.42
1:D:471:SER:C	1:D:473:ASP:H	2.23	0.42
1:E:287:LEU:HD22	1:E:311:ILE:HD11	2.01	0.42
1:F:287:LEU:HD22	1:F:311:ILE:HD11	2.02	0.42
1:F:271:ALA:CB	1:F:330:TRP:CZ3	3.03	0.42
1:F:471:SER:C	1:F:473:ASP:H	2.23	0.42
2:M:2:NAG:H83	2:M:2:NAG:O3	2.20	0.42
1:A:398:VAL:O	1:A:400:PRO:HD3	2.20	0.42
1:A:60:SER:CB	1:A:63:LYS:HB2	2.50	0.42
1:B:503:PHE:C	1:B:503:PHE:CD2	2.92	0.42
1:B:664:SER:OG	1:B:675:MSE:HB3	2.19	0.42
1:B:386:PRO:HG3	1:B:730:CYS:O	2.20	0.42
1:C:471:SER:C	1:C:473:ASP:N	2.73	0.42
1:C:512:THR:HA	1:C:513:PRO:HD3	1.76	0.42
1:D:271:ALA:CB	1:D:330:TRP:CZ3	3.03	0.42
1:D:398:VAL:O	1:D:400:PRO:HD3	2.20	0.42
1:D:413:THR:HG23	1:D:468:VAL:HG12	2.02	0.42
1:D:503:PHE:CD2	1:D:503:PHE:C	2.94	0.42
1:E:33:GLN:O	1:E:34:VAL:HG23	2.19	0.42
1:F:491:VAL:O	1:F:505:ASP:HA	2.20	0.42
1:F:69:LEU:HA	1:F:69:LEU:HD22	1.84	0.42
1:A:52:GLY:N	1:A:63:LYS:O	2.51	0.41
1:B:591:VAL:HA	1:B:592:PRO:HD3	1.80	0.41
1:C:445:TYR:CB	1:C:452:ALA:H	2.32	0.41
1:C:625:PRO:HD2	1:C:627:ARG:HH12	1.84	0.41
1:D:436:TYR:O	1:D:437:THR:HG23	2.20	0.41
1:E:513:PRO:HA	1:E:522:ILE:HG12	2.01	0.41
1:A:376:LYS:O	1:A:691:HIS:HE1	2.03	0.41
1:A:407:ILE:HG22	1:A:408:THR:N	2.34	0.41
1:B:489:MSE:HG3	1:B:508:VAL:HB	2.02	0.41
1:B:615:ALA:HA	1:B:616:PRO:HD3	1.56	0.41
1:B:657:SER:HA	1:B:732:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:LEU:HA	1:C:426:LEU:HD23	1.87	0.41
1:C:503:PHE:C	1:C:503:PHE:CD2	2.94	0.41
1:C:555:MSE:H	1:C:555:MSE:HE2	1.84	0.41
1:D:287:LEU:HD13	1:D:311:ILE:CD1	2.50	0.41
1:D:491:VAL:O	1:D:505:ASP:HA	2.20	0.41
1:F:413:THR:HG23	1:F:468:VAL:HG12	2.02	0.41
1:A:271:ALA:O	1:A:333:HIS:HE1	2.03	0.41
1:A:373:ILE:HA	1:A:374:PRO:HD2	1.91	0.41
1:A:657:SER:HA	1:A:732:LYS:HE3	2.01	0.41
1:A:6:PHE:HA	1:A:57:GLY:O	2.19	0.41
1:C:271:ALA:O	1:C:333:HIS:HE1	2.02	0.41
1:D:19:CYS:C	1:D:21:HIS:N	2.72	0.41
1:D:328:TYR:O	1:D:328:TYR:CD1	2.73	0.41
1:E:111:VAL:O	1:E:125:THR:HA	2.20	0.41
1:E:426:LEU:HD23	1:E:426:LEU:HA	1.88	0.41
1:E:453:GLN:CD	1:E:453:GLN:H	2.23	0.41
1:F:547:TYR:OH	1:F:560:PHE:HB3	2.19	0.41
1:A:287:LEU:HD13	1:A:311:ILE:CD1	2.49	0.41
1:A:300:LEU:CD1	1:A:337:ARG:HD3	2.50	0.41
1:B:19:CYS:C	1:B:21:HIS:N	2.72	0.41
1:C:51:PHE:CD2	1:C:80:MSE:SE	3.23	0.41
1:C:413:THR:HG21	1:C:595:GLN:HE22	1.83	0.41
1:D:102:LEU:HD11	1:D:155:TYR:CB	2.49	0.41
1:D:150:ILE:HG22	1:D:151:PRO:O	2.20	0.41
1:D:271:ALA:HB3	1:D:330:TRP:CZ3	2.55	0.41
1:D:334:GLU:HA	1:D:335:PRO:HD3	1.85	0.41
1:D:321:VAL:CG1	1:D:340:ALA:HB2	2.50	0.41
1:D:504:LEU:HB3	1:D:516:SER:HB2	2.03	0.41
1:D:691:HIS:HA	1:D:699:LEU:HD12	2.02	0.41
1:E:691:HIS:HA	1:E:699:LEU:HD12	2.02	0.41
1:A:552:TYR:HA	1:A:564:GLN:OE1	2.21	0.41
1:B:329:ILE:H	1:B:329:ILE:HG12	1.50	0.41
1:B:407:ILE:CG2	1:B:408:THR:N	2.84	0.41
1:C:493:LEU:HD23	1:C:493:LEU:HA	1.61	0.41
1:C:649:ARG:HG3	1:C:649:ARG:H	1.52	0.41
1:D:653:ALA:HB1	1:D:684:ARG:HD2	2.02	0.41
1:D:386:PRO:HG3	1:D:730:CYS:O	2.21	0.41
1:E:690:VAL:HG22	1:E:729:LEU:HD23	2.01	0.41
3:H:2:NAG:O3	3:H:3:BMA:H5	2.20	0.41
1:A:287:LEU:HD22	1:A:330:TRP:CE2	2.55	0.41
1:B:111:VAL:O	1:B:125:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:VAL:HG22	1:B:729:LEU:HD23	2.01	0.41
1:C:386:PRO:HB2	1:C:689:PRO:CG	2.50	0.41
1:C:407:ILE:CG2	1:C:408:THR:N	2.84	0.41
1:D:271:ALA:O	1:D:333:HIS:HE1	2.02	0.41
1:D:292:LEU:CD2	1:D:312:VAL:HG22	2.51	0.41
1:D:489:MSE:HE3	1:D:489:MSE:HB2	1.89	0.41
1:E:287:LEU:HD22	1:E:330:TRP:CE2	2.56	0.41
1:E:491:VAL:O	1:E:505:ASP:HA	2.20	0.41
1:F:652:ASP:C	1:F:654:PRO:HD2	2.40	0.41
1:F:6:PHE:HA	1:F:57:GLY:O	2.21	0.41
1:A:407:ILE:CG2	1:A:408:THR:N	2.84	0.41
1:B:327:GLU:HA	1:B:337:ARG:HB3	2.03	0.41
1:C:398:VAL:O	1:C:400:PRO:HD3	2.20	0.41
1:D:657:SER:HA	1:D:732:LYS:HE3	2.01	0.41
1:F:287:LEU:CD2	1:F:330:TRP:NE1	2.80	0.41
1:F:404:GLN:HA	1:F:482:ILE:HG12	2.02	0.41
1:F:489:MSE:HG3	1:F:508:VAL:HB	2.03	0.41
4:N:1:NAG:O3	4:N:2:NAG:C7	2.69	0.41
1:B:373:ILE:HA	1:B:374:PRO:HD2	1.90	0.41
1:B:413:THR:HG21	1:B:595:GLN:HE22	1.86	0.41
1:B:612:GLN:HG2	1:B:612:GLN:H	1.50	0.41
1:C:42:THR:CG2	1:C:104:LYS:HG3	2.51	0.41
1:C:271:ALA:HB3	1:C:330:TRP:CZ3	2.56	0.41
1:C:602:MSE:HE3	1:C:602:MSE:HB3	1.60	0.41
1:D:426:LEU:HA	1:D:426:LEU:HD23	1.89	0.41
1:E:51:PHE:CD2	1:E:80:MSE:SE	3.23	0.41
1:B:44:ARG:NH1	1:B:258:PRO:HB2	2.36	0.41
1:B:691:HIS:HA	1:B:699:LEU:HD12	2.03	0.41
1:C:35:TRP:HB2	1:C:44:ARG:HB3	2.02	0.41
1:C:6:PHE:CD2	1:C:6:PHE:N	2.88	0.41
1:D:108:GLY:CA	1:D:130:ILE:HB	2.46	0.41
1:D:547:TYR:OH	1:D:560:PHE:HB3	2.21	0.41
1:E:44:ARG:NH1	1:E:258:PRO:HB2	2.35	0.41
1:F:373:ILE:HA	1:F:374:PRO:HD2	1.91	0.41
3:P:2:NAG:H2	3:P:2:NAG:H83	1.94	0.41
1:B:411:PHE:CD1	1:B:411:PHE:C	2.93	0.41
1:B:544:VAL:N	1:B:612:GLN:HE22	2.18	0.41
1:C:19:CYS:C	1:C:21:HIS:N	2.73	0.41
1:C:287:LEU:HD22	1:C:311:ILE:HD11	2.03	0.41
1:D:111:VAL:O	1:D:125:THR:HA	2.21	0.41
1:D:287:LEU:CD2	1:D:330:TRP:NE1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:LYS:HA	1:D:557:PRO:HD3	1.90	0.41
1:D:552:TYR:HA	1:D:564:GLN:OE1	2.21	0.41
1:D:655:LEU:N	1:D:683:ASP:HB2	2.27	0.41
1:E:150:ILE:HG22	1:E:151:PRO:O	2.21	0.41
1:E:568:LEU:HD22	1:E:568:LEU:H	1.85	0.41
1:F:271:ALA:O	1:F:333:HIS:HE1	2.04	0.41
1:A:33:GLN:O	1:A:34:VAL:HG23	2.21	0.41
1:A:471:SER:C	1:A:473:ASP:H	2.24	0.41
1:B:287:LEU:CD2	1:B:330:TRP:CE2	3.04	0.41
1:C:287:LEU:CD2	1:C:330:TRP:NE1	2.82	0.41
1:C:547:TYR:OH	1:C:560:PHE:HB3	2.21	0.41
1:C:615:ALA:HA	1:C:616:PRO:HD3	1.55	0.41
1:C:657:SER:HA	1:C:732:LYS:HE3	2.02	0.41
1:D:148:LYS:HB3	1:D:150:ILE:CD1	2.51	0.41
1:D:44:ARG:NH1	1:D:258:PRO:HB2	2.36	0.41
1:E:287:LEU:HD13	1:E:311:ILE:CD1	2.50	0.41
1:E:287:LEU:CD2	1:E:330:TRP:CE2	3.03	0.41
1:E:471:SER:C	1:E:473:ASP:H	2.24	0.41
1:F:422:CYS:O	1:F:423:CYS:HB2	2.20	0.41
1:F:80:MSE:HE2	1:F:80:MSE:HB3	1.93	0.41
1:A:107:PRO:CG	1:A:108:GLY:N	2.84	0.40
1:A:150:ILE:HG22	1:A:151:PRO:O	2.21	0.40
1:A:422:CYS:O	1:A:423:CYS:HB2	2.20	0.40
1:A:413:THR:HG21	1:A:595:GLN:HE22	1.86	0.40
1:C:481:ALA:HB1	1:C:549:PHE:CE1	2.57	0.40
1:D:407:ILE:CG2	1:D:408:THR:N	2.83	0.40
1:E:69:LEU:HD22	1:E:69:LEU:HA	1.85	0.40
1:F:107:PRO:CG	1:F:108:GLY:N	2.85	0.40
1:F:143:PRO:HA	1:F:144:PRO:HD3	1.96	0.40
1:F:292:LEU:CD2	1:F:312:VAL:HG22	2.52	0.40
1:B:400:PRO:HB2	1:B:484:VAL:HG13	2.03	0.40
1:B:337:ARG:NH2	1:B:620:LYS:HE2	2.36	0.40
1:D:107:PRO:CG	1:D:108:GLY:N	2.84	0.40
1:D:361:TYR:HB2	1:D:381:ARG:HH21	1.86	0.40
1:D:35:TRP:HB2	1:D:44:ARG:HB3	2.02	0.40
1:D:471:SER:C	1:D:473:ASP:N	2.72	0.40
1:E:300:LEU:CD1	1:E:337:ARG:HD3	2.50	0.40
1:F:137:ARG:HH21	1:F:331:GLY:H	1.69	0.40
1:F:287:LEU:HD22	1:F:330:TRP:CE2	2.56	0.40
1:F:591:VAL:HA	1:F:592:PRO:HD3	1.80	0.40
1:A:146:HIS:N	1:A:146:HIS:CD2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:PRO:HA	1:B:144:PRO:HD3	1.95	0.40
1:B:432:ALA:O	1:B:433:HIS:HB3	2.22	0.40
1:B:447:PHE:CE1	1:B:455:PHE:HA	2.54	0.40
1:B:51:PHE:CD2	1:B:80:MSE:SE	3.25	0.40
1:B:552:TYR:HA	1:B:564:GLN:OE1	2.20	0.40
1:B:568:LEU:H	1:B:568:LEU:HD22	1.87	0.40
1:B:60:SER:CB	1:B:63:LYS:HB2	2.51	0.40
1:C:373:ILE:HA	1:C:374:PRO:HD2	1.91	0.40
1:C:654:PRO:HB3	1:C:684:ARG:H	1.87	0.40
1:D:544:VAL:N	1:D:612:GLN:HE22	2.19	0.40
1:F:287:LEU:CD2	1:F:330:TRP:CE2	3.04	0.40
1:F:407:ILE:CG2	1:F:408:THR:N	2.85	0.40
1:A:111:VAL:O	1:A:125:THR:HA	2.20	0.40
1:B:300:LEU:CD1	1:B:337:ARG:HD3	2.52	0.40
1:B:399:LEU:HD12	1:B:399:LEU:H	1.85	0.40
1:C:105:CYS:HA	1:C:106:PRO:HD3	1.89	0.40
1:C:292:LEU:CD2	1:C:312:VAL:HG22	2.51	0.40
1:C:300:LEU:CD1	1:C:337:ARG:HD3	2.51	0.40
1:C:71:GLN:C	1:C:73:HIS:H	2.25	0.40
1:D:71:GLN:C	1:D:73:HIS:H	2.24	0.40
1:F:108:GLY:CA	1:F:130:ILE:HB	2.48	0.40
1:F:489:MSE:HB2	1:F:489:MSE:HE3	1.91	0.40
1:F:92:ARG:HD3	1:F:92:ARG:HA	1.92	0.40
1:A:303:ASN:HA	1:A:304:PRO:HD3	1.84	0.40
1:A:547:TYR:OH	1:A:560:PHE:HB3	2.21	0.40
1:C:491:VAL:O	1:C:505:ASP:HA	2.21	0.40
1:C:530:PHE:CE2	1:C:617:PHE:HD1	2.40	0.40
1:D:398:VAL:HB	1:D:628:ALA:HB3	2.03	0.40
1:D:6:PHE:HA	1:D:57:GLY:O	2.22	0.40
1:E:432:ALA:O	1:E:433:HIS:HB3	2.21	0.40
1:E:471:SER:C	1:E:473:ASP:N	2.73	0.40
1:E:530:PHE:CE2	1:E:617:PHE:HD1	2.38	0.40
1:F:105:CYS:HA	1:F:106:PRO:HD3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	617/750 (82%)	501 (81%)	92 (15%)	24 (4%)	3	18
1	B	616/750 (82%)	499 (81%)	96 (16%)	21 (3%)	3	22
1	C	616/750 (82%)	500 (81%)	92 (15%)	24 (4%)	3	18
1	D	616/750 (82%)	502 (82%)	92 (15%)	22 (4%)	3	20
1	E	617/750 (82%)	505 (82%)	90 (15%)	22 (4%)	3	20
1	F	612/750 (82%)	503 (82%)	87 (14%)	22 (4%)	3	20
All	All	3694/4500 (82%)	3010 (82%)	549 (15%)	135 (4%)	3	20

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	117	SER
1	A	434	ALA
1	A	650	THR
1	A	730	CYS
1	B	106	PRO
1	B	117	SER
1	B	434	ALA
1	B	650	THR
1	B	730	CYS
1	C	106	PRO
1	C	117	SER
1	C	434	ALA
1	C	447	PHE
1	C	650	THR
1	C	730	CYS
1	D	106	PRO
1	D	117	SER
1	D	434	ALA
1	D	650	THR

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Mol	Chain	Res	Type
1	D	730	CYS
1	E	106	PRO
1	E	117	SER
1	E	434	ALA
1	E	650	THR
1	E	730	CYS
1	F	106	PRO
1	F	117	SER
1	F	434	ALA
1	F	447	PHE
1	F	650	THR
1	F	730	CYS
1	A	80	MSE
1	A	107	PRO
1	A	446	PRO
1	A	450	GLY
1	A	515	THR
1	B	80	MSE
1	B	107	PRO
1	B	515	THR
1	C	80	MSE
1	C	107	PRO
1	C	515	THR
1	D	80	MSE
1	D	107	PRO
1	D	515	THR
1	E	80	MSE
1	E	107	PRO
1	E	515	THR
1	F	80	MSE
1	F	107	PRO
1	F	515	THR
1	A	257	LEU
1	A	624	ASN
1	B	255	LEU
1	B	257	LEU
1	B	624	ASN
1	C	257	LEU
1	C	624	ASN
1	D	257	LEU
1	D	624	ASN
1	E	257	LEU

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Mol	Chain	Res	Type
1	E	423	CYS
1	E	624	ASN
1	F	624	ASN
1	A	70	LYS
1	A	322	ASP
1	A	386	PRO
1	A	423	CYS
1	A	721	PRO
1	B	322	ASP
1	B	332	ASN
1	B	423	CYS
1	B	721	PRO
1	C	22	THR
1	C	136	GLY
1	C	322	ASP
1	C	423	CYS
1	C	721	PRO
1	D	322	ASP
1	D	332	ASN
1	D	423	CYS
1	D	721	PRO
1	E	322	ASP
1	E	453	GLN
1	E	721	PRO
1	F	22	THR
1	F	136	GLY
1	F	322	ASP
1	F	332	ASN
1	F	423	CYS
1	F	721	PRO
1	A	22	THR
1	A	332	ASN
1	A	430	PRO
1	B	70	LYS
1	B	136	GLY
1	B	386	PRO
1	B	430	PRO
1	C	70	LYS
1	C	386	PRO
1	C	430	PRO
1	D	70	LYS
1	D	386	PRO

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Mol	Chain	Res	Type
1	D	430	PRO
1	E	70	LYS
1	E	136	GLY
1	E	332	ASN
1	E	386	PRO
1	E	430	PRO
1	F	70	LYS
1	F	386	PRO
1	F	430	PRO
1	A	119	ASN
1	A	136	GLY
1	B	444	VAL
1	C	332	ASN
1	C	449	TRP
1	C	653	ALA
1	D	22	THR
1	D	119	ASN
1	D	136	GLY
1	E	119	ASN
1	F	119	ASN
1	F	444	VAL
1	A	444	VAL
1	C	444	VAL
1	D	444	VAL
1	E	444	VAL
1	F	610	PRO
1	E	610	PRO
1	A	610	PRO
1	C	610	PRO
1	D	610	PRO
1	B	610	PRO

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	534/630 (85%)	468 (88%)	66 (12%)	4	19
1	B	533/630 (85%)	466 (87%)	67 (13%)	4	19
1	C	533/630 (85%)	466 (87%)	67 (13%)	4	19
1	D	533/630 (85%)	469 (88%)	64 (12%)	5	20
1	E	532/630 (84%)	466 (88%)	66 (12%)	4	19
1	F	529/630 (84%)	464 (88%)	65 (12%)	4	20
All	All	3194/3780 (84%)	2799 (88%)	395 (12%)	4	19

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	20	HIS
1	A	68	SER
1	A	69	LEU
1	A	71	GLN
1	A	72	ASP
1	A	74	THR
1	A	77	GLU
1	A	93	ARG
1	A	94	LEU
1	A	109	ASP
1	A	120	SER
1	A	122	THR
1	A	125	THR
1	A	146	HIS
1	A	261	LEU
1	A	262	ILE
1	A	267	MSE
1	A	268	VAL
1	A	282	HIS
1	A	288	ASP
1	A	289	THR
1	A	293	THR
1	A	294	LEU
1	A	295	LEU
1	A	296	THR
1	A	308	THR

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Mol	Chain	Res	Type
1	A	317	ARG
1	A	329	ILE
1	A	333	HIS
1	A	336	VAL
1	A	341	GLN
1	A	343	SER
1	A	387	LEU
1	A	394	MSE
1	A	402	THR
1	A	405	GLU
1	A	407	ILE
1	A	409	CYS
1	A	413	THR
1	A	428	CYS
1	A	437	THR
1	A	438	CYS
1	A	474	CYS
1	A	490	LYS
1	A	497	TYR
1	A	505	ASP
1	A	516	SER
1	A	518	ASP
1	A	519	LEU
1	A	541	ARG
1	A	548	ASP
1	A	555	MSE
1	A	563	ILE
1	A	567	SER
1	A	573	LEU
1	A	578	ASP
1	A	602	MSE
1	A	609	ARG
1	A	611	LEU
1	A	612	GLN
1	A	626	LEU
1	A	649	ARG
1	A	651	SER
1	A	652	ASP
1	A	655	LEU
1	B	17	SER
1	B	20	HIS
1	B	68	SER

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	71	GLN
1	B	72	ASP
1	B	74	THR
1	B	77	GLU
1	B	93	ARG
1	B	94	LEU
1	B	109	ASP
1	B	120	SER
1	B	122	THR
1	B	125	THR
1	B	146	HIS
1	B	261	LEU
1	B	262	ILE
1	B	267	MSE
1	B	268	VAL
1	B	282	HIS
1	B	288	ASP
1	B	289	THR
1	B	293	THR
1	B	294	LEU
1	B	295	LEU
1	B	296	THR
1	B	308	THR
1	B	312	VAL
1	B	317	ARG
1	B	329	ILE
1	B	333	HIS
1	B	336	VAL
1	B	341	GLN
1	B	387	LEU
1	B	394	MSE
1	B	402	THR
1	B	405	GLU
1	B	407	ILE
1	B	409	CYS
1	B	413	THR
1	B	428	CYS
1	B	437	THR
1	B	438	CYS
1	B	474	CYS
1	B	490	LYS

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Mol	Chain	Res	Type
1	B	497	TYR
1	B	505	ASP
1	B	516	SER
1	B	518	ASP
1	B	519	LEU
1	B	541	ARG
1	B	548	ASP
1	B	555	MSE
1	B	563	ILE
1	B	567	SER
1	B	573	LEU
1	B	578	ASP
1	B	597	SER
1	B	602	MSE
1	B	609	ARG
1	B	611	LEU
1	B	612	GLN
1	B	626	LEU
1	B	649	ARG
1	B	651	SER
1	B	652	ASP
1	B	655	LEU
1	C	17	SER
1	C	20	HIS
1	C	68	SER
1	C	69	LEU
1	C	71	GLN
1	C	72	ASP
1	C	74	THR
1	C	77	GLU
1	C	93	ARG
1	C	94	LEU
1	C	109	ASP
1	C	120	SER
1	C	122	THR
1	C	125	THR
1	C	146	HIS
1	C	255	LEU
1	C	261	LEU
1	C	262	ILE
1	C	267	MSE
1	C	268	VAL

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Mol	Chain	Res	Type
1	C	282	HIS
1	C	288	ASP
1	C	289	THR
1	C	293	THR
1	C	294	LEU
1	C	295	LEU
1	C	296	THR
1	C	308	THR
1	C	317	ARG
1	C	329	ILE
1	C	333	HIS
1	C	336	VAL
1	C	341	GLN
1	C	387	LEU
1	C	394	MSE
1	C	402	THR
1	C	405	GLU
1	C	407	ILE
1	C	409	CYS
1	C	413	THR
1	C	428	CYS
1	C	437	THR
1	C	438	CYS
1	C	447	PHE
1	C	448	MSE
1	C	474	CYS
1	C	490	LYS
1	C	497	TYR
1	C	505	ASP
1	C	516	SER
1	C	518	ASP
1	C	519	LEU
1	C	541	ARG
1	C	548	ASP
1	C	555	MSE
1	C	563	ILE
1	C	567	SER
1	C	573	LEU
1	C	578	ASP
1	C	597	SER
1	C	602	MSE
1	C	611	LEU

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Mol	Chain	Res	Type
1	C	612	GLN
1	C	626	LEU
1	C	649	ARG
1	C	651	SER
1	C	652	ASP
1	D	17	SER
1	D	20	HIS
1	D	68	SER
1	D	69	LEU
1	D	71	GLN
1	D	72	ASP
1	D	74	THR
1	D	77	GLU
1	D	93	ARG
1	D	94	LEU
1	D	109	ASP
1	D	120	SER
1	D	122	THR
1	D	125	THR
1	D	146	HIS
1	D	261	LEU
1	D	262	ILE
1	D	267	MSE
1	D	268	VAL
1	D	282	HIS
1	D	288	ASP
1	D	289	THR
1	D	293	THR
1	D	294	LEU
1	D	295	LEU
1	D	296	THR
1	D	308	THR
1	D	317	ARG
1	D	329	ILE
1	D	333	HIS
1	D	336	VAL
1	D	387	LEU
1	D	394	MSE
1	D	402	THR
1	D	405	GLU
1	D	407	ILE
1	D	409	CYS

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Mol	Chain	Res	Type
1	D	413	THR
1	D	428	CYS
1	D	437	THR
1	D	438	CYS
1	D	474	CYS
1	D	490	LYS
1	D	497	TYR
1	D	505	ASP
1	D	516	SER
1	D	518	ASP
1	D	519	LEU
1	D	541	ARG
1	D	548	ASP
1	D	555	MSE
1	D	563	ILE
1	D	567	SER
1	D	573	LEU
1	D	578	ASP
1	D	602	MSE
1	D	609	ARG
1	D	611	LEU
1	D	612	GLN
1	D	626	LEU
1	D	649	ARG
1	D	651	SER
1	D	652	ASP
1	D	655	LEU
1	E	17	SER
1	E	20	HIS
1	E	68	SER
1	E	69	LEU
1	E	71	GLN
1	E	72	ASP
1	E	74	THR
1	E	77	GLU
1	E	93	ARG
1	E	94	LEU
1	E	109	ASP
1	E	120	SER
1	E	122	THR
1	E	125	THR
1	E	146	HIS

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Mol	Chain	Res	Type
1	E	261	LEU
1	E	262	ILE
1	E	267	MSE
1	E	268	VAL
1	E	282	HIS
1	E	288	ASP
1	E	289	THR
1	E	293	THR
1	E	294	LEU
1	E	295	LEU
1	E	296	THR
1	E	308	THR
1	E	312	VAL
1	E	317	ARG
1	E	329	ILE
1	E	333	HIS
1	E	336	VAL
1	E	387	LEU
1	E	394	MSE
1	E	402	THR
1	E	405	GLU
1	E	407	ILE
1	E	409	CYS
1	E	413	THR
1	E	428	CYS
1	E	437	THR
1	E	438	CYS
1	E	474	CYS
1	E	490	LYS
1	E	497	TYR
1	E	505	ASP
1	E	516	SER
1	E	518	ASP
1	E	519	LEU
1	E	541	ARG
1	E	548	ASP
1	E	555	MSE
1	E	563	ILE
1	E	567	SER
1	E	573	LEU
1	E	578	ASP
1	E	597	SER

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Mol	Chain	Res	Type
1	E	602	MSE
1	E	609	ARG
1	E	611	LEU
1	E	612	GLN
1	E	626	LEU
1	E	649	ARG
1	E	651	SER
1	E	652	ASP
1	E	655	LEU
1	F	17	SER
1	F	20	HIS
1	F	68	SER
1	F	69	LEU
1	F	71	GLN
1	F	72	ASP
1	F	74	THR
1	F	77	GLU
1	F	93	ARG
1	F	94	LEU
1	F	109	ASP
1	F	120	SER
1	F	122	THR
1	F	125	THR
1	F	146	HIS
1	F	261	LEU
1	F	262	ILE
1	F	267	MSE
1	F	268	VAL
1	F	282	HIS
1	F	288	ASP
1	F	289	THR
1	F	293	THR
1	F	294	LEU
1	F	295	LEU
1	F	296	THR
1	F	308	THR
1	F	317	ARG
1	F	329	ILE
1	F	333	HIS
1	F	336	VAL
1	F	341	GLN
1	F	387	LEU

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Mol	Chain	Res	Type
1	F	394	MSE
1	F	402	THR
1	F	405	GLU
1	F	407	ILE
1	F	409	CYS
1	F	413	THR
1	F	428	CYS
1	F	437	THR
1	F	438	CYS
1	F	448	MSE
1	F	474	CYS
1	F	490	LYS
1	F	497	TYR
1	F	505	ASP
1	F	516	SER
1	F	518	ASP
1	F	519	LEU
1	F	541	ARG
1	F	548	ASP
1	F	555	MSE
1	F	563	ILE
1	F	567	SER
1	F	573	LEU
1	F	578	ASP
1	F	597	SER
1	F	602	MSE
1	F	611	LEU
1	F	612	GLN
1	F	626	LEU
1	F	649	ARG
1	F	651	SER
1	F	655	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	50	GLN
1	A	62	ASN
1	A	146	HIS
1	A	291	HIS
1	A	332	ASN

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Mol	Chain	Res	Type
1	A	333	HIS
1	A	453	GLN
1	A	540	HIS
1	A	546	ASN
1	A	595	GLN
1	A	612	GLN
1	A	691	HIS
1	A	715	HIS
1	B	46	GLN
1	B	50	GLN
1	B	62	ASN
1	B	146	HIS
1	B	291	HIS
1	B	332	ASN
1	B	333	HIS
1	B	460	ASN
1	B	540	HIS
1	B	546	ASN
1	B	595	GLN
1	B	612	GLN
1	B	715	HIS
1	C	46	GLN
1	C	50	GLN
1	C	62	ASN
1	C	146	HIS
1	C	256	HIS
1	C	291	HIS
1	C	332	ASN
1	C	333	HIS
1	C	540	HIS
1	C	546	ASN
1	C	595	GLN
1	C	612	GLN
1	C	691	HIS
1	C	715	HIS
1	D	46	GLN
1	D	50	GLN
1	D	62	ASN
1	D	146	HIS
1	D	291	HIS
1	D	332	ASN
1	D	333	HIS

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Mol	Chain	Res	Type
1	D	453	GLN
1	D	540	HIS
1	D	546	ASN
1	D	595	GLN
1	D	612	GLN
1	D	691	HIS
1	D	715	HIS
1	E	46	GLN
1	E	50	GLN
1	E	62	ASN
1	E	146	HIS
1	E	291	HIS
1	E	332	ASN
1	E	333	HIS
1	E	540	HIS
1	E	546	ASN
1	E	595	GLN
1	E	612	GLN
1	E	691	HIS
1	E	715	HIS
1	F	46	GLN
1	F	50	GLN
1	F	62	ASN
1	F	146	HIS
1	F	291	HIS
1	F	332	ASN
1	F	333	HIS
1	F	540	HIS
1	F	546	ASN
1	F	595	GLN
1	F	612	GLN
1	F	691	HIS
1	F	715	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 (i)

50 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	1,2	14,14,15	0.40	0	17,19,21	2.12	3 (17%)
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	2.04	5 (29%)
2	BMA	G	3	2	11,11,12	1.76	3 (27%)	15,15,17	4.51	12 (80%)
2	MAN	G	4	2	11,11,12	0.92	1 (9%)	15,15,17	2.34	4 (26%)
3	NAG	H	1	1,3	14,14,15	0.70	0	17,19,21	1.38	2 (11%)
3	NAG	H	2	3	14,14,15	0.49	0	17,19,21	1.14	1 (5%)
3	BMA	H	3	3	11,11,12	2.17	4 (36%)	15,15,17	3.23	9 (60%)
3	MAN	H	4	3	11,11,12	0.42	0	15,15,17	1.56	2 (13%)
3	MAN	H	5	3	11,11,12	0.52	0	15,15,17	1.47	2 (13%)
2	NAG	I	1	1,2	14,14,15	0.78	0	17,19,21	1.08	1 (5%)
2	NAG	I	2	2	14,14,15	0.81	0	17,19,21	1.95	3 (17%)
2	BMA	I	3	2	11,11,12	2.26	5 (45%)	15,15,17	3.12	9 (60%)
2	MAN	I	4	2	11,11,12	0.54	0	15,15,17	1.13	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.55	0	17,19,21	1.43	2 (11%)
2	NAG	J	2	2	14,14,15	0.59	0	17,19,21	1.58	4 (23%)
2	BMA	J	3	2	11,11,12	1.87	3 (27%)	15,15,17	3.82	9 (60%)
2	MAN	J	4	2	11,11,12	0.63	0	15,15,17	0.85	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.70	0	17,19,21	1.22	2 (11%)
2	NAG	K	2	2	14,14,15	0.64	0	17,19,21	0.96	2 (11%)
2	BMA	K	3	2	11,11,12	2.11	4 (36%)	15,15,17	3.96	10 (66%)
2	MAN	K	4	2	11,11,12	0.80	1 (9%)	15,15,17	1.93	7 (46%)
2	NAG	L	1	1,2	14,14,15	0.47	0	17,19,21	1.97	4 (23%)
2	NAG	L	2	2	14,14,15	0.48	0	17,19,21	2.88	5 (29%)
2	BMA	L	3	2	11,11,12	1.87	3 (27%)	15,15,17	3.60	8 (53%)
2	MAN	L	4	2	11,11,12	0.45	0	15,15,17	1.82	3 (20%)
2	NAG	M	1	1,2	14,14,15	0.75	0	17,19,21	2.26	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	M	2	2	14,14,15	0.59	0	17,19,21	1.69	5 (29%)
2	BMA	M	3	2	11,11,12	1.95	4 (36%)	15,15,17	3.61	12 (80%)
2	MAN	M	4	2	11,11,12	0.56	0	15,15,17	1.02	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.39	0	17,19,21	2.15	3 (17%)
4	NAG	N	2	4	14,14,15	0.51	0	17,19,21	1.29	3 (17%)
4	BMA	N	3	4	11,11,12	2.06	4 (36%)	15,15,17	3.53	10 (66%)
2	NAG	O	1	1,2	14,14,15	0.63	0	17,19,21	0.89	0
2	NAG	O	2	2	14,14,15	0.67	0	17,19,21	1.85	4 (23%)
2	BMA	O	3	2	11,11,12	2.02	4 (36%)	15,15,17	3.94	10 (66%)
2	MAN	O	4	2	11,11,12	0.67	0	15,15,17	0.78	0
3	NAG	P	1	1,3	14,14,15	0.49	0	17,19,21	2.21	3 (17%)
3	NAG	P	2	3	14,14,15	0.62	1 (7%)	17,19,21	2.54	6 (35%)
3	BMA	P	3	3	11,11,12	1.86	3 (27%)	15,15,17	4.13	8 (53%)
3	MAN	P	4	3	11,11,12	0.59	0	15,15,17	1.20	2 (13%)
3	MAN	P	5	3	11,11,12	0.63	0	15,15,17	0.62	0
2	NAG	Q	1	1,2	14,14,15	0.66	0	17,19,21	1.87	3 (17%)
2	NAG	Q	2	2	14,14,15	0.49	0	17,19,21	3.22	5 (29%)
2	BMA	Q	3	2	11,11,12	2.11	4 (36%)	15,15,17	4.48	10 (66%)
2	MAN	Q	4	2	11,11,12	0.52	0	15,15,17	1.43	2 (13%)
3	NAG	R	1	1,3	14,14,15	0.44	0	17,19,21	1.93	3 (17%)
3	NAG	R	2	3	14,14,15	0.45	0	17,19,21	2.20	3 (17%)
3	BMA	R	3	3	11,11,12	2.15	4 (36%)	15,15,17	2.30	7 (46%)
3	MAN	R	4	3	11,11,12	0.62	0	15,15,17	0.72	0
3	MAN	R	5	3	11,11,12	0.47	0	15,15,17	1.62	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	1/1/5/7	6/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	MAN	H	4	3	-	1/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	1/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	1/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	BMA	M	3	2	-	2/2/19/22	0/1/1/1
2	MAN	M	4	2	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	2/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
3	MAN	P	4	3	-	0/2/19/22	1/1/1/1
3	MAN	P	5	3	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	1,2	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	2/2/19/22	1/1/1/1
3	NAG	R	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	BMA	R	3	3	-	1/2/19/22	0/1/1/1
3	MAN	R	4	3	-	1/2/19/22	0/1/1/1
3	MAN	R	5	3	-	2/2/19/22	1/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	3	BMA	C4-C5	4.37	1.62	1.53
2	I	3	BMA	C4-C5	4.29	1.62	1.53
3	H	3	BMA	C4-C5	4.13	1.61	1.53
4	N	3	BMA	C4-C5	4.04	1.61	1.53
3	R	3	BMA	C4-C5	3.92	1.61	1.53
2	K	3	BMA	C2-C3	-3.89	1.46	1.52
2	L	3	BMA	O4-C4	3.82	1.52	1.43
2	Q	3	BMA	O4-C4	3.80	1.51	1.43
2	G	3	BMA	O4-C4	3.74	1.51	1.43
2	J	3	BMA	O4-C4	3.73	1.51	1.43
4	N	3	BMA	O4-C4	3.70	1.51	1.43
3	P	3	BMA	O4-C4	3.64	1.51	1.43
2	K	3	BMA	O4-C4	3.60	1.51	1.43
2	M	3	BMA	O4-C4	3.59	1.51	1.43
2	O	3	BMA	C4-C5	3.56	1.60	1.53
3	R	3	BMA	O4-C4	3.56	1.51	1.43
2	O	3	BMA	O4-C4	3.52	1.51	1.43
3	H	3	BMA	O4-C4	3.51	1.51	1.43
2	J	3	BMA	C4-C5	3.49	1.60	1.53
2	M	3	BMA	C4-C5	3.43	1.60	1.53
2	I	3	BMA	O4-C4	3.43	1.51	1.43
2	K	3	BMA	C4-C5	3.43	1.60	1.53
2	L	3	BMA	C4-C5	3.41	1.60	1.53
3	P	3	BMA	C4-C5	3.26	1.59	1.53
2	I	3	BMA	C2-C3	-3.16	1.47	1.52
3	R	3	BMA	C2-C3	-3.16	1.47	1.52
2	G	3	BMA	C4-C5	3.15	1.59	1.53
2	I	3	BMA	C4-C3	2.97	1.59	1.52
2	M	3	BMA	C2-C3	-2.91	1.48	1.52
2	O	3	BMA	C2-C3	-2.88	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	BMA	C4-C3	2.83	1.59	1.52
3	P	3	BMA	C2-C3	-2.82	1.48	1.52
3	H	3	BMA	C2-C3	-2.80	1.48	1.52
4	N	3	BMA	C2-C3	-2.78	1.48	1.52
2	Q	3	BMA	C4-C3	2.78	1.59	1.52
2	L	3	BMA	C4-C3	2.54	1.58	1.52
3	R	3	BMA	C4-C3	2.43	1.58	1.52
2	O	3	BMA	C4-C3	2.42	1.58	1.52
2	J	3	BMA	C4-C3	2.39	1.58	1.52
2	G	4	MAN	O5-C1	-2.39	1.39	1.43
4	N	3	BMA	C4-C3	2.32	1.58	1.52
2	M	3	BMA	C4-C3	2.29	1.58	1.52
2	K	3	BMA	C4-C3	2.24	1.58	1.52
2	I	3	BMA	C1-C2	-2.23	1.47	1.52
2	K	4	MAN	O5-C1	-2.22	1.40	1.43
2	Q	3	BMA	C2-C3	-2.17	1.49	1.52
3	P	2	NAG	C1-C2	2.09	1.55	1.52
2	G	3	BMA	C2-C3	-2.03	1.49	1.52

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	2	NAG	C4-C3-C2	-10.25	96.00	111.02
2	Q	3	BMA	C1-O5-C5	-9.55	99.26	112.19
3	P	3	BMA	O5-C5-C6	9.28	121.75	107.20
2	G	3	BMA	O5-C5-C6	8.80	121.01	107.20
2	L	2	NAG	C1-O5-C5	8.25	123.36	112.19
2	M	3	BMA	O5-C5-C6	8.17	120.02	107.20
2	Q	3	BMA	O5-C5-C6	8.05	119.83	107.20
3	H	3	BMA	C1-O5-C5	-8.03	101.31	112.19
2	K	3	BMA	O5-C5-C6	7.77	119.39	107.20
2	O	3	BMA	O5-C5-C6	7.74	119.34	107.20
2	O	3	BMA	C1-O5-C5	-7.68	101.78	112.19
2	L	3	BMA	O5-C5-C6	7.64	119.18	107.20
4	N	1	NAG	C1-O5-C5	7.55	122.42	112.19
2	G	3	BMA	O3-C3-C2	7.55	124.44	109.99
2	J	3	BMA	O3-C3-C2	7.52	124.40	109.99
3	R	2	NAG	C1-O5-C5	7.47	122.31	112.19
3	P	3	BMA	O3-C3-C2	7.45	124.27	109.99
2	G	1	NAG	C1-O5-C5	7.18	121.92	112.19
3	P	2	NAG	C1-O5-C5	6.83	121.45	112.19
2	J	3	BMA	O5-C5-C6	6.83	117.91	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	3	BMA	O5-C5-C6	6.69	117.69	107.20
2	G	3	BMA	O4-C4-C5	6.67	125.87	109.30
2	I	3	BMA	C1-O5-C5	-6.62	103.23	112.19
3	P	1	NAG	C1-O5-C5	6.54	121.06	112.19
2	L	1	NAG	C1-O5-C5	6.23	120.64	112.19
2	Q	3	BMA	C1-C2-C3	-6.18	102.07	109.67
2	I	3	BMA	O5-C5-C6	6.17	116.88	107.20
2	L	2	NAG	C4-C3-C2	-6.09	102.09	111.02
2	Q	3	BMA	O3-C3-C2	6.06	121.61	109.99
2	G	3	BMA	O4-C4-C3	5.87	123.93	110.35
3	H	3	BMA	O5-C5-C6	5.81	116.32	107.20
2	K	3	BMA	O4-C4-C5	5.79	123.68	109.30
2	K	3	BMA	O4-C4-C3	5.79	123.73	110.35
4	N	3	BMA	C1-O5-C5	-5.77	104.37	112.19
3	P	3	BMA	O4-C4-C5	5.73	123.52	109.30
2	M	1	NAG	O4-C4-C3	5.71	123.55	110.35
2	L	4	MAN	C1-O5-C5	5.69	119.90	112.19
2	K	3	BMA	C2-C3-C4	-5.61	101.19	110.89
3	R	1	NAG	C1-O5-C5	5.58	119.75	112.19
2	G	4	MAN	O5-C1-C2	-5.55	102.21	110.77
4	N	3	BMA	O4-C4-C5	5.53	123.03	109.30
2	L	3	BMA	O3-C3-C2	5.51	120.55	109.99
2	J	3	BMA	O4-C4-C3	5.47	123.01	110.35
2	G	2	NAG	C1-O5-C5	5.40	119.51	112.19
2	M	3	BMA	O4-C4-C5	5.39	122.69	109.30
2	J	3	BMA	O4-C4-C5	5.36	122.60	109.30
2	G	3	BMA	C3-C4-C5	-5.29	100.80	110.24
2	Q	2	NAG	O4-C4-C3	5.27	122.54	110.35
2	L	3	BMA	O4-C4-C5	5.22	122.25	109.30
2	Q	1	NAG	C1-O5-C5	5.10	119.10	112.19
2	K	3	BMA	O3-C3-C4	5.05	122.02	110.35
3	P	2	NAG	C4-C3-C2	-5.03	103.65	111.02
2	L	3	BMA	C1-O5-C5	-5.02	105.39	112.19
2	O	3	BMA	O4-C4-C5	4.98	121.66	109.30
2	M	3	BMA	O4-C4-C3	4.96	121.82	110.35
2	I	2	NAG	O5-C1-C2	-4.95	103.48	111.29
3	P	3	BMA	O4-C4-C3	4.78	121.40	110.35
2	Q	3	BMA	O4-C4-C5	4.71	121.00	109.30
4	N	3	BMA	O3-C3-C2	4.69	118.97	109.99
3	H	5	MAN	C1-O5-C5	4.68	118.54	112.19
3	R	3	BMA	O5-C5-C6	4.58	114.38	107.20
2	L	3	BMA	O4-C4-C3	4.56	120.89	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	2	NAG	C2-N2-C7	-4.53	116.46	122.90
2	G	4	MAN	C3-C4-C5	4.44	118.16	110.24
3	H	4	MAN	C1-O5-C5	4.32	118.04	112.19
2	O	3	BMA	O4-C4-C3	4.20	120.06	110.35
2	O	2	NAG	O5-C1-C2	-4.11	104.80	111.29
3	P	3	BMA	C2-C3-C4	-4.11	103.79	110.89
2	Q	4	MAN	C1-O5-C5	4.10	117.74	112.19
2	M	3	BMA	O3-C3-C2	4.04	117.73	109.99
2	O	3	BMA	O3-C3-C2	4.00	117.64	109.99
4	N	3	BMA	O4-C4-C3	3.97	119.52	110.35
2	G	3	BMA	C2-C3-C4	-3.94	104.08	110.89
2	M	2	NAG	C1-O5-C5	-3.83	107.01	112.19
3	R	5	MAN	C1-O5-C5	3.82	117.37	112.19
2	J	3	BMA	O3-C3-C4	3.75	119.03	110.35
2	I	3	BMA	C3-C4-C5	3.75	116.93	110.24
2	O	2	NAG	C4-C3-C2	-3.74	105.54	111.02
2	Q	3	BMA	O2-C2-C1	3.73	116.78	109.15
2	O	2	NAG	C2-N2-C7	-3.72	117.61	122.90
2	K	4	MAN	C3-C4-C5	3.72	116.87	110.24
2	I	2	NAG	C3-C4-C5	3.69	116.82	110.24
2	J	3	BMA	C2-C3-C4	-3.67	104.55	110.89
3	P	1	NAG	C4-C3-C2	-3.66	105.65	111.02
2	M	3	BMA	O3-C3-C4	3.63	118.74	110.35
2	K	1	NAG	O5-C1-C2	-3.59	105.62	111.29
3	R	3	BMA	O4-C4-C5	3.56	118.15	109.30
3	R	3	BMA	O5-C1-C2	-3.56	105.28	110.77
3	H	1	NAG	C4-C3-C2	3.56	116.23	111.02
2	G	2	NAG	C3-C4-C5	3.49	116.46	110.24
2	K	3	BMA	O3-C3-C2	3.46	116.62	109.99
3	P	3	BMA	C1-O5-C5	-3.42	107.55	112.19
2	J	1	NAG	O5-C1-C2	-3.41	105.90	111.29
2	O	3	BMA	O3-C3-C4	3.41	118.22	110.35
3	R	2	NAG	O5-C5-C4	3.37	119.02	110.83
2	G	4	MAN	C1-C2-C3	-3.34	105.56	109.67
2	K	3	BMA	O2-C2-C1	3.33	115.97	109.15
2	G	2	NAG	O5-C5-C4	3.33	118.92	110.83
2	Q	3	BMA	O2-C2-C3	3.32	116.79	110.14
4	N	3	BMA	O3-C3-C4	3.29	117.94	110.35
2	O	3	BMA	C1-C2-C3	-3.28	105.64	109.67
2	O	3	BMA	C6-C5-C4	3.28	120.68	113.00
3	R	1	NAG	C4-C3-C2	-3.27	106.23	111.02
2	L	2	NAG	O4-C4-C3	3.24	117.84	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	1	NAG	C3-C4-C5	-3.23	104.47	110.24
3	H	3	BMA	O4-C4-C5	3.23	117.33	109.30
2	K	3	BMA	C3-C4-C5	-3.23	104.48	110.24
2	G	3	BMA	O3-C3-C4	3.15	117.64	110.35
2	G	4	MAN	C1-O5-C5	-3.11	107.98	112.19
2	K	3	BMA	C6-C5-C4	3.10	120.27	113.00
2	Q	1	NAG	O4-C4-C3	3.10	117.51	110.35
4	N	3	BMA	C6-C5-C4	3.08	120.22	113.00
3	R	3	BMA	C3-C4-C5	3.07	115.72	110.24
2	M	1	NAG	C1-O5-C5	3.06	116.33	112.19
2	I	3	BMA	O2-C2-C3	3.05	116.24	110.14
3	P	3	BMA	C1-C2-C3	3.04	113.40	109.67
2	Q	3	BMA	O4-C4-C3	3.03	117.36	110.35
2	I	2	NAG	C2-N2-C7	-3.02	118.60	122.90
2	M	3	BMA	C1-O5-C5	-3.00	108.12	112.19
2	L	1	NAG	O5-C5-C4	3.00	118.13	110.83
2	J	2	NAG	C1-O5-C5	-3.00	108.13	112.19
3	R	5	MAN	O5-C5-C6	3.00	111.90	107.20
3	P	1	NAG	O4-C4-C3	2.99	117.26	110.35
2	J	3	BMA	C3-C4-C5	-2.98	104.93	110.24
2	G	3	BMA	C6-C5-C4	2.95	119.92	113.00
3	P	4	MAN	C1-O5-C5	2.94	116.18	112.19
2	M	1	NAG	C4-C3-C2	-2.93	106.72	111.02
2	Q	4	MAN	O5-C5-C6	2.91	111.76	107.20
3	H	4	MAN	C2-C3-C4	-2.88	105.91	110.89
2	I	3	BMA	O4-C4-C5	2.86	116.41	109.30
2	O	3	BMA	O2-C2-C3	2.84	115.82	110.14
3	H	3	BMA	O3-C3-C4	2.84	116.91	110.35
3	H	3	BMA	O2-C2-C3	2.83	115.80	110.14
2	M	2	NAG	C3-C4-C5	2.82	115.28	110.24
3	H	2	NAG	C1-O5-C5	2.81	116.00	112.19
3	P	2	NAG	O4-C4-C3	2.78	116.78	110.35
3	P	2	NAG	O5-C1-C2	2.77	115.66	111.29
2	K	4	MAN	C6-C5-C4	-2.76	106.53	113.00
3	P	3	BMA	C3-C4-C5	-2.76	105.32	110.24
3	P	4	MAN	O5-C5-C6	2.76	111.52	107.20
2	M	2	NAG	O5-C1-C2	-2.75	106.94	111.29
2	M	3	BMA	C6-C5-C4	2.75	119.45	113.00
2	G	1	NAG	O5-C5-C6	2.74	111.51	107.20
2	K	4	MAN	O5-C5-C4	2.73	117.46	110.83
2	M	3	BMA	C2-C3-C4	-2.72	106.18	110.89
2	J	3	BMA	C6-C5-C4	2.70	119.34	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	3	BMA	O3-C3-C4	2.69	116.58	110.35
2	O	3	BMA	O2-C2-C1	2.69	114.66	109.15
4	N	1	NAG	O5-C5-C4	2.69	117.38	110.83
2	M	1	NAG	C2-N2-C7	-2.66	119.11	122.90
2	L	3	BMA	O2-C2-C1	2.65	114.58	109.15
2	L	2	NAG	C2-N2-C7	-2.65	119.14	122.90
2	J	3	BMA	O2-C2-C3	2.65	115.44	110.14
2	J	1	NAG	C1-O5-C5	2.64	115.77	112.19
2	J	2	NAG	C4-C3-C2	2.63	114.88	111.02
2	L	4	MAN	O5-C5-C6	2.62	111.32	107.20
2	K	4	MAN	O5-C1-C2	-2.61	106.75	110.77
2	G	3	BMA	O5-C5-C4	-2.60	104.50	110.83
2	Q	1	NAG	O5-C5-C6	2.60	111.28	107.20
3	H	3	BMA	O3-C3-C2	2.59	114.95	109.99
4	N	3	BMA	C2-C3-C4	-2.58	106.42	110.89
2	L	3	BMA	C6-C5-C4	2.58	119.05	113.00
2	J	2	NAG	C3-C4-C5	2.58	114.84	110.24
2	M	1	NAG	O5-C5-C6	2.57	111.23	107.20
3	H	1	NAG	C3-C4-C5	2.56	114.81	110.24
3	H	5	MAN	O5-C5-C6	2.54	111.19	107.20
2	J	2	NAG	O5-C5-C6	2.53	111.17	107.20
2	L	3	BMA	O2-C2-C3	2.52	115.19	110.14
4	N	2	NAG	O5-C1-C2	-2.49	107.35	111.29
2	K	4	MAN	O5-C5-C6	-2.49	103.30	107.20
2	L	2	NAG	O5-C5-C4	2.48	116.85	110.83
3	R	5	MAN	C3-C4-C5	-2.48	105.82	110.24
3	R	1	NAG	O5-C5-C4	2.47	116.83	110.83
2	L	1	NAG	O5-C5-C6	-2.46	103.35	107.20
2	K	2	NAG	C1-C2-N2	2.46	114.68	110.49
2	G	3	BMA	O5-C1-C2	2.45	114.56	110.77
3	R	3	BMA	O3-C3-C2	2.43	114.64	109.99
2	I	1	NAG	O5-C5-C6	2.41	110.99	107.20
4	N	2	NAG	O5-C5-C6	2.40	110.96	107.20
2	K	4	MAN	C1-O5-C5	2.39	115.44	112.19
2	G	3	BMA	O2-C2-C3	2.39	114.92	110.14
3	H	3	BMA	O4-C4-C3	2.36	115.82	110.35
3	R	3	BMA	O4-C4-C3	2.35	115.78	110.35
2	G	3	BMA	C1-C2-C3	2.35	112.55	109.67
2	M	3	BMA	O2-C2-C1	2.34	113.94	109.15
2	O	2	NAG	C3-C4-C5	2.34	114.41	110.24
2	M	2	NAG	O5-C5-C6	2.33	110.86	107.20
2	Q	2	NAG	O3-C3-C4	2.32	115.72	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	3	BMA	O3-C3-C2	2.32	114.44	109.99
2	K	4	MAN	C1-C2-C3	-2.32	106.82	109.67
3	P	2	NAG	O5-C5-C6	2.31	110.83	107.20
3	H	3	BMA	C6-C5-C4	2.30	118.40	113.00
2	Q	2	NAG	O5-C1-C2	-2.29	107.67	111.29
2	G	1	NAG	O5-C5-C4	2.26	116.33	110.83
4	N	3	BMA	O2-C2-C3	2.26	114.67	110.14
2	Q	3	BMA	C6-C5-C4	2.26	118.30	113.00
2	I	4	MAN	C1-O5-C5	2.26	115.25	112.19
2	M	2	NAG	C2-N2-C7	-2.25	119.70	122.90
3	R	5	MAN	C2-C3-C4	-2.25	107.00	110.89
2	G	2	NAG	C4-C3-C2	2.24	114.31	111.02
3	H	3	BMA	C3-C4-C5	2.23	114.21	110.24
2	J	4	MAN	O5-C5-C6	2.22	110.69	107.20
3	R	2	NAG	C3-C4-C5	2.22	114.20	110.24
2	L	4	MAN	C1-C2-C3	2.22	112.39	109.67
3	P	2	NAG	O4-C4-C5	2.21	114.78	109.30
2	M	3	BMA	C3-C4-C5	-2.20	106.31	110.24
4	N	3	BMA	O2-C2-C1	2.20	113.66	109.15
4	N	2	NAG	C3-C4-C5	2.18	114.12	110.24
3	R	3	BMA	O2-C2-C1	2.17	113.60	109.15
2	M	3	BMA	O2-C2-C3	2.14	114.43	110.14
2	K	3	BMA	O5-C5-C4	-2.10	105.73	110.83
2	G	2	NAG	C6-C5-C4	-2.09	108.11	113.00
2	Q	3	BMA	O3-C3-C4	2.08	115.17	110.35
2	L	1	NAG	C2-N2-C7	-2.08	119.94	122.90
2	I	3	BMA	O2-C2-C1	2.06	113.37	109.15
2	M	3	BMA	O5-C5-C4	-2.05	105.83	110.83
4	N	1	NAG	O5-C5-C6	2.04	110.41	107.20
2	M	4	MAN	C2-C3-C4	-2.02	107.39	110.89
2	I	3	BMA	C6-C5-C4	2.02	117.74	113.00
2	M	1	NAG	O5-C1-C2	2.02	114.47	111.29
2	K	2	NAG	O5-C1-C2	-2.02	108.11	111.29
2	K	1	NAG	O5-C5-C6	2.00	110.34	107.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	Q	1	NAG	C1

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C3-C2-N2-C7
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	R	2	NAG	C8-C7-N2-C2
3	R	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	J	3	BMA	O5-C5-C6-O6
2	J	4	MAN	O5-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
2	Q	3	BMA	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	C1-C2-N2-C7
3	R	5	MAN	C4-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
2	M	3	BMA	C4-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
2	J	4	MAN	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
2	O	4	MAN	O5-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
2	O	4	MAN	C4-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
4	N	2	NAG	O5-C5-C6-O6
2	I	3	BMA	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	Q	4	MAN	C4-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	R	5	MAN	O5-C5-C6-O6
3	R	3	BMA	C4-C5-C6-O6
2	Q	4	MAN	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	L	3	BMA	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	Q	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	M	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
3	R	1	NAG	C4-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
2	G	1	NAG	C1-C2-N2-C7
4	N	1	NAG	O7-C7-N2-C2
3	R	4	MAN	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	4	MAN	C1-C2-C3-C4-C5-O5
3	P	4	MAN	C1-C2-C3-C4-C5-O5
3	R	5	MAN	C1-C2-C3-C4-C5-O5
3	H	5	MAN	C1-C2-C3-C4-C5-O5
2	Q	4	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	5	MAN	2	0
2	L	3	BMA	1	0
2	G	1	NAG	1	0
2	K	2	NAG	2	0
2	G	3	BMA	1	0
3	H	2	NAG	1	0
2	L	1	NAG	1	0
2	M	2	NAG	1	0
3	R	1	NAG	4	0
4	N	2	NAG	1	0
2	J	3	BMA	2	0
4	N	1	NAG	2	0
3	R	2	NAG	4	0
3	P	2	NAG	1	0
3	H	5	MAN	1	0

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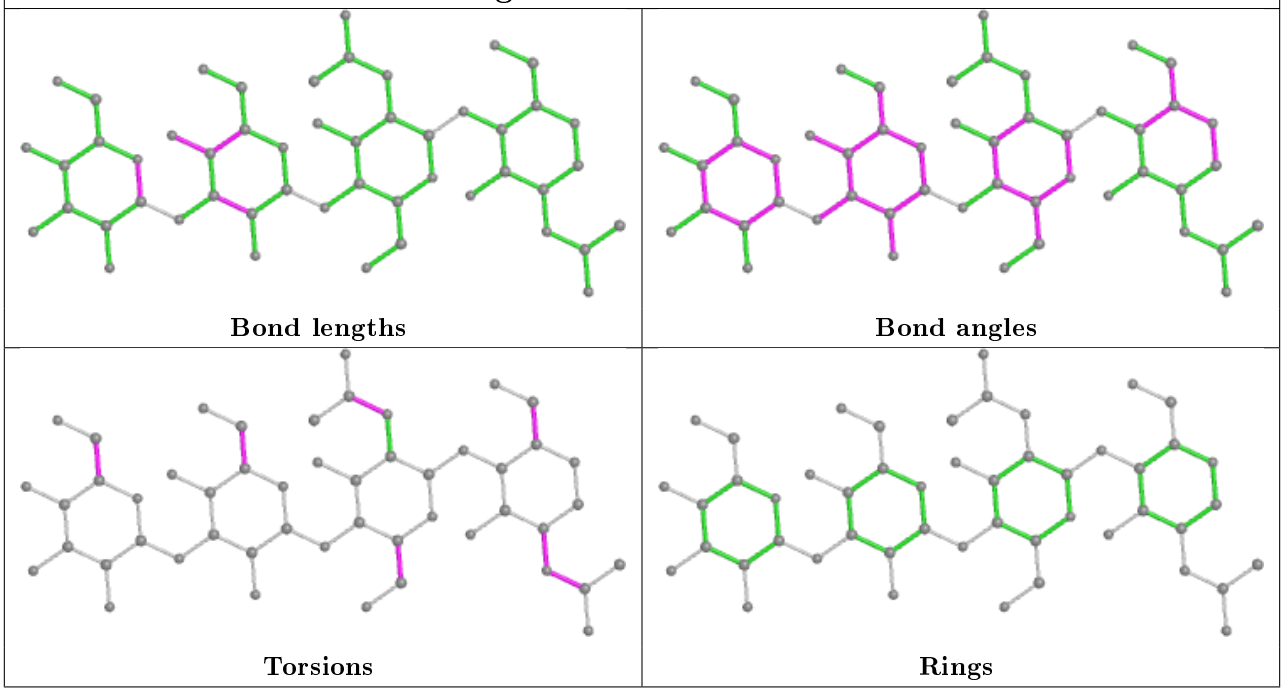
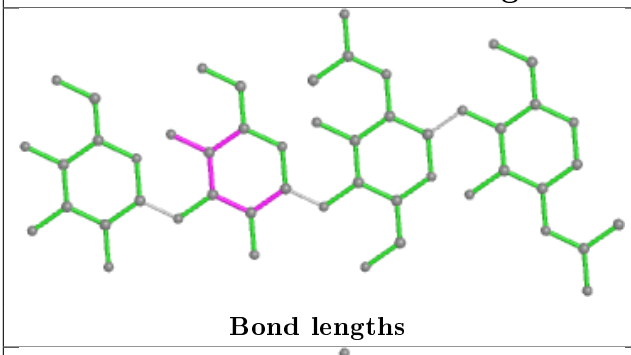
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	3	BMA	1	0
2	L	2	NAG	1	0
2	G	4	MAN	1	0
3	H	4	MAN	1	0
2	J	4	MAN	2	0
3	H	3	BMA	2	0
2	K	1	NAG	2	0

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

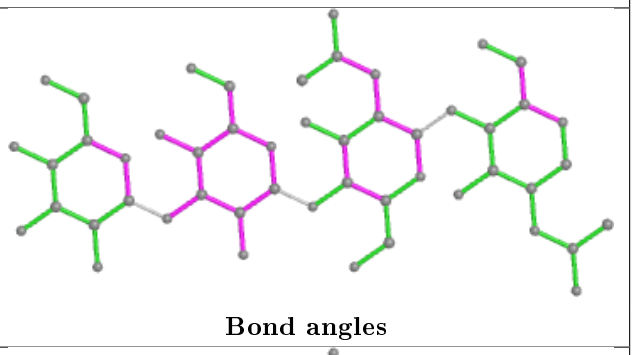
Oligosaccharide Chain G



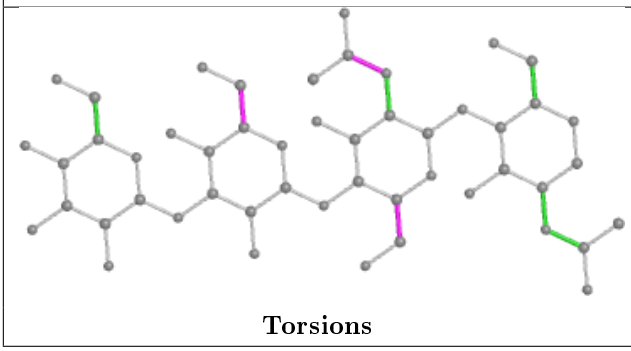
Oligosaccharide Chain I



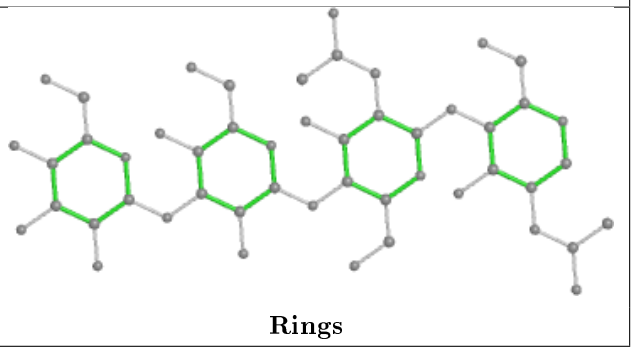
Bond lengths



Bond angles

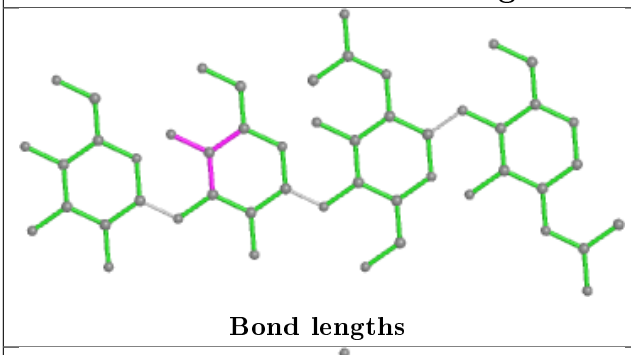


Torsions

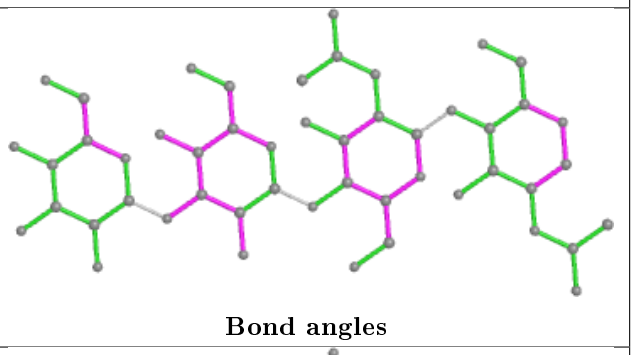


Rings

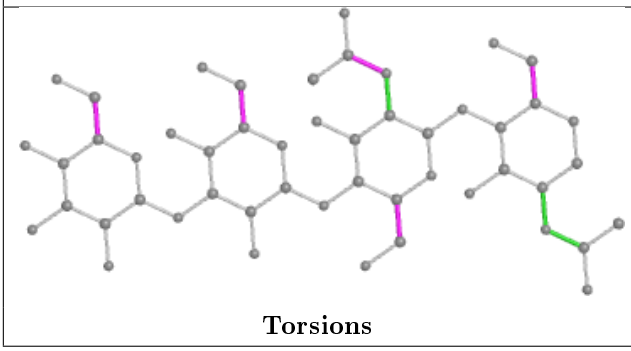
Oligosaccharide Chain J



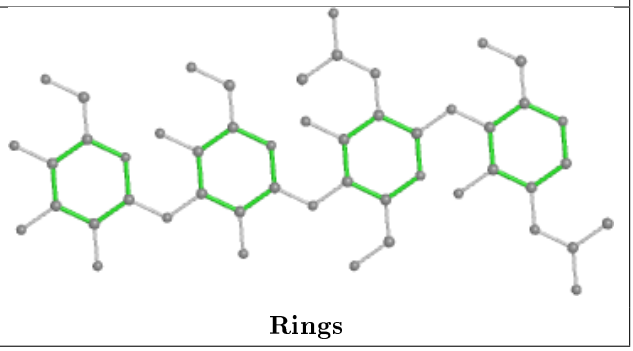
Bond lengths



Bond angles

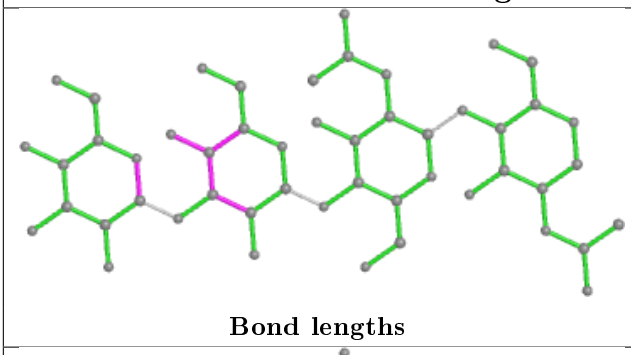


Torsions

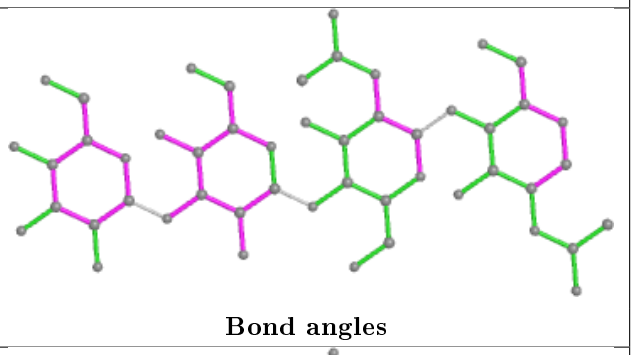


Rings

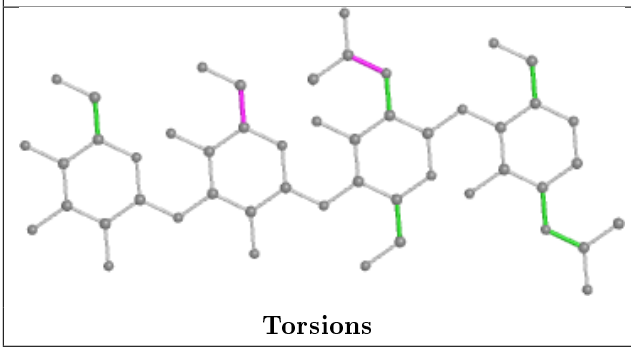
Oligosaccharide Chain K



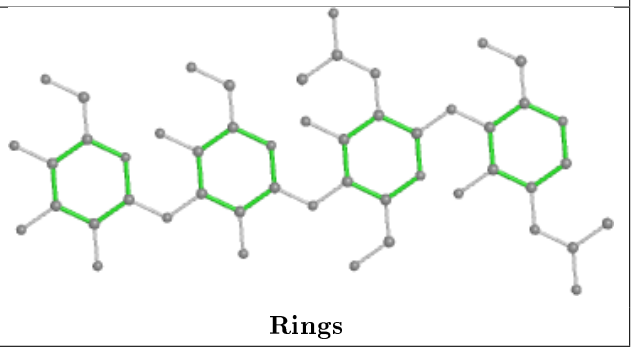
Bond lengths



Bond angles

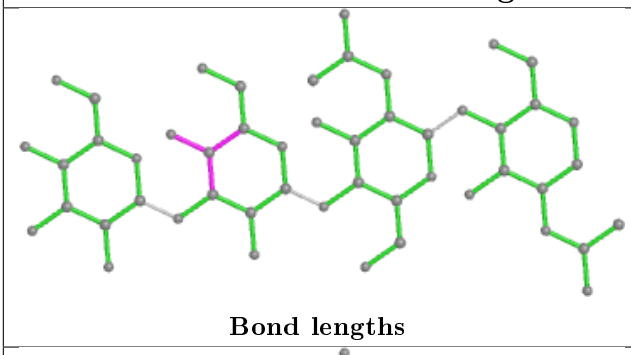


Torsions

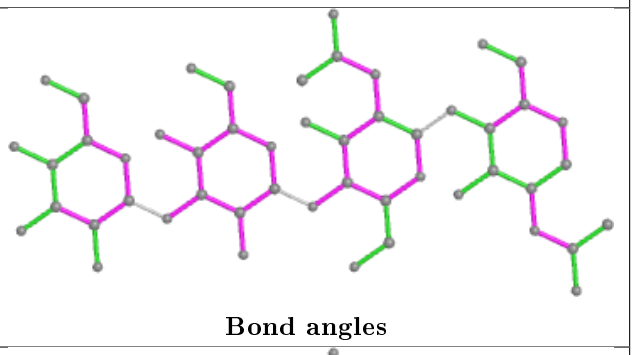


Rings

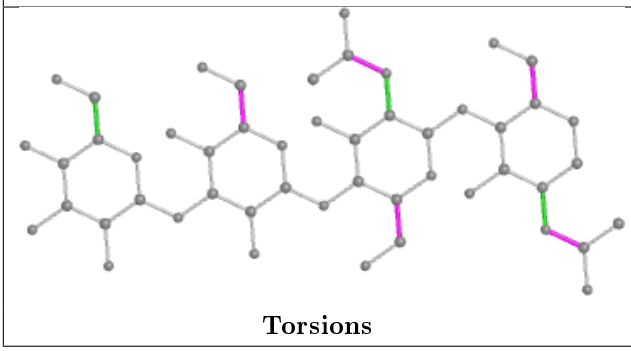
Oligosaccharide Chain L



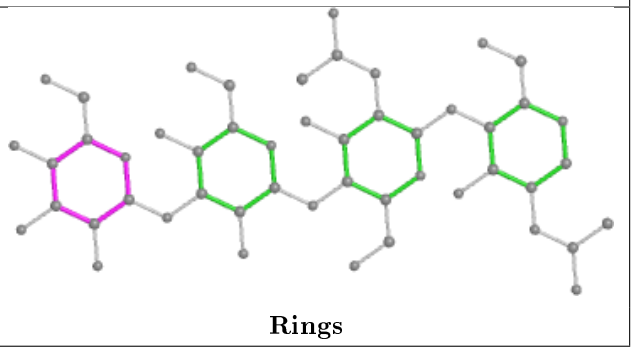
Bond lengths



Bond angles

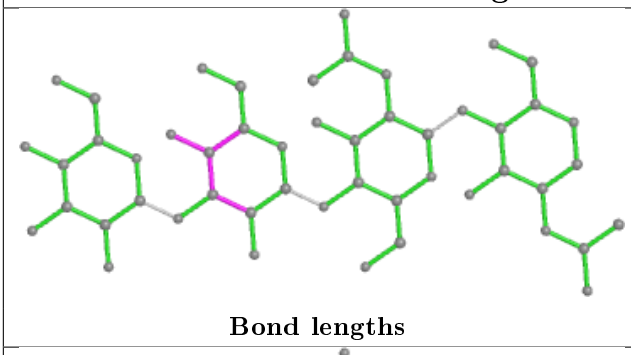


Torsions

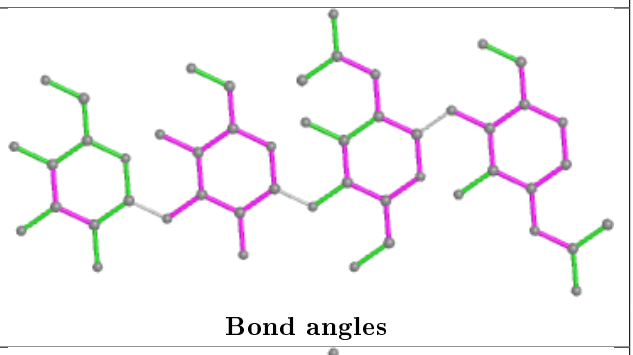


Rings

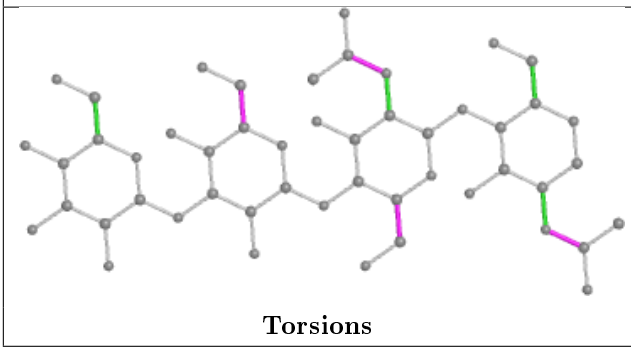
Oligosaccharide Chain M



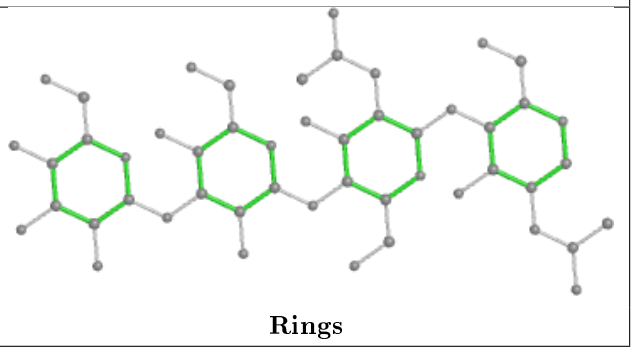
Bond lengths



Bond angles

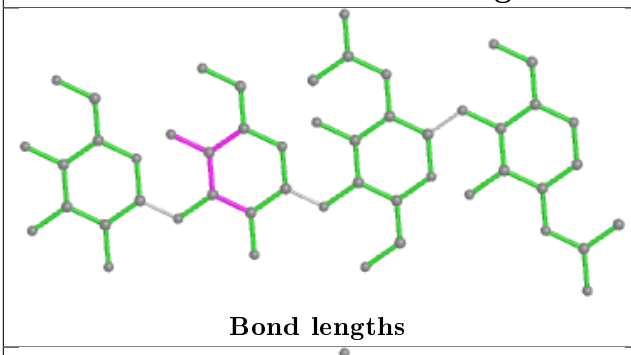


Torsions

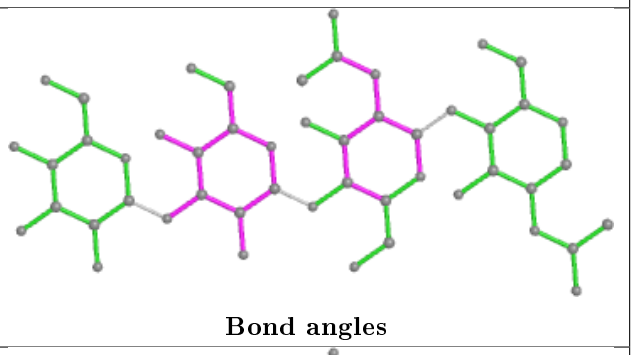


Rings

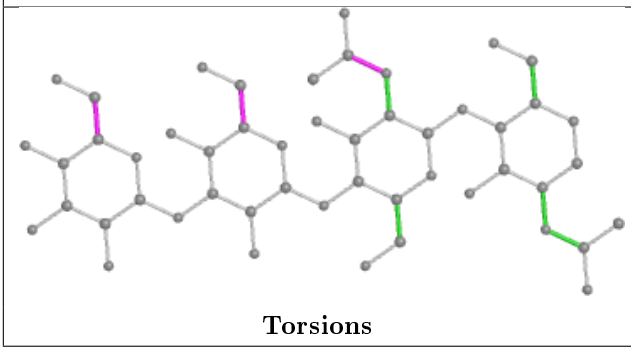
Oligosaccharide Chain O



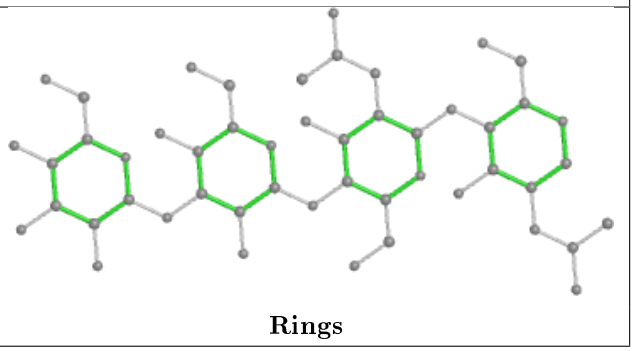
Bond lengths



Bond angles

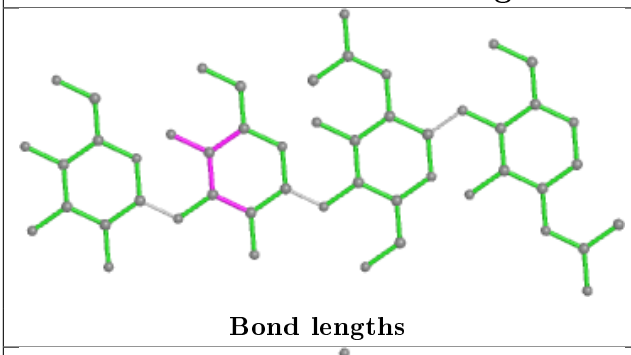


Torsions

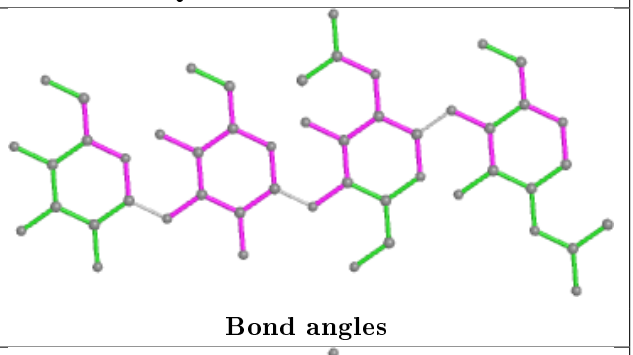


Rings

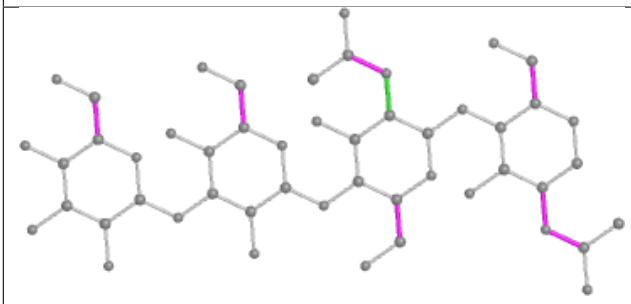
Oligosaccharide Chain Q



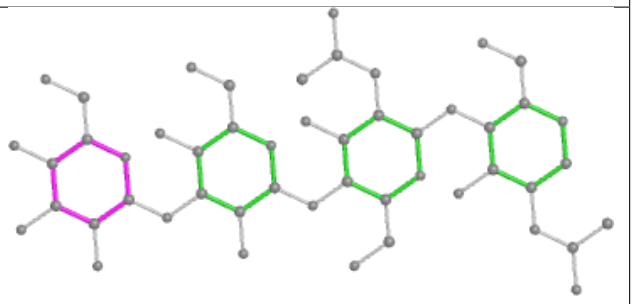
Bond lengths



Bond angles

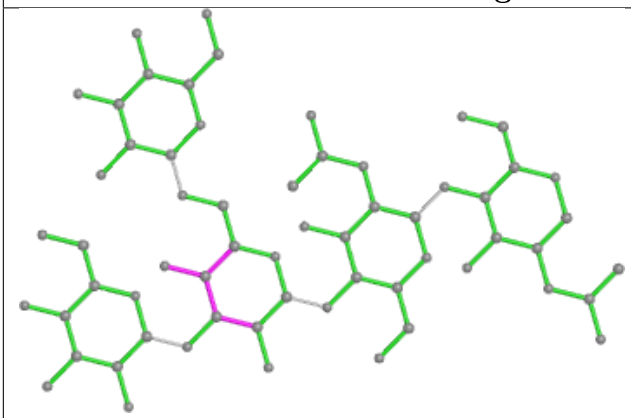


Torsions

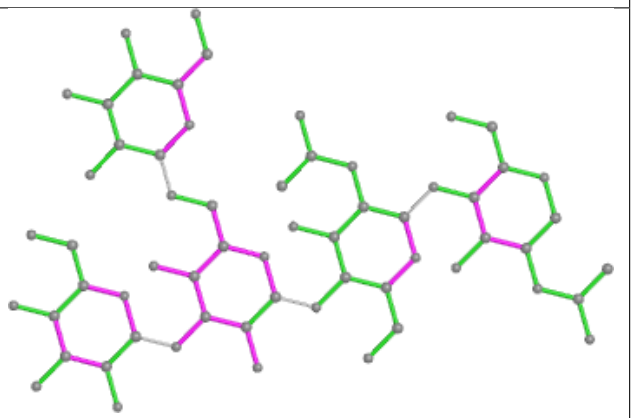


Rings

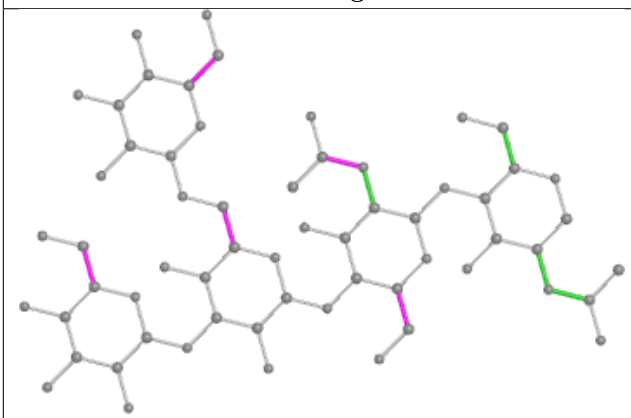
Oligosaccharide Chain H



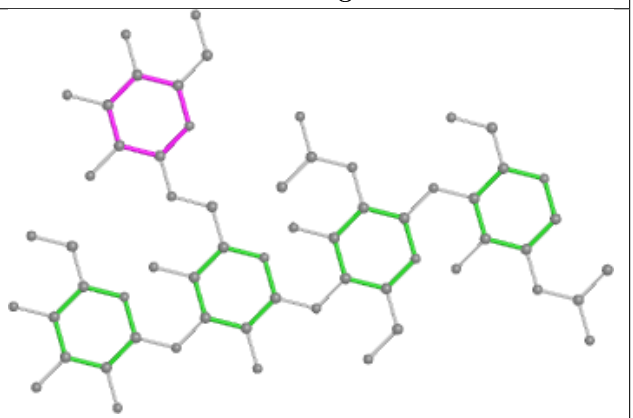
Bond lengths



Bond angles

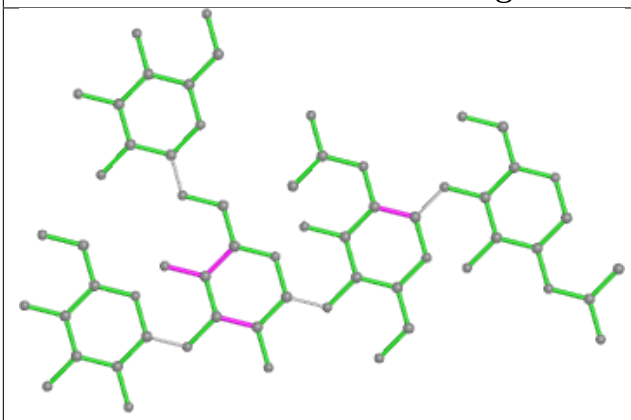


Torsions

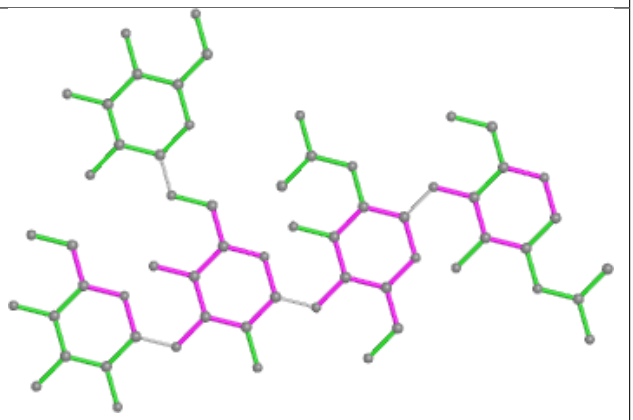


Rings

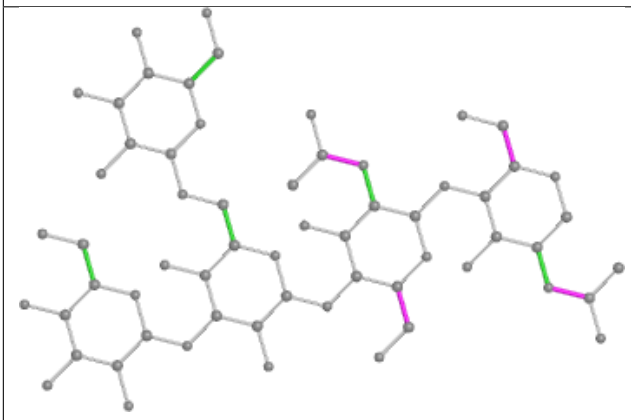
Oligosaccharide Chain P



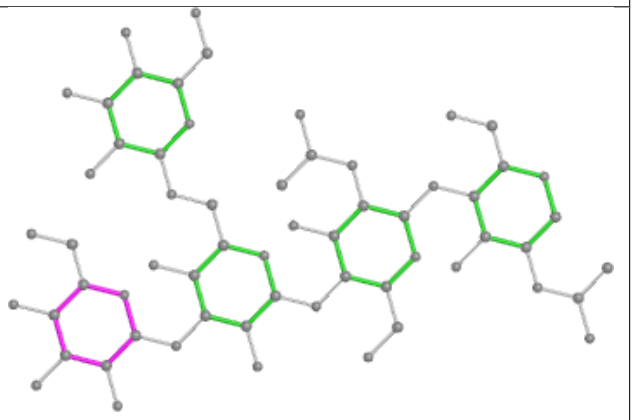
Bond lengths



Bond angles

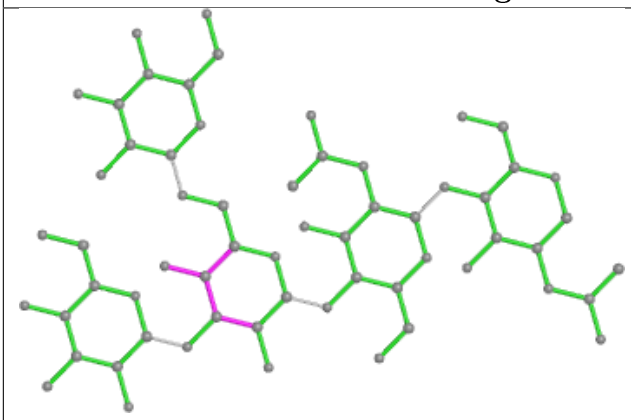


Torsions

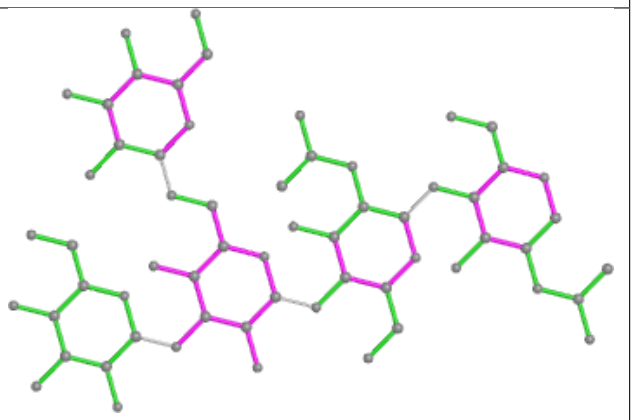


Rings

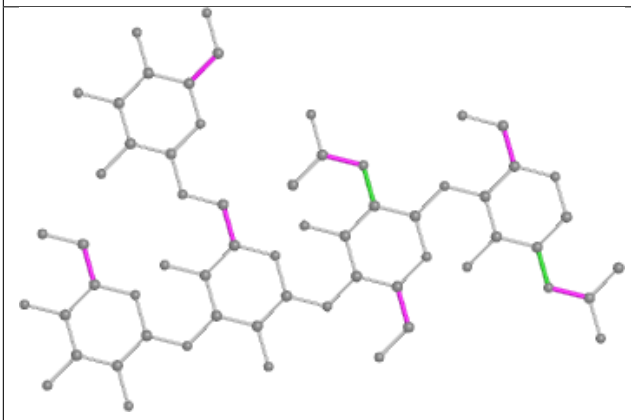
Oligosaccharide Chain R



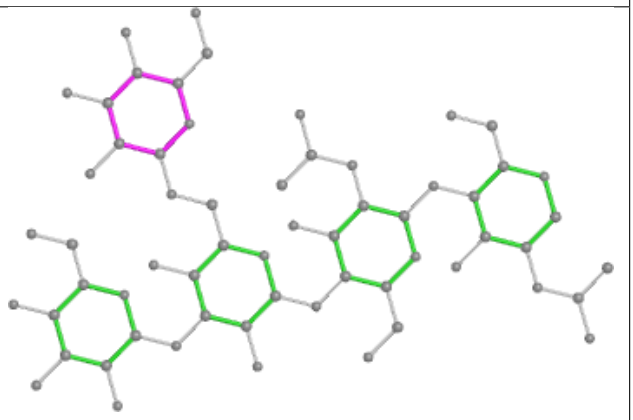
Bond lengths



Bond angles

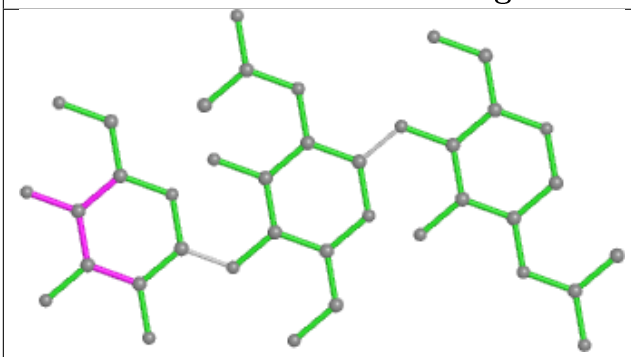


Torsions

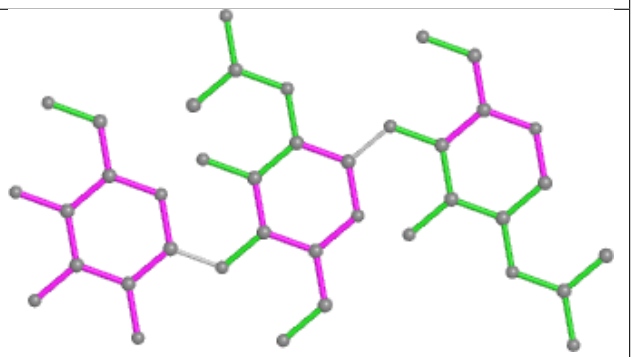


Rings

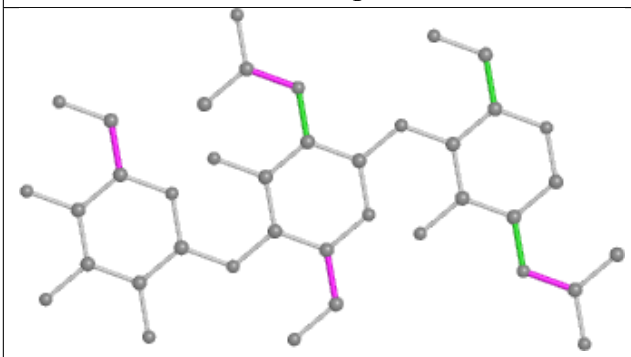
Oligosaccharide Chain N



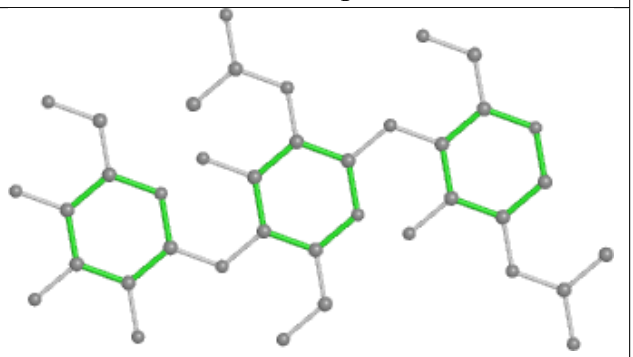
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	613/750 (81%)	0.69	60 (9%) 7 7	52, 123, 277, 384	0
1	B	612/750 (81%)	0.70	66 (10%) 5 5	53, 123, 278, 384	0
1	C	612/750 (81%)	0.69	61 (9%) 7 7	53, 123, 276, 384	0
1	D	612/750 (81%)	0.73	79 (12%) 3 3	52, 123, 275, 384	0
1	E	613/750 (81%)	0.67	72 (11%) 4 4	52, 123, 278, 384	0
1	F	608/750 (81%)	0.70	68 (11%) 5 5	52, 122, 277, 377	0
All	All	3670/4500 (81%)	0.69	406 (11%) 5 5	52, 123, 278, 384	0

All (406) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	706	VAL	13.3
1	C	705	HIS	13.2
1	D	706	VAL	13.1
1	B	720	SER	12.9
1	F	705	HIS	11.7
1	A	705	HIS	10.8
1	E	666	CYS	10.7
1	D	683	ASP	10.6
1	D	714	VAL	10.5
1	A	706	VAL	10.4
1	F	714	VAL	10.3
1	D	705	HIS	9.4
1	E	683	ASP	9.4
1	B	706	VAL	9.4
1	E	705	HIS	9.1
1	C	698	THR	8.9
1	C	686	GLY	8.5
1	A	736	CYS	8.3
1	E	449	TRP	8.1

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Mol	Chain	Res	Type	RSRZ
1	E	720	SER	8.0
1	F	704	VAL	7.7
1	A	704	VAL	7.6
1	F	449	TRP	7.6
1	C	689	PRO	7.4
1	C	696	THR	7.3
1	E	704	VAL	7.3
1	A	723	ALA	7.3
1	E	667	THR	7.1
1	B	705	HIS	7.0
1	C	704	VAL	7.0
1	D	686	GLY	6.9
1	D	655	LEU	6.7
1	C	736	CYS	6.6
1	B	714	VAL	6.5
1	F	71	GLN	6.5
1	B	725	PHE	6.5
1	D	723	ALA	6.4
1	B	719	ALA	6.3
1	B	669	SER	6.0
1	B	666	CYS	6.0
1	A	686	GLY	5.9
1	D	449	TRP	5.9
1	D	667	THR	5.9
1	F	723	ALA	5.9
1	D	724	ASN	5.9
1	A	667	THR	5.8
1	F	451	GLY	5.8
1	B	713	THR	5.7
1	E	71	GLN	5.7
1	A	727	VAL	5.7
1	D	659	VAL	5.7
1	B	712	VAL	5.5
1	D	704	VAL	5.5
1	A	725	PHE	5.5
1	B	727	VAL	5.4
1	D	727	VAL	5.4
1	F	667	THR	5.4
1	E	722	GLN	5.4
1	E	706	VAL	5.3
1	D	736	CYS	5.3
1	C	695	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	723	ALA	5.3
1	F	420	ILE	5.2
1	B	420	ILE	5.2
1	C	714	VAL	5.2
1	E	712	VAL	5.2
1	F	706	VAL	5.1
1	B	726	ILE	5.1
1	E	714	VAL	5.0
1	A	666	CYS	4.9
1	C	420	ILE	4.9
1	C	449	TRP	4.9
1	C	676	ALA	4.8
1	E	713	THR	4.8
1	A	740	CYS	4.7
1	E	716	PHE	4.7
1	E	658	THR	4.7
1	E	709	LYS	4.6
1	A	420	ILE	4.6
1	D	457	ASP	4.6
1	B	450	GLY	4.5
1	E	659	VAL	4.5
1	D	451	GLY	4.5
1	E	740	CYS	4.4
1	A	720	SER	4.4
1	B	686	GLY	4.4
1	F	713	THR	4.4
1	B	724	ASN	4.4
1	B	683	ASP	4.3
1	D	666	CYS	4.3
1	C	659	VAL	4.3
1	B	716	PHE	4.2
1	F	668	TYR	4.2
1	A	669	SER	4.2
1	C	71	GLN	4.2
1	F	676	ALA	4.2
1	C	671	ASP	4.2
1	C	101	LEU	4.2
1	C	720	SER	4.1
1	B	723	ALA	4.1
1	F	461	SER	4.1
1	A	726	ILE	4.1
1	B	696	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	720	SER	4.1
1	E	72	ASP	4.0
1	F	712	VAL	4.0
1	B	671	ASP	4.0
1	D	713	THR	4.0
1	C	717	SER	4.0
1	E	723	ALA	4.0
1	E	668	TYR	4.0
1	D	679	GLN	3.9
1	F	450	GLY	3.9
1	D	725	PHE	3.9
1	E	719	ALA	3.9
1	A	71	GLN	3.9
1	B	499	ASN	3.9
1	B	721	PRO	3.9
1	C	683	ASP	3.9
1	E	739	GLU	3.9
1	F	722	GLN	3.9
1	A	72	ASP	3.9
1	D	676	ALA	3.9
1	E	698	THR	3.8
1	F	731	GLY	3.8
1	F	689	PRO	3.8
1	D	586	ALA	3.8
1	B	668	TYR	3.8
1	E	724	ASN	3.8
1	C	72	ASP	3.7
1	F	673	GLY	3.7
1	A	56	SER	3.7
1	A	101	LEU	3.7
1	C	658	THR	3.6
1	F	432	ALA	3.6
1	D	712	VAL	3.6
1	E	717	SER	3.6
1	F	72	ASP	3.6
1	D	739	GLU	3.6
1	F	730	CYS	3.6
1	A	255	LEU	3.5
1	F	740	CYS	3.5
1	B	689	PRO	3.5
1	C	739	GLU	3.5
1	B	715	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	720	SER	3.5
1	D	716	PHE	3.5
1	A	457	ASP	3.5
1	F	696	THR	3.5
1	C	702	SER	3.5
1	B	447	PHE	3.4
1	E	255	LEU	3.4
1	F	426	LEU	3.4
1	D	671	ASP	3.4
1	A	95	SER	3.4
1	A	713	THR	3.4
1	C	699	LEU	3.4
1	F	425	SER	3.4
1	D	721	PRO	3.4
1	D	740	CYS	3.3
1	D	707	LEU	3.3
1	C	668	TYR	3.3
1	D	469	GLU	3.3
1	A	668	TYR	3.3
1	D	95	SER	3.3
1	C	740	CYS	3.3
1	C	721	PRO	3.3
1	A	447	PHE	3.3
1	E	432	ALA	3.3
1	C	408	THR	3.3
1	F	678	LEU	3.3
1	C	419	LYS	3.2
1	E	515	THR	3.2
1	C	679	GLN	3.2
1	E	457	ASP	3.2
1	F	586	ALA	3.2
1	E	113	VAL	3.2
1	A	421	LYS	3.2
1	D	432	ALA	3.2
1	F	736	CYS	3.2
1	F	725	PHE	3.1
1	B	739	GLU	3.1
1	E	119	ASN	3.1
1	C	661	CYS	3.1
1	F	698	THR	3.1
1	B	704	VAL	3.1
1	D	450	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	432	ALA	3.1
1	A	698	THR	3.1
1	A	714	VAL	3.1
1	D	726	ILE	3.1
1	D	729	LEU	3.1
1	B	83	ILE	3.0
1	C	724	ASN	3.0
1	D	69	LEU	3.0
1	D	722	GLN	3.0
1	C	731	GLY	3.0
1	E	75	VAL	3.0
1	F	367	VAL	3.0
1	B	419	LYS	3.0
1	F	96	TYR	3.0
1	C	655	LEU	3.0
1	B	426	LEU	2.9
1	F	659	VAL	2.9
1	B	72	ASP	2.9
1	F	31	ILE	2.9
1	D	515	THR	2.9
1	B	113	VAL	2.9
1	B	71	GLN	2.9
1	B	27	SER	2.8
1	B	461	SER	2.8
1	F	29	VAL	2.8
1	C	69	LEU	2.8
1	D	715	HIS	2.8
1	A	449	TRP	2.8
1	D	445	TYR	2.8
1	D	657	SER	2.8
1	F	719	ALA	2.8
1	C	666	CYS	2.8
1	E	673	GLY	2.8
1	A	113	VAL	2.8
1	B	70	LYS	2.8
1	D	97	LYS	2.8
1	E	418	PRO	2.8
1	F	575	ALA	2.8
1	E	727	VAL	2.8
1	F	360	GLY	2.8
1	B	29	VAL	2.8
1	E	669	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	575	ALA	2.7
1	A	504	LEU	2.7
1	B	101	LEU	2.7
1	B	45	ILE	2.7
1	F	95	SER	2.7
1	F	26	PHE	2.7
1	B	462	GLN	2.7
1	C	725	PHE	2.7
1	E	736	CYS	2.7
1	B	649	ARG	2.7
1	C	450	GLY	2.7
1	B	698	THR	2.7
1	D	493	LEU	2.7
1	A	739	GLU	2.7
1	B	728	SER	2.7
1	C	713	THR	2.7
1	F	97	LYS	2.7
1	D	29	VAL	2.7
1	D	113	VAL	2.7
1	C	591	VAL	2.6
1	C	563	ILE	2.6
1	D	640	ILE	2.6
1	B	367	VAL	2.6
1	C	422	CYS	2.6
1	E	721	PRO	2.6
1	E	679	GLN	2.6
1	C	283	ILE	2.6
1	B	737	ASN	2.6
1	D	734	THR	2.6
1	B	451	GLY	2.6
1	F	739	GLU	2.6
1	F	119	ASN	2.6
1	D	656	VAL	2.6
1	D	735	THR	2.6
1	A	455	PHE	2.6
1	F	636	ILE	2.6
1	C	367	VAL	2.6
1	F	27	SER	2.5
1	E	674	GLY	2.5
1	F	457	ASP	2.5
1	E	672	PHE	2.5
1	D	678	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	724	ASN	2.5
1	D	388	ASN	2.5
1	C	407	ILE	2.5
1	A	96	TYR	2.5
1	B	703	THR	2.5
1	D	695	SER	2.5
1	A	97	LYS	2.5
1	A	734	THR	2.5
1	E	493	LEU	2.5
1	A	31	ILE	2.5
1	B	718	THR	2.5
1	E	661	CYS	2.5
1	F	388	ASN	2.4
1	A	388	ASN	2.4
1	E	419	LYS	2.4
1	E	450	GLY	2.4
1	A	737	ASN	2.4
1	D	660	LYS	2.4
1	F	69	LEU	2.4
1	F	671	ASP	2.4
1	E	431	ALA	2.4
1	D	731	GLY	2.4
1	C	672	PHE	2.4
1	D	668	TYR	2.4
1	F	75	VAL	2.4
1	A	733	LYS	2.4
1	D	647	PHE	2.4
1	E	689	PRO	2.4
1	E	671	ASP	2.4
1	F	464	SER	2.4
1	A	712	VAL	2.4
1	B	418	PRO	2.4
1	A	683	ASP	2.4
1	A	716	PHE	2.4
1	F	10	SER	2.4
1	B	7	THR	2.4
1	D	83	ILE	2.4
1	E	408	THR	2.4
1	D	565	ALA	2.3
1	D	129	LYS	2.3
1	A	450	GLY	2.3
1	B	457	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	452	ALA	2.3
1	E	45	ILE	2.3
1	E	407	ILE	2.3
1	E	678	LEU	2.3
1	B	679	GLN	2.3
1	D	71	GLN	2.3
1	D	696	THR	2.3
1	F	726	ILE	2.3
1	A	418	PRO	2.3
1	D	75	VAL	2.3
1	E	447	PHE	2.3
1	D	698	THR	2.3
1	B	722	GLN	2.3
1	F	419	LYS	2.3
1	B	693	HIS	2.3
1	C	678	LEU	2.3
1	C	680	TYR	2.3
1	A	367	VAL	2.3
1	B	495	ILE	2.3
1	A	586	ALA	2.3
1	F	418	PRO	2.3
1	E	10	SER	2.3
1	B	515	THR	2.3
1	E	464	SER	2.3
1	B	736	CYS	2.3
1	D	328	TYR	2.3
1	E	97	LYS	2.3
1	E	665	GLU	2.3
1	A	678	LEU	2.3
1	D	101	LEU	2.3
1	A	674	GLY	2.2
1	D	72	ASP	2.2
1	C	421	LYS	2.2
1	D	7	THR	2.2
1	E	686	GLY	2.2
1	C	94	LEU	2.2
1	E	49	ALA	2.2
1	F	716	PHE	2.2
1	B	95	SER	2.2
1	A	722	GLN	2.2
1	E	101	LEU	2.2
1	F	733	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	680	TYR	2.2
1	D	658	THR	2.2
1	A	78	GLY	2.2
1	A	26	PHE	2.2
1	B	469	GLU	2.1
1	C	113	VAL	2.1
1	B	119	ASN	2.1
1	F	729	LEU	2.1
1	F	703	THR	2.1
1	C	700	GLN	2.1
1	D	636	ILE	2.1
1	E	623	VAL	2.1
1	C	457	ASP	2.1
1	D	111	VAL	2.1
1	E	415	VAL	2.1
1	F	495	ILE	2.1
1	A	445	TYR	2.1
1	D	26	PHE	2.1
1	F	653	ALA	2.1
1	D	8	LEU	2.1
1	C	565	ALA	2.1
1	E	711	ALA	2.1
1	A	636	ILE	2.1
1	C	29	VAL	2.1
1	E	681	VAL	2.1
1	A	426	LEU	2.1
1	B	628	ALA	2.1
1	D	391	ILE	2.1
1	E	283	ILE	2.1
1	F	686	GLY	2.1
1	C	95	SER	2.1
1	D	526	ILE	2.1
1	E	657	SER	2.1
1	F	113	VAL	2.1
1	A	642	ILE	2.1
1	B	731	GLY	2.1
1	E	47	THR	2.1
1	C	712	VAL	2.1
1	A	703	THR	2.0
1	D	420	ILE	2.0
1	E	655	LEU	2.0
1	F	283	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	657	SER	2.0
1	B	729	LEU	2.0
1	D	717	SER	2.0
1	C	431	ALA	2.0
1	F	328	TYR	2.0
1	E	499	ASN	2.0
1	C	623	VAL	2.0
1	D	27	SER	2.0
1	E	69	LEU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	R	5	11/12	0.44	0.30	209,236,246,247	0
2	BMA	L	3	11/12	0.51	0.22	138,178,231,243	0
3	NAG	H	2	14/15	0.60	0.26	218,228,238,243	0
2	MAN	J	4	11/12	0.61	0.35	244,259,266,268	0
3	BMA	H	3	11/12	0.61	0.23	194,229,252,253	0
3	MAN	H	4	11/12	0.62	0.48	176,202,226,228	0
3	MAN	H	5	11/12	0.65	0.31	174,195,201,207	0
2	NAG	L	2	14/15	0.66	0.24	218,236,246,251	0
2	MAN	G	4	11/12	0.68	0.31	225,228,240,247	0
2	MAN	L	4	11/12	0.68	0.21	248,250,254,260	0
3	BMA	P	3	11/12	0.70	0.17	195,214,225,225	0
3	MAN	P	5	11/12	0.71	0.25	193,208,213,216	0
2	MAN	I	4	11/12	0.72	0.61	164,189,195,195	0
3	MAN	R	4	11/12	0.75	0.29	241,253,263,265	0
2	NAG	J	2	14/15	0.75	0.20	165,190,204,219	0
2	MAN	K	4	11/12	0.77	0.32	177,187,197,202	0
4	BMA	N	3	11/12	0.77	0.21	176,193,202,203	0
3	NAG	R	2	14/15	0.78	0.16	199,205,211,212	0
3	BMA	R	3	11/12	0.79	0.16	195,209,234,236	0

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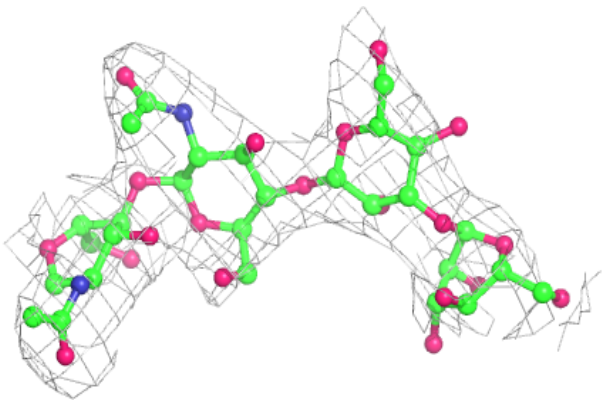
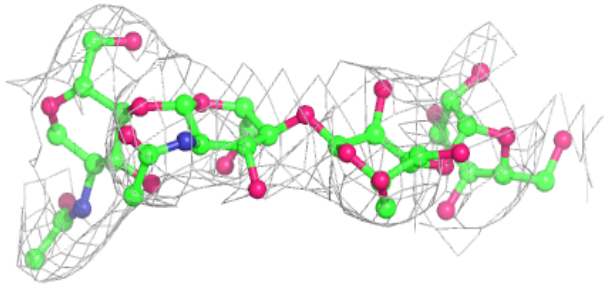
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	P	1	14/15	0.79	0.22	144,163,174,188	0
2	BMA	J	3	11/12	0.80	0.17	234,243,255,256	0
2	BMA	M	3	11/12	0.80	0.23	176,190,223,224	0
2	BMA	I	3	11/12	0.81	0.21	185,193,201,201	0
3	NAG	P	2	14/15	0.81	0.18	189,205,217,222	0
2	BMA	Q	3	11/12	0.82	0.20	137,172,188,193	0
2	MAN	M	4	11/12	0.82	0.40	176,185,193,194	0
2	NAG	G	2	14/15	0.83	0.23	113,136,144,151	0
2	BMA	O	3	11/12	0.83	0.14	173,180,196,200	0
2	NAG	K	2	14/15	0.83	0.32	124,164,186,188	0
2	NAG	L	1	14/15	0.84	0.16	127,150,176,205	0
4	NAG	N	2	14/15	0.84	0.19	184,194,201,202	0
3	MAN	P	4	11/12	0.84	0.28	114,174,187,188	0
2	NAG	I	2	14/15	0.85	0.24	113,130,175,175	0
2	NAG	J	1	14/15	0.85	0.20	144,161,170,183	0
2	MAN	Q	4	11/12	0.85	0.20	185,192,197,199	0
4	NAG	N	1	14/15	0.85	0.18	154,177,186,194	0
2	NAG	Q	2	14/15	0.86	0.25	98,134,160,166	0
2	NAG	M	2	14/15	0.87	0.25	110,131,162,178	0
3	NAG	R	1	14/15	0.87	0.17	129,152,172,190	0
2	BMA	G	3	11/12	0.87	0.22	165,169,197,213	0
2	BMA	K	3	11/12	0.88	0.12	159,180,190,193	0
2	NAG	Q	1	14/15	0.88	0.18	78,105,124,134	0
2	MAN	O	4	11/12	0.88	0.51	191,196,204,207	0
3	NAG	H	1	14/15	0.90	0.20	138,164,178,204	0
2	NAG	G	1	14/15	0.91	0.16	77,100,126,131	0
2	NAG	O	1	14/15	0.91	0.14	93,108,125,132	0
2	NAG	K	1	14/15	0.91	0.18	92,108,127,134	0
2	NAG	I	1	14/15	0.92	0.19	91,98,122,133	0
2	NAG	M	1	14/15	0.93	0.18	92,103,130,136	0
2	NAG	O	2	14/15	0.93	0.18	113,124,164,165	0

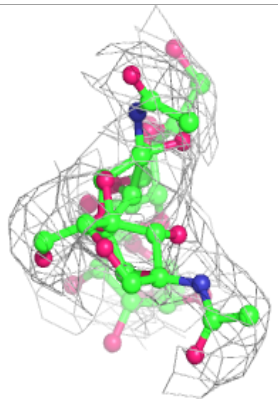
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

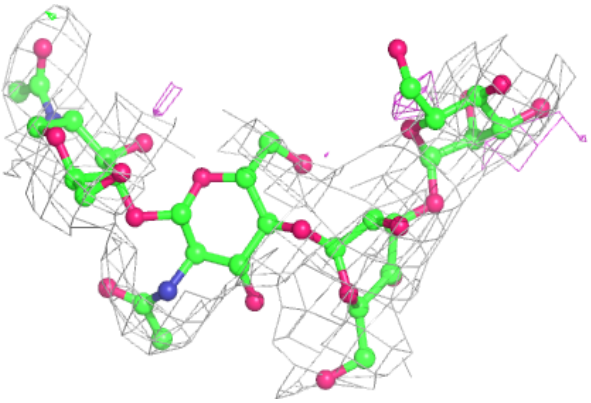


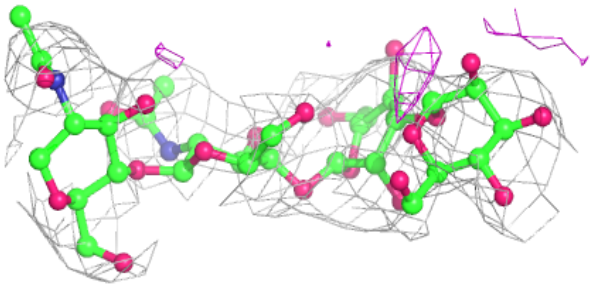


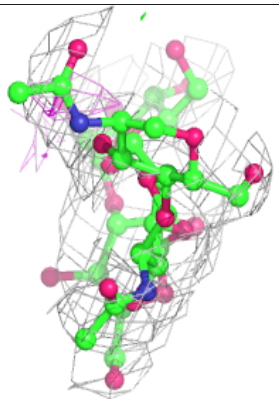


Electron density around Chain I:

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

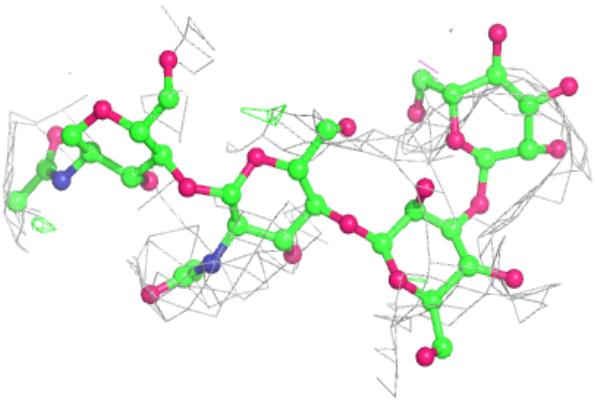


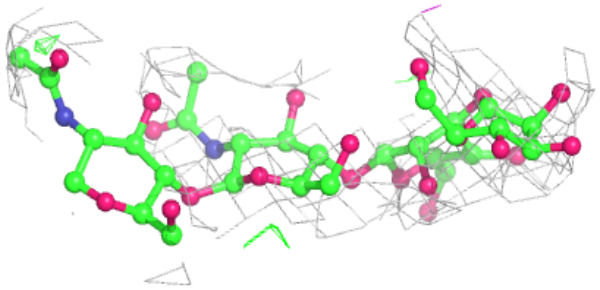


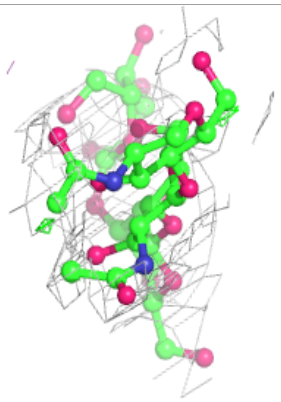


Electron density around Chain J:

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

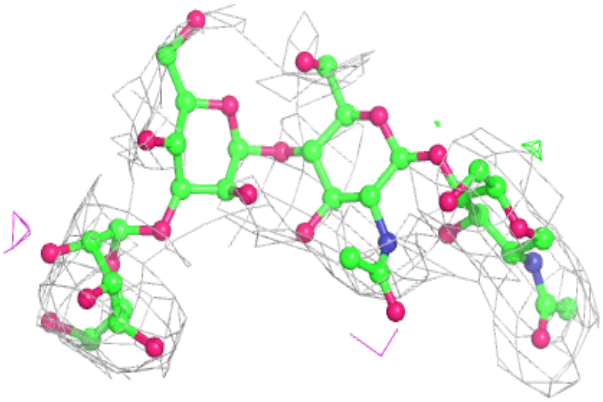


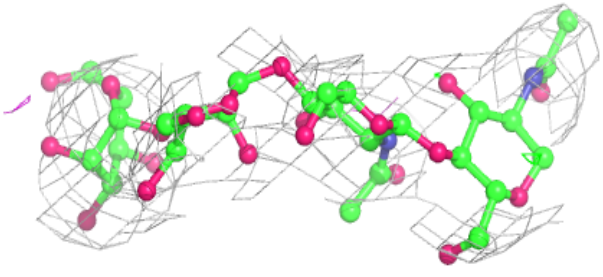


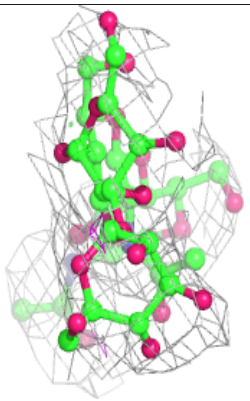


Electron density around Chain K:

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

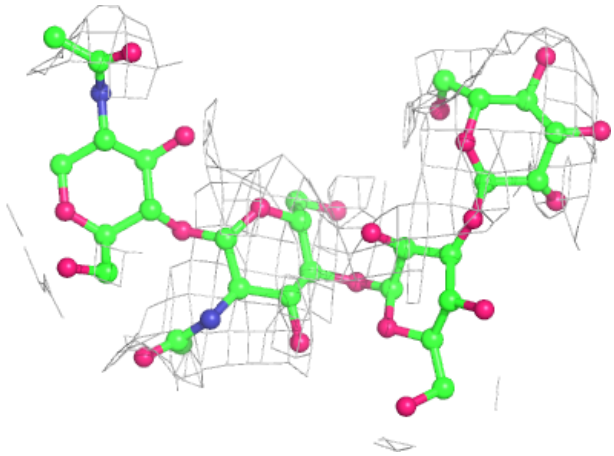


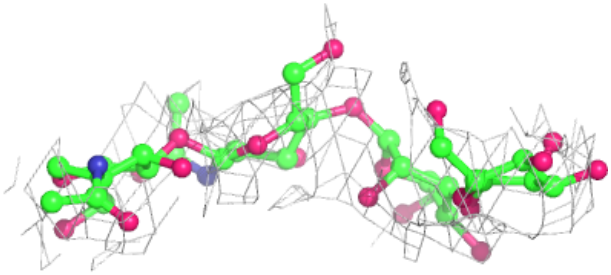


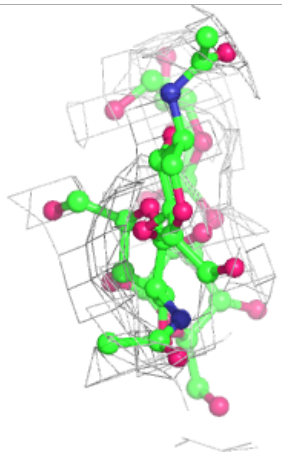


Electron density around Chain L:

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

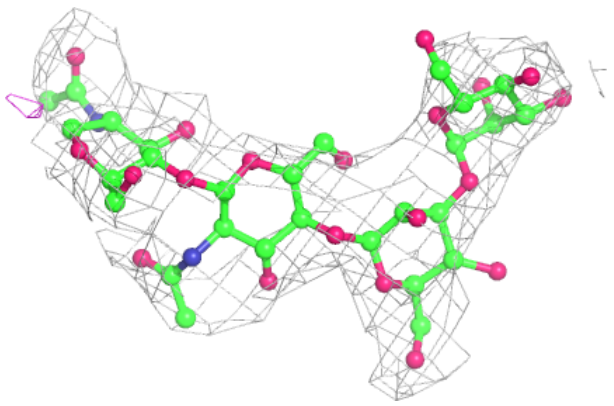


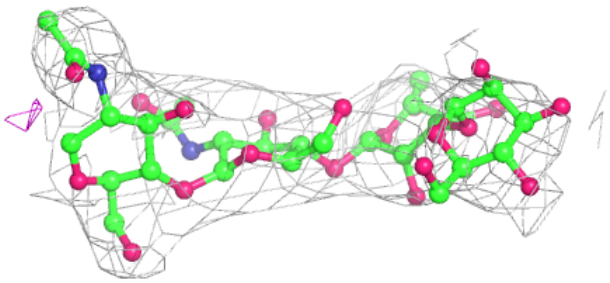


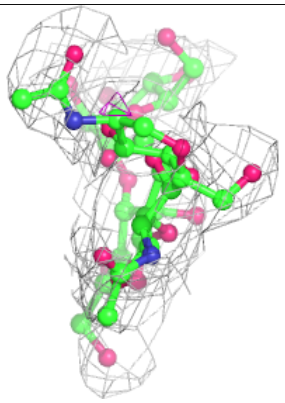


Electron density around Chain M:

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

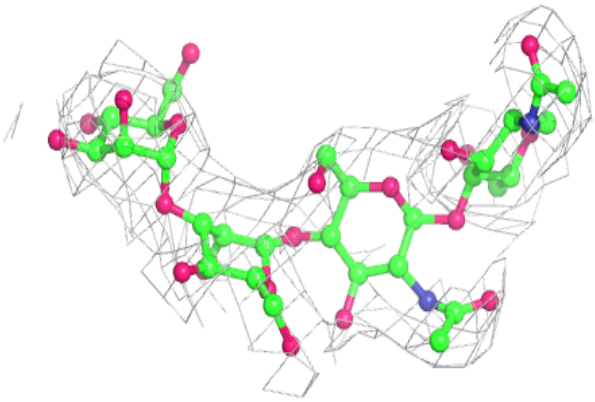


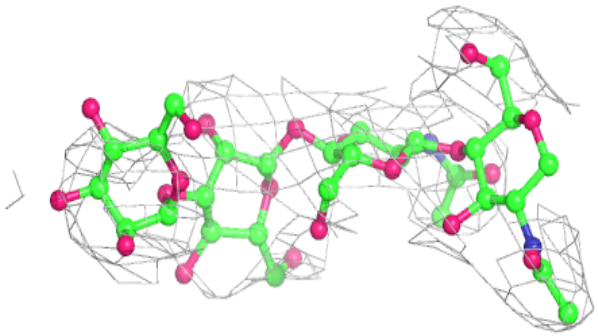


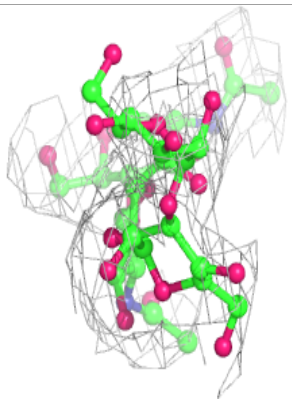


Electron density around Chain O:

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

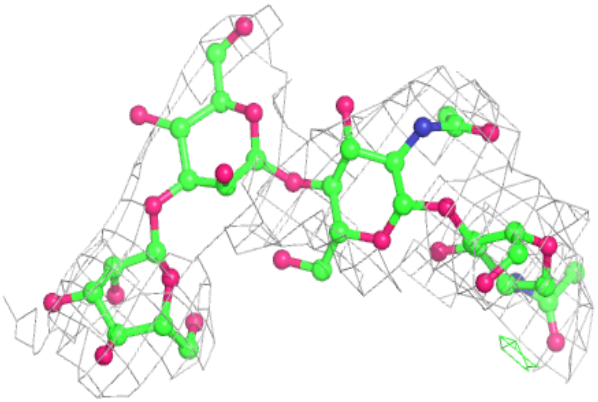


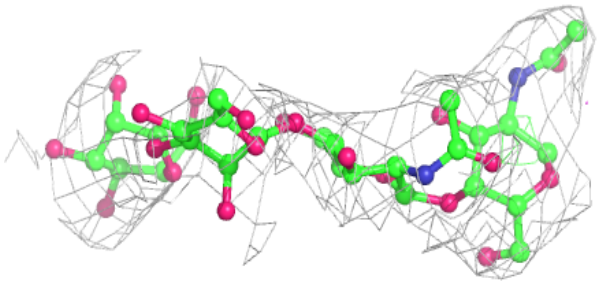


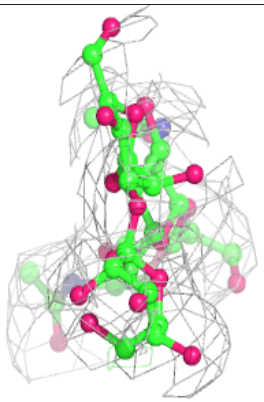


Electron density around Chain Q:

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

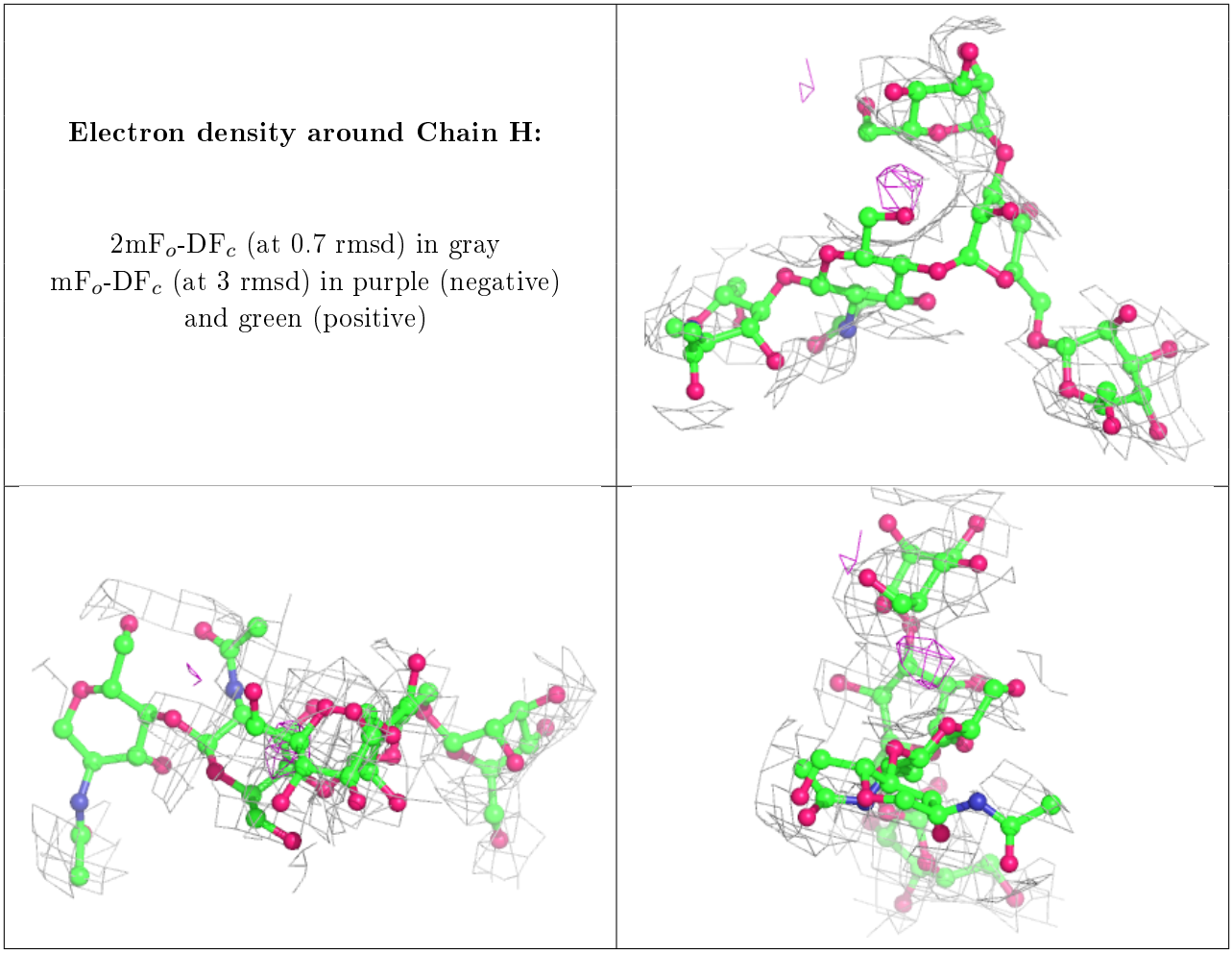






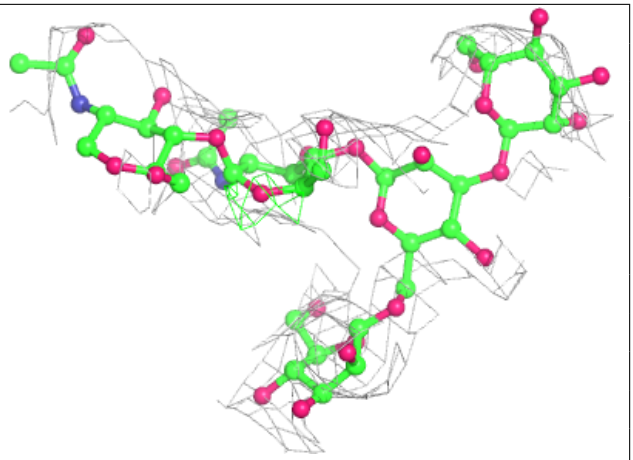
Electron density around Chain H:

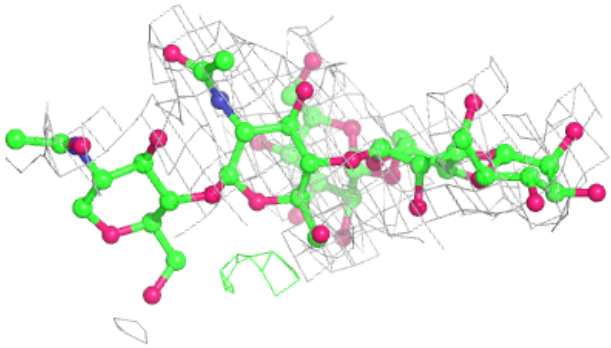
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

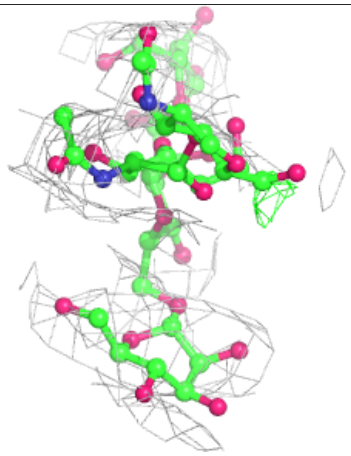


Electron density around Chain P:

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

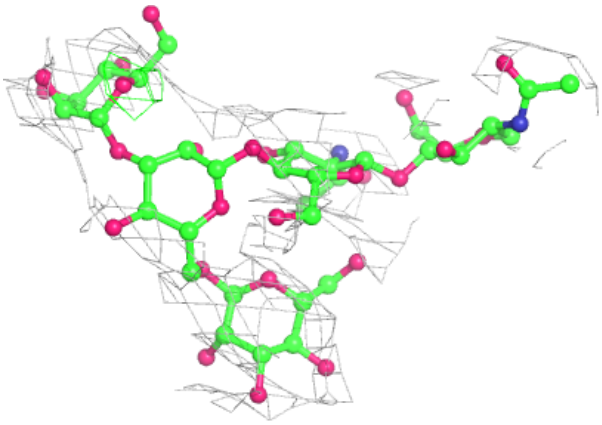


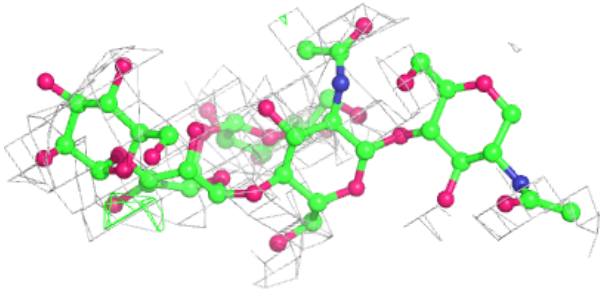


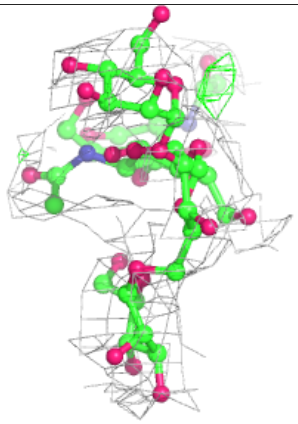


Electron density around Chain R:

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

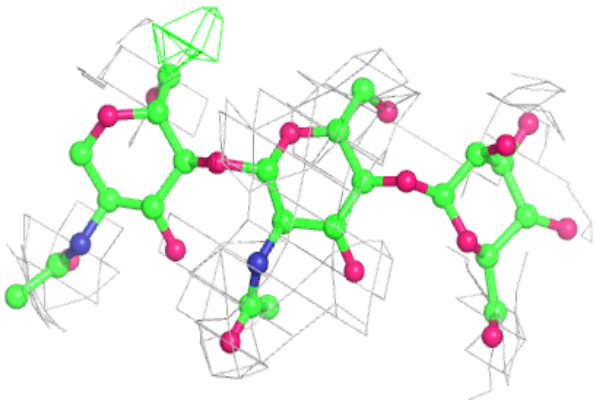


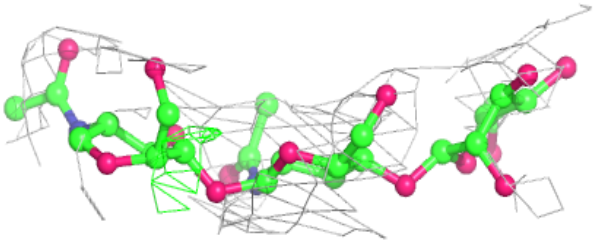


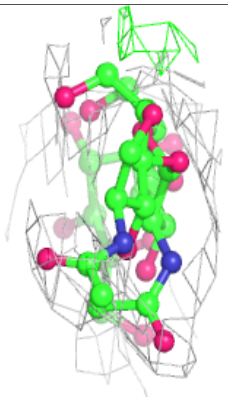


Electron density around Chain N:

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







6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.