Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:30 PM BST

PDB ID	:	3KQ4
Title	:	Structure of Intrinsic Factor-Cobalamin bound to its receptor Cubilin
Authors	:	Andersen, C.B.F.; Madsen, M.; Moestrup, S.K.; Andersen, G.R.
Deposited on	:	2009-11-17
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

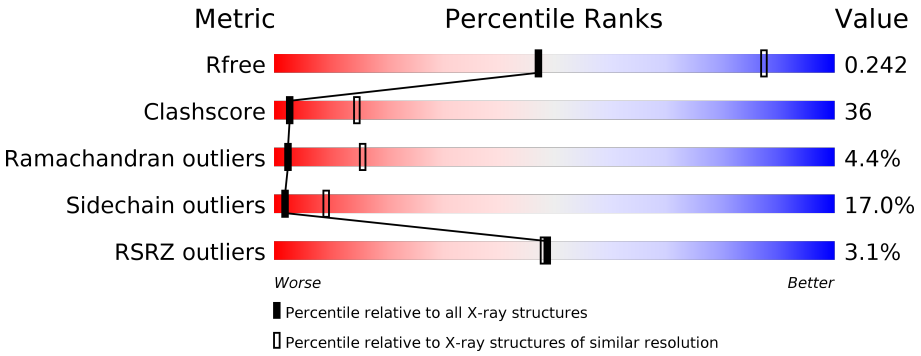
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.30 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	393	2% 53% 35% 10%
1	C	393	% 54% 34% 9%
1	E	393	2% 54% 34% 10%
2	B	457	5% 38% 48% 13%
2	D	457	4% 38% 48% 13%
2	F	457	5% 37% 49% 13%

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Mol	Chain	Length	Quality of chain
3	G	5	60% 40%
3	H	5	20% 80%
3	J	5	60% 40%
3	K	5	20% 80%
3	M	5	60% 40%
3	N	5	20% 80%
4	I	2	100%
4	L	2	100%
4	O	2	100%

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
5	NAG	A	2001	X	-	X	-
5	NAG	B	2001	X	-	-	-
5	NAG	B	2008	X	-	-	-
5	NAG	B	2009	-	-	-	X
5	NAG	C	2001	X	-	X	-
5	NAG	D	2001	X	-	-	-
5	NAG	D	2008	X	-	-	-
5	NAG	D	2009	-	-	-	X
5	NAG	E	2001	X	-	X	-
5	NAG	F	2001	X	-	-	-
5	NAG	F	2008	X	-	-	-
6	B12	A	2007	X	-	X	-
6	B12	C	2007	X	-	X	-
6	B12	E	2007	X	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20793 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 Gastric intrinsic factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	3	0	0
			2950	1870	488	573	19			
1	C	385	Total	C	N	O	S	3	0	0
			2950	1870	488	573	19			
1	E	385	Total	C	N	O	S	3	0	0
			2950	1870	488	573	19			

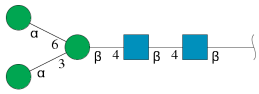
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	HIS	GLN	SEE REMARK 999	UNP P27352
C	91	HIS	GLN	SEE REMARK 999	UNP P27352
E	91	HIS	GLN	SEE REMARK 999	UNP P27352

- Molecule 2 is a protein called Cubilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	457	Total	C	N	O	S	0	0	0
			3638	2311	598	709	20			
2	D	457	Total	C	N	O	S	0	0	0
			3638	2311	598	709	20			
2	F	457	Total	C	N	O	S	0	0	0
			3638	2311	598	709	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.

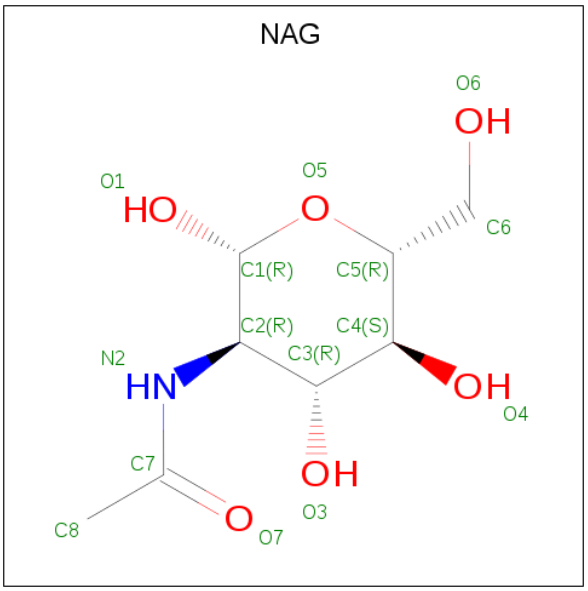


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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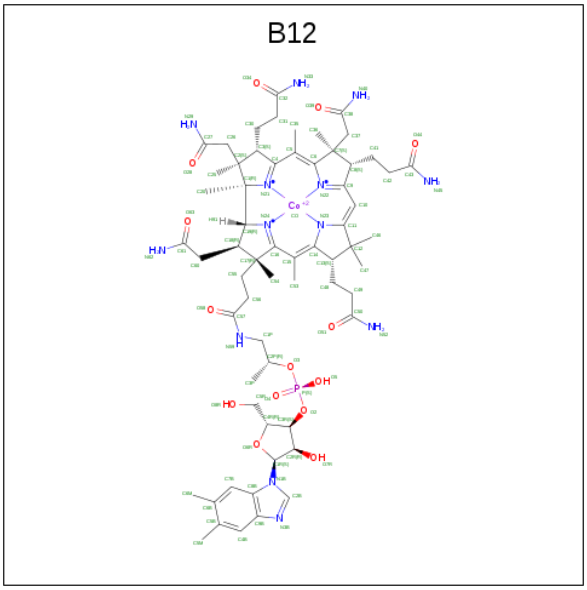
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Co N O P 91 62 1 13 14 1	0	0
6	C	1	Total C Co N O P 91 62 1 13 14 1	0	0
6	E	1	Total C Co N O P 91 62 1 13 14 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

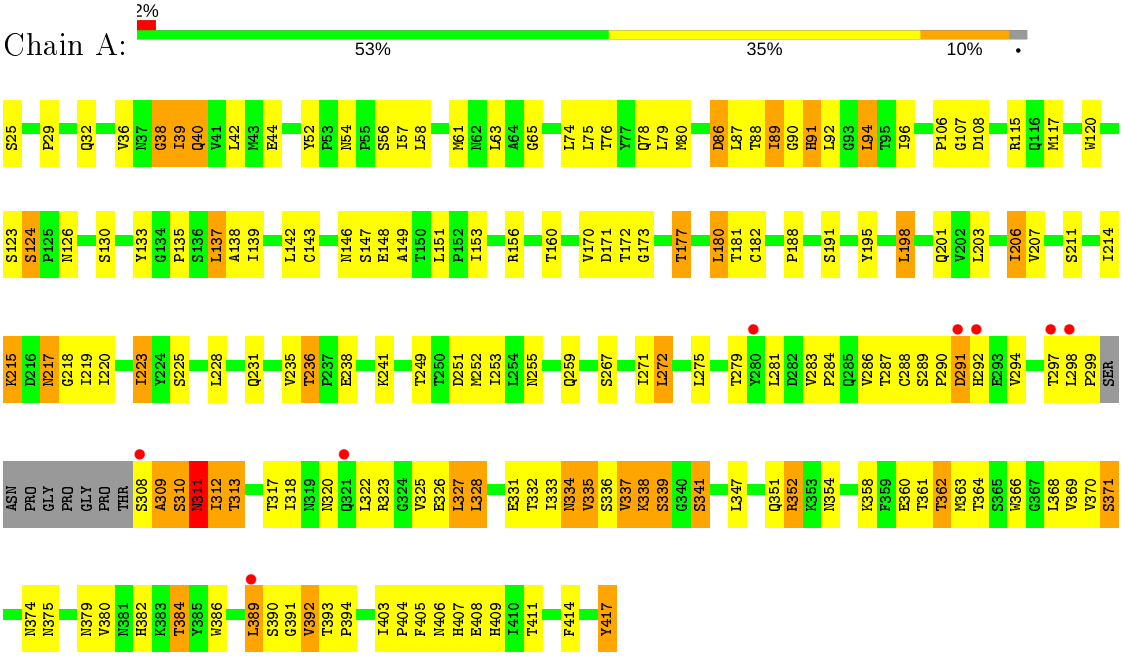
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	4	Total Ca 4 4	0	0
7	D	4	Total Ca 4 4	0	0
7	F	4	Total Ca 4 4	0	0

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.

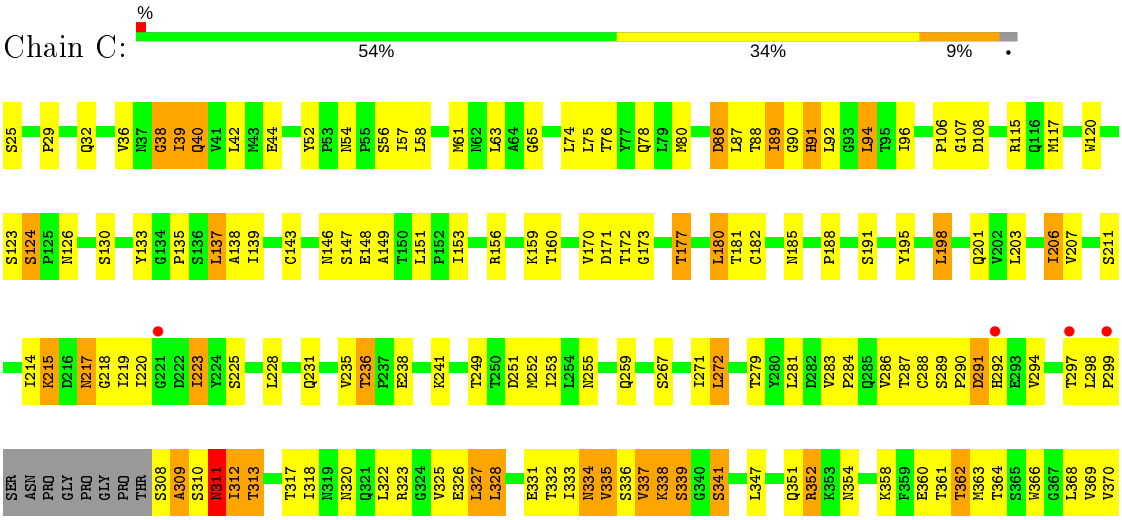
- Molecule 1: Gastric intrinsic factor

Chain A:



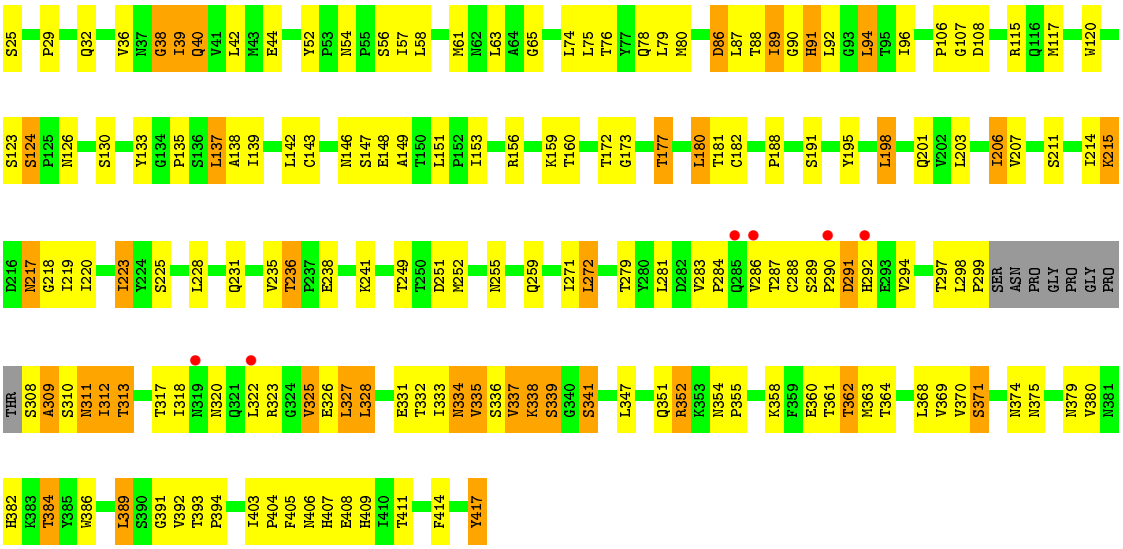
- Molecule 1: Gastric intrinsic factor

Chain C:



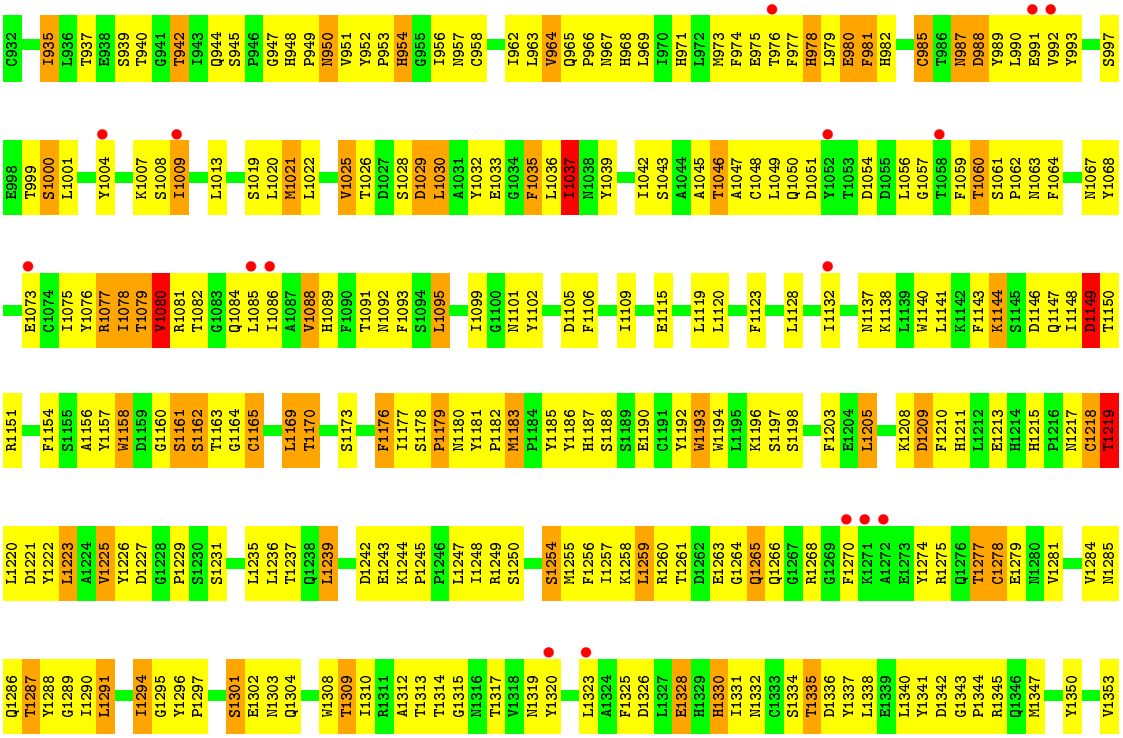
- Molecule 1: Gastric intrinsic factor

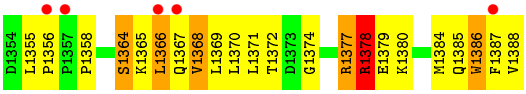
Chain E:



- Molecule 2: Cubilin

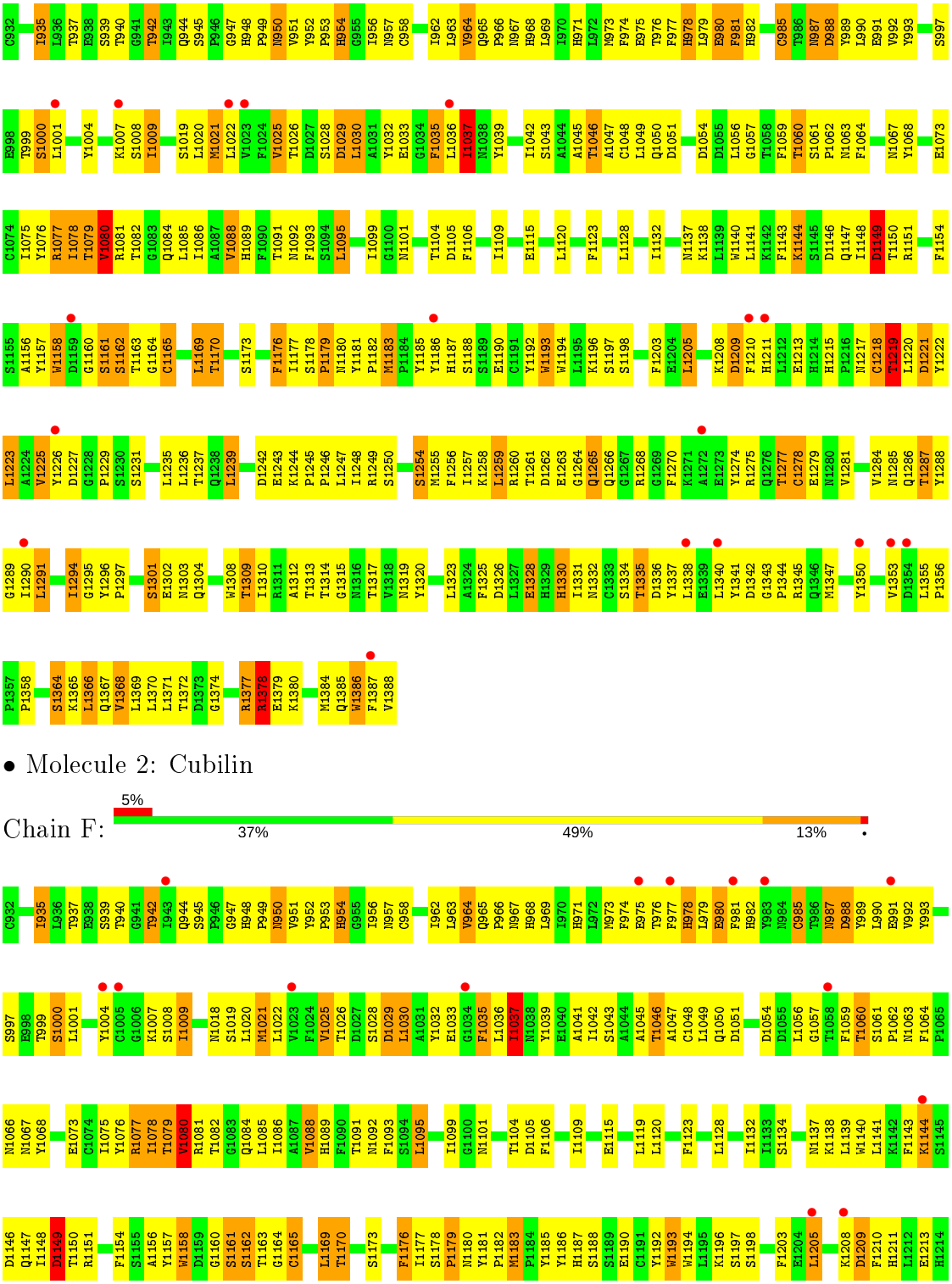
Chain B:





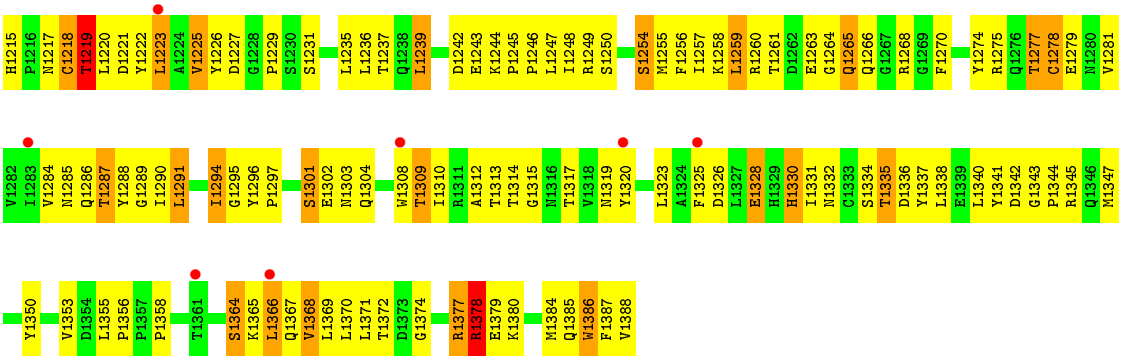
- Molecule 2: Cubilin

Chain D:



- Molecule 2: Cubilin

Chain F:



• 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 G:

• 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

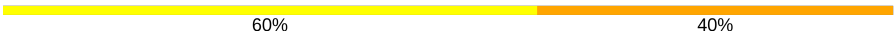
Chain J:

• 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 K:

• 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 M:



• 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 N:

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

Chain I:

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

Chain L:

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

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	117.68Å 204.18Å 410.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.85 – 3.30 47.85 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.85-3.30) 96.6 (47.85-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.242 0.207 , 0.242	Depositor DCC
R_{free} test set	1102 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å^2)	93.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.428 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.437 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20793	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: CA, BMA, B12, 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	0.67	1/3007 (0.0%)	0.80	1/4090 (0.0%)
1	C	0.67	1/3007 (0.0%)	0.80	1/4090 (0.0%)
1	E	0.67	1/3007 (0.0%)	0.80	0/4090
2	B	0.55	0/3748	0.74	0/5110
2	D	0.55	0/3748	0.74	0/5110
2	F	0.55	0/3748	0.74	0/5110
All	All	0.60	3/20265 (0.0%)	0.77	2/27600 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	360	GLU	CG-CD	5.96	1.60	1.51
1	A	360	GLU	CG-CD	5.94	1.60	1.51
1	C	360	GLU	CG-CD	5.92	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	311	ASN	CB-CA-C	5.42	121.24	110.40
1	A	311	ASN	CB-CA-C	5.12	120.65	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2950	0	2961	150	0
1	C	2950	0	2961	149	0
1	E	2950	0	2961	147	0
2	B	3638	0	3373	308	0
2	D	3638	0	3373	305	0
2	F	3638	0	3373	309	0
3	G	61	0	52	3	0
3	H	61	0	52	5	0
3	J	61	0	52	3	0
3	K	61	0	52	5	0
3	M	61	0	52	4	0
3	N	61	0	52	5	0
4	I	28	0	25	3	0
4	L	28	0	25	3	0
4	O	28	0	25	3	0
5	A	14	0	13	7	0
5	B	84	0	78	7	0
5	C	14	0	13	8	0
5	D	84	0	78	7	0
5	E	14	0	13	7	0
5	F	84	0	78	8	0
6	A	91	0	87	29	0
6	C	91	0	87	26	0
6	E	91	0	87	25	0
7	B	4	0	0	0	0
7	D	4	0	0	0	0
7	F	4	0	0	0	0
All	All	20793	0	19923	1450	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 36.

All (1450) 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:C:311:ASN:HB2	1:C:337:VAL:HA	1.19	1.18
1:A:311:ASN:HB2	1:A:337:VAL:HA	1.19	1.11
1:E:223:ILE:HD12	1:E:223:ILE:H	1.10	1.10
1:E:311:ASN:HB2	1:E:337:VAL:HA	1.19	1.08
1:A:223:ILE:H	1:A:223:ILE:HD12	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1079:THR:HG23	2:F:1138:LYS:HG2	1.34	1.06
1:C:223:ILE:H	1:C:223:ILE:HD12	1.10	1.06
2:B:1079:THR:HG23	2:B:1138:LYS:HG2	1.34	1.05
2:D:1079:THR:HG23	2:D:1138:LYS:HG2	1.33	1.03
1:E:352:ARG:HG3	1:E:352:ARG:HH11	1.24	1.00
1:C:352:ARG:HH11	1:C:352:ARG:HG3	1.22	1.00
6:A:2007:B12:H531	6:A:2007:B12:H552	1.44	0.99
6:E:2007:B12:H531	6:E:2007:B12:H552	1.44	0.99
2:B:1294:ILE:HD11	2:B:1301:SER:OG	1.62	0.99
1:A:352:ARG:HH11	1:A:352:ARG:HG3	1.25	0.98
6:C:2007:B12:H552	6:C:2007:B12:H531	1.44	0.98
2:D:1294:ILE:HD11	2:D:1301:SER:OG	1.62	0.97
2:F:1294:ILE:HD11	2:F:1301:SER:OG	1.62	0.97
1:A:40:GLN:HG2	1:A:272:LEU:HD11	1.47	0.97
1:E:40:GLN:HG2	1:E:272:LEU:HD11	1.47	0.96
2:D:1057:GLY:HA2	2:D:1158:TRP:NE1	1.81	0.95
1:C:40:GLN:HG2	1:C:272:LEU:HD11	1.47	0.95
2:B:1057:GLY:HA2	2:B:1158:TRP:NE1	1.81	0.95
6:E:2007:B12:H312	6:E:2007:B12:H353	1.50	0.94
6:C:2007:B12:H312	6:C:2007:B12:H353	1.50	0.94
6:A:2007:B12:H353	6:A:2007:B12:H312	1.50	0.93
2:F:1057:GLY:HA2	2:F:1158:TRP:NE1	1.81	0.93
1:E:362:THR:HG22	1:E:371:SER:HB3	1.49	0.93
1:C:362:THR:HG22	1:C:371:SER:HB3	1.50	0.92
1:A:362:THR:HG22	1:A:371:SER:HB3	1.50	0.92
2:B:1330:HIS:CE1	2:B:1332:ASN:H	1.88	0.91
1:C:312:ILE:HG21	1:C:406:ASN:HA	1.51	0.91
2:D:1330:HIS:CE1	2:D:1332:ASN:H	1.88	0.91
1:A:312:ILE:HG21	1:A:406:ASN:HA	1.52	0.90
1:E:312:ILE:HG21	1:E:406:ASN:HA	1.51	0.90
2:F:1330:HIS:CE1	2:F:1332:ASN:H	1.89	0.90
1:E:223:ILE:CD1	1:E:223:ILE:H	1.84	0.90
1:A:223:ILE:H	1:A:223:ILE:CD1	1.84	0.89
1:C:223:ILE:H	1:C:223:ILE:CD1	1.84	0.88
2:B:1084:GLN:HG3	2:B:1163:THR:H	1.39	0.88
2:F:1084:GLN:HG3	2:F:1163:THR:H	1.39	0.87
2:D:1084:GLN:HG3	2:D:1163:THR:H	1.39	0.87
1:A:337:VAL:HG22	5:A:2001:NAG:O7	1.76	0.85
2:B:1319:ASN:HB2	2:B:1387:PHE:HD2	1.40	0.85
2:D:1319:ASN:HB2	2:D:1387:PHE:HD2	1.42	0.85
1:A:362:THR:CG2	1:A:371:SER:HB3	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ARG:O	1:E:160:THR:HG23	1.77	0.84
2:F:1067:ASN:HB3	2:F:1150:THR:CG2	2.08	0.84
2:F:1319:ASN:HB2	2:F:1387:PHE:HD2	1.41	0.84
1:E:362:THR:CG2	1:E:371:SER:HB3	2.07	0.84
2:F:1313:THR:HG22	5:F:2009:NAG:H82	1.59	0.84
2:D:974:PHE:CE1	2:D:1037:ILE:HD12	2.13	0.84
1:C:156:ARG:O	1:C:160:THR:HG23	1.78	0.84
1:C:362:THR:CG2	1:C:371:SER:HB3	2.07	0.83
1:E:317:THR:HG23	1:E:331:GLU:HG3	1.60	0.83
2:F:974:PHE:CE1	2:F:1037:ILE:HD12	2.13	0.83
2:B:974:PHE:CE1	2:B:1037:ILE:HD12	2.13	0.83
2:D:1067:ASN:HB3	2:D:1150:THR:CG2	2.08	0.83
2:D:1313:THR:HG22	5:D:2009:NAG:H82	1.59	0.83
2:B:1067:ASN:HB3	2:B:1150:THR:CG2	2.08	0.83
2:B:1313:THR:HG22	5:B:2009:NAG:H82	1.59	0.83
2:F:1078:ILE:HD11	2:F:1086:ILE:HG12	1.60	0.83
1:A:317:THR:HG23	1:A:331:GLU:HG3	1.59	0.82
2:B:1078:ILE:HD11	2:B:1086:ILE:HG12	1.60	0.82
2:D:1078:ILE:HD11	2:D:1086:ILE:HG12	1.60	0.82
1:C:317:THR:HG23	1:C:331:GLU:HG3	1.60	0.81
1:E:223:ILE:HD12	1:E:223:ILE:N	1.94	0.81
1:A:223:ILE:N	1:A:223:ILE:HD12	1.94	0.81
2:F:1035:PHE:O	2:F:1035:PHE:HD1	1.63	0.81
1:C:223:ILE:N	1:C:223:ILE:HD12	1.94	0.81
2:F:1342:ASP:HB2	2:F:1347:MET:HE2	1.62	0.81
2:F:1297:PRO:O	2:F:1380:LYS:HD3	1.82	0.80
2:B:1342:ASP:HB2	2:B:1347:MET:HE2	1.63	0.80
2:D:1035:PHE:HD1	2:D:1035:PHE:O	1.63	0.80
2:D:1297:PRO:O	2:D:1380:LYS:HD3	1.82	0.80
1:E:92:LEU:O	1:E:96:ILE:HG13	1.82	0.80
2:F:1323:LEU:HD11	2:F:1385:GLN:HG3	1.64	0.80
2:B:1035:PHE:O	2:B:1035:PHE:HD1	1.63	0.80
2:B:1323:LEU:HD11	2:B:1385:GLN:HG3	1.64	0.80
2:B:1297:PRO:O	2:B:1380:LYS:HD3	1.82	0.80
2:D:1342:ASP:HB3	2:D:1345:ARG:HG2	1.62	0.80
2:D:1323:LEU:HD11	2:D:1385:GLN:HG3	1.64	0.80
1:A:177:THR:HG22	1:A:206:ILE:HG21	1.63	0.80
1:E:337:VAL:HG22	5:E:2001:NAG:O7	1.81	0.80
3:N:3:BMA:H61	3:N:5:MAN:H5	1.64	0.79
1:A:92:LEU:O	1:A:96:ILE:HG13	1.82	0.79
2:F:1342:ASP:HB3	2:F:1345:ARG:HG2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1342:ASP:HB3	2:B:1345:ARG:HG2	1.62	0.79
1:C:337:VAL:HG22	5:C:2001:NAG:O7	1.83	0.79
6:C:2007:B12:C53	6:C:2007:B12:H552	2.12	0.79
2:D:1342:ASP:HB2	2:D:1347:MET:HE2	1.65	0.78
2:D:1378:ARG:N	2:D:1378:ARG:HD2	1.98	0.78
2:F:1378:ARG:HD2	2:F:1378:ARG:N	1.97	0.78
2:F:1187:HIS:HB3	2:F:1266:GLN:NE2	1.99	0.78
3:H:3:BMA:H61	3:H:5:MAN:H5	1.64	0.78
1:C:312:ILE:O	1:C:335:VAL:HA	1.82	0.78
3:K:3:BMA:H61	3:K:5:MAN:H5	1.64	0.78
2:B:1187:HIS:HB3	2:B:1266:GLN:NE2	1.99	0.78
1:C:92:LEU:O	1:C:96:ILE:HG13	1.82	0.78
1:E:312:ILE:O	1:E:335:VAL:HA	1.84	0.78
1:C:177:THR:HG22	1:C:206:ILE:HG21	1.63	0.78
2:D:1187:HIS:HB3	2:D:1266:GLN:NE2	1.99	0.78
2:B:1078:ILE:O	2:B:1078:ILE:HG13	1.83	0.77
1:A:312:ILE:O	1:A:335:VAL:HA	1.84	0.77
1:E:177:THR:HG22	1:E:206:ILE:HG21	1.63	0.77
2:D:1078:ILE:O	2:D:1078:ILE:HG13	1.83	0.77
2:F:1078:ILE:O	2:F:1078:ILE:HG13	1.83	0.77
1:E:160:THR:HG21	2:F:1099:ILE:HG21	1.67	0.77
6:E:2007:B12:C53	6:E:2007:B12:H552	2.12	0.77
2:B:1378:ARG:HD2	2:B:1378:ARG:N	1.97	0.77
6:E:2007:B12:H203	6:E:2007:B12:H302	1.66	0.77
6:C:2007:B12:H203	6:C:2007:B12:H302	1.66	0.76
2:F:1330:HIS:CG	2:F:1331:ILE:N	2.52	0.76
1:A:156:ARG:O	1:A:160:THR:HG23	1.85	0.76
2:D:1330:HIS:CG	2:D:1331:ILE:N	2.52	0.76
2:F:1082:THR:HG23	2:F:1186:TYR:CD2	2.21	0.76
2:B:1309:THR:HG23	2:B:1367:GLN:HG2	1.66	0.76
2:F:1309:THR:HG23	2:F:1367:GLN:HG2	1.66	0.76
3:G:3:BMA:H4	3:G:5:MAN:H2	1.66	0.76
2:D:1309:THR:HG23	2:D:1367:GLN:HG2	1.66	0.76
2:F:1330:HIS:CG	2:F:1331:ILE:H	2.04	0.76
3:J:3:BMA:H4	3:J:5:MAN:H2	1.66	0.76
1:A:160:THR:CG2	2:B:1099:ILE:HG21	2.15	0.76
2:B:1035:PHE:O	2:B:1035:PHE:CD1	2.38	0.76
2:B:1082:THR:HG23	2:B:1186:TYR:CD2	2.21	0.76
2:F:1035:PHE:O	2:F:1035:PHE:CD1	2.38	0.76
3:M:3:BMA:H4	3:M:5:MAN:H2	1.66	0.76
2:D:1335:THR:HG23	2:D:1336:ASP:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:THR:CG2	2:D:1099:ILE:HG21	2.16	0.75
6:A:2007:B12:H203	6:A:2007:B12:H302	1.66	0.75
2:B:1330:HIS:CG	2:B:1331:ILE:N	2.52	0.75
1:C:160:THR:HG21	2:D:1099:ILE:HG21	1.66	0.75
1:C:352:ARG:NH1	1:C:352:ARG:HG3	1.93	0.75
1:E:160:THR:CG2	2:F:1099:ILE:HG21	2.16	0.75
6:A:2007:B12:C53	6:A:2007:B12:H552	2.12	0.75
2:B:1330:HIS:CG	2:B:1331:ILE:H	2.03	0.75
2:B:1304:GLN:H	2:B:1372:THR:HG23	1.52	0.75
2:D:1082:THR:HG23	2:D:1186:TYR:CD2	2.21	0.75
4:L:1:NAG:O3	4:L:2:NAG:H2	1.87	0.75
2:B:1194:TRP:HE1	2:B:1254:SER:HB3	1.52	0.75
2:B:1335:THR:HG23	2:B:1336:ASP:H	1.51	0.75
2:F:1335:THR:HG23	2:F:1336:ASP:H	1.51	0.75
4:O:1:NAG:O3	4:O:2:NAG:H2	1.87	0.75
2:D:1222:TYR:CE2	2:D:1260:ARG:HB3	2.21	0.74
6:E:2007:B12:H362	6:E:2007:B12:H351	1.69	0.74
2:B:1222:TYR:CE2	2:B:1260:ARG:HB3	2.21	0.74
2:F:1222:TYR:CE2	2:F:1260:ARG:HB3	2.21	0.74
2:D:1035:PHE:CD1	2:D:1035:PHE:O	2.38	0.74
2:F:1194:TRP:HE1	2:F:1254:SER:HB3	1.51	0.74
2:F:1304:GLN:H	2:F:1372:THR:HG23	1.52	0.74
1:A:160:THR:HG21	2:B:1099:ILE:HG21	1.69	0.74
4:I:1:NAG:O3	4:I:2:NAG:H2	1.87	0.74
1:E:352:ARG:HG3	1:E:352:ARG:NH1	1.95	0.74
1:E:389:LEU:HB3	1:E:394:PRO:HA	1.70	0.74
2:D:1304:GLN:H	2:D:1372:THR:HG23	1.52	0.73
2:D:1194:TRP:HE1	2:D:1254:SER:HB3	1.51	0.73
1:A:389:LEU:HB3	1:A:394:PRO:HA	1.70	0.73
2:B:999:THR:HG22	2:B:1000:SER:H	1.53	0.73
2:D:1181:TYR:CD1	2:D:1182:PRO:HA	2.24	0.73
6:A:2007:B12:H351	6:A:2007:B12:H362	1.69	0.73
1:E:297:THR:HG22	1:E:299:PRO:HD3	1.71	0.73
1:A:311:ASN:HB2	1:A:337:VAL:CA	2.11	0.72
6:C:2007:B12:H362	6:C:2007:B12:H351	1.69	0.72
3:H:3:BMA:H61	3:H:5:MAN:C5	2.18	0.72
6:C:2007:B12:N22	6:C:2007:B12:H4B	2.04	0.72
2:D:999:THR:HG22	2:D:1000:SER:H	1.53	0.72
2:F:1181:TYR:CD1	2:F:1182:PRO:HA	2.24	0.72
6:A:2007:B12:N22	6:A:2007:B12:H4B	2.04	0.72
2:D:1330:HIS:CG	2:D:1331:ILE:H	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:999:THR:HG22	2:F:1000:SER:H	1.53	0.72
2:F:954:HIS:CD2	2:F:954:HIS:H	2.06	0.72
2:F:944:GLN:HA	2:F:944:GLN:OE1	1.90	0.72
1:A:352:ARG:NH1	1:A:352:ARG:HG3	1.96	0.72
2:B:1181:TYR:CD1	2:B:1182:PRO:HA	2.24	0.72
1:A:297:THR:HG22	1:A:299:PRO:HD3	1.71	0.72
6:E:2007:B12:N22	6:E:2007:B12:H4B	2.04	0.72
2:D:1185:TYR:CE1	2:D:1266:GLN:HG3	2.25	0.72
1:C:389:LEU:HB3	1:C:394:PRO:HA	1.70	0.72
2:B:944:GLN:OE1	2:B:944:GLN:HA	1.90	0.71
2:B:954:HIS:H	2:B:954:HIS:CD2	2.06	0.71
2:D:1243:GLU:HA	2:D:1243:GLU:OE1	1.90	0.71
2:D:954:HIS:CD2	2:D:954:HIS:H	2.06	0.71
3:N:3:BMA:H61	3:N:5:MAN:C5	2.18	0.71
2:B:1243:GLU:OE1	2:B:1243:GLU:HA	1.90	0.71
2:D:944:GLN:HA	2:D:944:GLN:OE1	1.90	0.71
2:B:1185:TYR:CE1	2:B:1266:GLN:HG3	2.25	0.71
2:F:953:PRO:HB2	2:F:956:ILE:HD11	1.73	0.71
2:B:1182:PRO:HB3	2:B:1268:ARG:HH21	1.56	0.71
1:C:297:THR:HG22	1:C:299:PRO:HD3	1.71	0.71
2:F:1182:PRO:HB3	2:F:1268:ARG:HH21	1.56	0.71
2:D:1182:PRO:HB3	2:D:1268:ARG:HH21	1.56	0.71
2:B:1308:TRP:HB2	2:B:1368:VAL:CG2	2.21	0.71
2:B:978:HIS:HB2	2:B:1033:GLU:OE2	1.90	0.71
2:D:1308:TRP:HB2	2:D:1368:VAL:CG2	2.21	0.71
2:B:953:PRO:HB2	2:B:956:ILE:HD11	1.73	0.70
2:D:1319:ASN:HB2	2:D:1387:PHE:CD2	2.26	0.70
2:F:1243:GLU:HA	2:F:1243:GLU:OE1	1.90	0.70
2:B:1188:SER:HA	2:B:1261:THR:O	1.92	0.70
2:F:1188:SER:HA	2:F:1261:THR:O	1.92	0.70
2:F:978:HIS:HB2	2:F:1033:GLU:OE2	1.91	0.70
2:D:978:HIS:HB2	2:D:1033:GLU:OE2	1.91	0.70
2:F:1277:THR:HG22	2:F:1279:GLU:H	1.56	0.70
2:F:1308:TRP:HB2	2:F:1368:VAL:CG2	2.21	0.70
2:F:1319:ASN:HB2	2:F:1387:PHE:CD2	2.25	0.70
2:D:1057:GLY:HA2	2:D:1158:TRP:HE1	1.56	0.70
2:D:953:PRO:HB2	2:D:956:ILE:HD11	1.73	0.70
1:E:87:LEU:HD22	1:E:91:HIS:HB3	1.73	0.70
2:F:1185:TYR:CE1	2:F:1266:GLN:HG3	2.25	0.70
2:F:1277:THR:HG22	2:F:1278:CYS:H	1.56	0.70
2:B:1277:THR:HG22	2:B:1279:GLU:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:HA	1:A:334:ASN:O	1.92	0.69
2:B:1277:THR:HG22	2:B:1278:CYS:H	1.56	0.69
2:D:1277:THR:HG22	2:D:1278:CYS:H	1.56	0.69
1:E:311:ASN:HB2	1:E:337:VAL:CA	2.12	0.69
3:K:3:BMA:H61	3:K:5:MAN:C5	2.18	0.69
2:D:1188:SER:HA	2:D:1261:THR:O	1.92	0.69
1:E:313:THR:HA	1:E:334:ASN:O	1.92	0.69
2:D:1277:THR:HG22	2:D:1279:GLU:H	1.56	0.69
1:A:87:LEU:HD22	1:A:91:HIS:HB3	1.73	0.69
2:F:951:VAL:HB	2:F:1032:TYR:O	1.92	0.69
1:A:173:GLY:O	1:A:177:THR:HG23	1.93	0.69
6:C:2007:B12:C6	6:C:2007:B12:H4B	2.23	0.69
1:C:173:GLY:O	1:C:177:THR:HG23	1.93	0.69
2:F:1057:GLY:HA2	2:F:1158:TRP:HE1	1.56	0.69
2:F:1177:ILE:HG23	2:F:1181:TYR:HB3	1.75	0.68
6:A:2007:B12:H4B	6:A:2007:B12:C6	2.23	0.68
1:C:87:LEU:HD22	1:C:91:HIS:HB3	1.73	0.68
2:F:1304:GLN:HB2	2:F:1372:THR:HG22	1.75	0.68
2:B:1177:ILE:HG23	2:B:1181:TYR:HB3	1.75	0.68
2:B:951:VAL:HB	2:B:1032:TYR:O	1.92	0.68
2:F:1057:GLY:HA3	2:F:1157:TYR:HA	1.75	0.68
2:B:1057:GLY:HA2	2:B:1158:TRP:HE1	1.56	0.68
1:C:313:THR:HA	1:C:334:ASN:O	1.92	0.68
2:D:1304:GLN:HB2	2:D:1372:THR:HG22	1.75	0.68
2:D:935:ILE:O	2:D:935:ILE:HG13	1.94	0.68
6:E:2007:B12:C6	6:E:2007:B12:H4B	2.23	0.68
1:E:173:GLY:O	1:E:177:THR:HG23	1.93	0.68
2:B:1319:ASN:HB2	2:B:1387:PHE:CD2	2.26	0.68
1:C:311:ASN:HB2	1:C:337:VAL:CA	2.13	0.67
2:B:1057:GLY:HA3	2:B:1157:TYR:HA	1.75	0.67
1:C:156:ARG:HG3	2:D:1099:ILE:HD12	1.77	0.67
2:D:1177:ILE:HG23	2:D:1181:TYR:HB3	1.75	0.67
2:D:951:VAL:HB	2:D:1032:TYR:O	1.93	0.67
1:E:156:ARG:HG3	2:F:1099:ILE:HD12	1.77	0.67
2:B:935:ILE:HG13	2:B:935:ILE:O	1.94	0.67
2:D:1060:THR:CG2	2:D:1064:PHE:HB3	2.24	0.67
2:D:1057:GLY:HA3	2:D:1157:TYR:HA	1.75	0.67
2:F:1213:GLU:OE2	2:F:1265:GLN:HB3	1.95	0.67
2:F:1060:THR:CG2	2:F:1064:PHE:HB3	2.24	0.67
2:F:1084:GLN:HG3	2:F:1162:SER:N	2.10	0.67
2:B:1084:GLN:HG3	2:B:1162:SER:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1213:GLU:OE2	2:D:1265:GLN:HB3	1.95	0.67
2:B:1213:GLU:OE2	2:B:1265:GLN:HB3	1.95	0.66
1:E:211:SER:HA	1:E:214:ILE:HD12	1.77	0.66
2:F:1008:SER:HB3	2:F:1182:PRO:O	1.95	0.66
2:F:935:ILE:HG13	2:F:935:ILE:O	1.94	0.66
2:D:999:THR:HG22	2:D:1000:SER:N	2.11	0.66
2:B:1060:THR:CG2	2:B:1064:PHE:HB3	2.24	0.66
2:D:1294:ILE:HD11	2:D:1301:SER:HG	1.59	0.66
2:B:1304:GLN:HB2	2:B:1372:THR:HG22	1.75	0.66
1:A:156:ARG:HG3	2:B:1099:ILE:HD12	1.77	0.66
2:D:1084:GLN:HG3	2:D:1162:SER:N	2.10	0.66
1:A:211:SER:HA	1:A:214:ILE:HD12	1.77	0.66
2:F:1109:ILE:HG12	2:F:1141:LEU:HD22	1.78	0.66
2:B:999:THR:HG22	2:B:1000:SER:N	2.11	0.66
2:B:1109:ILE:HG12	2:B:1141:LEU:HD22	1.78	0.65
2:D:1109:ILE:HG12	2:D:1141:LEU:HD22	1.78	0.65
2:B:1366:LEU:HD22	2:B:1366:LEU:C	2.17	0.65
2:D:1008:SER:HB3	2:D:1182:PRO:O	1.95	0.65
1:E:318:ILE:HG13	1:E:318:ILE:O	1.97	0.65
2:F:1294:ILE:HD11	2:F:1301:SER:HG	1.59	0.65
2:B:1089:HIS:O	2:B:1156:ALA:HB1	1.97	0.65
2:D:1109:ILE:HG23	2:D:1141:LEU:HD21	1.78	0.65
2:D:1341:TYR:HB2	2:D:1367:GLN:HB2	1.79	0.65
2:B:1008:SER:HB3	2:B:1182:PRO:O	1.95	0.65
2:F:999:THR:HG22	2:F:1000:SER:N	2.11	0.65
2:F:1259:LEU:HD23	2:F:1259:LEU:O	1.97	0.65
2:B:1341:TYR:HB2	2:B:1367:GLN:HB2	1.79	0.65
2:D:1182:PRO:HB3	2:D:1268:ARG:NH2	2.12	0.65
2:D:1366:LEU:HD22	2:D:1366:LEU:C	2.17	0.65
2:F:1084:GLN:HG2	2:F:1161:SER:HA	1.79	0.65
2:F:1089:HIS:O	2:F:1156:ALA:HB1	1.97	0.65
1:A:318:ILE:O	1:A:318:ILE:HG13	1.97	0.65
2:B:1109:ILE:HG23	2:B:1141:LEU:HD21	1.78	0.65
1:C:318:ILE:O	1:C:318:ILE:HG13	1.97	0.65
1:C:211:SER:HA	1:C:214:ILE:HD12	1.77	0.65
2:D:1308:TRP:HB2	2:D:1368:VAL:HG23	1.79	0.65
2:D:956:ILE:HG22	2:D:958:CYS:H	1.62	0.64
2:D:1089:HIS:O	2:D:1156:ALA:HB1	1.97	0.64
2:F:1308:TRP:HB2	2:F:1368:VAL:HG23	1.79	0.64
2:B:1182:PRO:HB3	2:B:1268:ARG:NH2	2.12	0.64
2:B:956:ILE:HG22	2:B:958:CYS:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ILE:HG22	1:C:313:THR:H	1.63	0.64
2:F:1366:LEU:C	2:F:1366:LEU:HD22	2.17	0.64
2:B:1294:ILE:HD11	2:B:1301:SER:HG	1.60	0.64
2:B:1049:LEU:CD2	2:B:1075:ILE:HB	2.28	0.64
2:B:1308:TRP:HB2	2:B:1368:VAL:HG23	1.79	0.64
2:D:993:TYR:HB3	2:D:1021:MET:HB2	1.79	0.64
6:A:2007:B12:N22	6:A:2007:B12:C4B	2.60	0.64
2:F:1049:LEU:CD2	2:F:1075:ILE:HB	2.28	0.64
2:F:1341:TYR:HB2	2:F:1367:GLN:HB2	1.79	0.64
6:E:2007:B12:C4B	6:E:2007:B12:N22	2.60	0.64
1:E:203:LEU:O	1:E:207:VAL:HG23	1.98	0.64
1:A:317:THR:HG1	1:A:409:HIS:HE2	1.45	0.64
1:C:203:LEU:O	1:C:207:VAL:HG23	1.98	0.64
2:B:1285:ASN:HD21	5:B:2009:NAG:H61	1.63	0.63
2:D:1049:LEU:CD2	2:D:1075:ILE:HB	2.28	0.63
2:D:1259:LEU:O	2:D:1259:LEU:HD23	1.97	0.63
2:D:1285:ASN:HD21	5:D:2009:NAG:H61	1.63	0.63
2:F:1109:ILE:HG23	2:F:1141:LEU:HD21	1.78	0.63
6:C:2007:B12:N22	6:C:2007:B12:C4B	2.60	0.63
2:D:1084:GLN:HG2	2:D:1161:SER:HA	1.79	0.63
2:F:956:ILE:HG22	2:F:958:CYS:H	1.62	0.63
2:B:1259:LEU:HD23	2:B:1259:LEU:O	1.97	0.63
2:D:1296:TYR:CG	2:D:1297:PRO:HA	2.34	0.63
2:F:1060:THR:HG23	2:F:1064:PHE:HB3	1.79	0.63
2:B:1049:LEU:HD23	2:B:1075:ILE:HB	1.81	0.63
2:B:1296:TYR:CG	2:B:1297:PRO:HA	2.34	0.63
1:E:389:LEU:HD23	1:E:389:LEU:H	1.62	0.63
2:F:1296:TYR:CG	2:F:1297:PRO:HA	2.34	0.63
2:B:1287:THR:O	2:B:1388:VAL:HG23	1.99	0.63
1:C:389:LEU:H	1:C:389:LEU:HD23	1.62	0.63
2:D:1287:THR:O	2:D:1388:VAL:HG23	1.99	0.63
1:A:389:LEU:HD23	1:A:389:LEU:H	1.62	0.63
2:F:1287:THR:O	2:F:1388:VAL:HG23	1.99	0.63
2:F:993:TYR:HB3	2:F:1021:MET:HB2	1.79	0.63
2:F:1182:PRO:HB3	2:F:1268:ARG:NH2	2.12	0.63
1:A:203:LEU:O	1:A:207:VAL:HG23	1.98	0.63
2:B:1060:THR:HG23	2:B:1064:PHE:HB3	1.79	0.63
1:E:312:ILE:HG22	1:E:313:THR:H	1.64	0.63
1:A:312:ILE:HG22	1:A:313:THR:H	1.63	0.62
2:D:1060:THR:HG23	2:D:1064:PHE:HB3	1.79	0.62
2:B:1084:GLN:HG2	2:B:1161:SER:HA	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:993:TYR:HB3	2:B:1021:MET:HB2	1.79	0.62
2:F:1049:LEU:HD23	2:F:1075:ILE:HB	1.81	0.62
2:B:1076:TYR:HB2	2:B:1141:LEU:HB2	1.82	0.62
1:A:308:SER:O	1:A:309:ALA:HB2	2.00	0.62
1:C:317:THR:HG1	1:C:409:HIS:HE2	1.46	0.62
2:D:1076:TYR:HB2	2:D:1141:LEU:HB2	1.82	0.62
2:D:1067:ASN:HA	2:D:1151:ARG:O	1.99	0.62
1:E:317:THR:HG1	1:E:409:HIS:HE2	1.48	0.62
1:E:337:VAL:HG13	5:E:2001:NAG:H2	1.81	0.62
2:D:1049:LEU:HD23	2:D:1075:ILE:HB	1.81	0.62
2:B:1106:PHE:CZ	2:B:1144:LYS:HB2	2.35	0.62
2:D:1277:THR:HG22	2:D:1278:CYS:N	2.15	0.62
2:D:1325:PHE:HB2	2:D:1355:LEU:HD12	1.82	0.62
2:F:1340:LEU:CD2	2:F:1368:VAL:HG12	2.30	0.62
2:F:1285:ASN:HD21	5:F:2009:NAG:H61	1.63	0.61
2:B:1067:ASN:HA	2:B:1151:ARG:O	1.99	0.61
2:D:1106:PHE:CZ	2:D:1144:LYS:HB2	2.35	0.61
2:D:1340:LEU:CD2	2:D:1368:VAL:HG12	2.30	0.61
2:F:1067:ASN:HA	2:F:1151:ARG:O	1.99	0.61
2:B:1325:PHE:HB2	2:B:1355:LEU:HD12	1.82	0.61
2:B:1340:LEU:CD2	2:B:1368:VAL:HG12	2.30	0.61
2:F:1106:PHE:CZ	2:F:1144:LYS:HB2	2.35	0.61
2:F:1076:TYR:HB2	2:F:1141:LEU:HB2	1.82	0.61
1:A:337:VAL:HG13	5:A:2001:NAG:H2	1.83	0.61
2:B:1277:THR:HG22	2:B:1278:CYS:N	2.15	0.61
6:E:2007:B12:H601	6:E:2007:B12:H262	1.82	0.61
1:E:76:THR:O	1:E:80:MET:HG3	2.01	0.61
1:A:290:PRO:O	1:A:291:ASP:HB2	2.01	0.61
1:C:308:SER:O	1:C:309:ALA:HB2	2.00	0.61
2:B:1320:TYR:OH	2:B:1366:LEU:HD23	2.00	0.61
2:F:1277:THR:HG22	2:F:1278:CYS:N	2.15	0.61
2:D:978:HIS:O	2:D:979:LEU:HD23	2.01	0.61
2:F:1325:PHE:HB2	2:F:1355:LEU:HD12	1.82	0.61
2:B:1079:THR:HG23	2:B:1138:LYS:CG	2.23	0.60
1:E:308:SER:O	1:E:309:ALA:HB2	2.00	0.60
2:F:1320:TYR:OH	2:F:1366:LEU:HD23	2.02	0.60
2:F:1225:VAL:CG1	2:F:1236:LEU:HB2	2.32	0.60
6:A:2007:B12:H601	6:A:2007:B12:H262	1.82	0.60
1:A:76:THR:O	1:A:80:MET:HG3	2.01	0.60
2:B:1225:VAL:CG1	2:B:1236:LEU:HB2	2.32	0.60
6:C:2007:B12:H262	6:C:2007:B12:H601	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1320:TYR:OH	2:D:1366:LEU:HD23	2.02	0.60
2:D:954:HIS:CD2	2:D:954:HIS:N	2.70	0.60
2:B:1182:PRO:CB	2:B:1268:ARG:HH21	2.15	0.60
1:C:290:PRO:O	1:C:291:ASP:HB2	2.01	0.60
1:C:76:THR:O	1:C:80:MET:HG3	2.01	0.60
6:E:2007:B12:C55	6:E:2007:B12:H531	2.23	0.60
1:E:379:ASN:H	1:E:384:THR:HG22	1.67	0.60
2:D:1182:PRO:CB	2:D:1268:ARG:HH21	2.15	0.60
2:B:971:HIS:HB2	2:B:1042:ILE:HD12	1.83	0.59
6:C:2007:B12:C55	6:C:2007:B12:H531	2.23	0.59
2:D:971:HIS:HB2	2:D:1042:ILE:HD12	1.84	0.59
2:F:978:HIS:O	2:F:979:LEU:HD23	2.02	0.59
1:A:379:ASN:H	1:A:384:THR:HG22	1.67	0.59
2:B:954:HIS:CD2	2:B:954:HIS:N	2.70	0.59
1:E:320:ASN:HB3	1:E:328:LEU:HG	1.83	0.59
2:B:978:HIS:O	2:B:979:LEU:HD23	2.02	0.59
2:D:1225:VAL:CG1	2:D:1236:LEU:HB2	2.32	0.59
2:F:1182:PRO:CB	2:F:1268:ARG:HH21	2.15	0.59
1:C:405:PHE:CZ	1:C:408:GLU:HG3	2.37	0.59
1:C:379:ASN:H	1:C:384:THR:HG22	1.67	0.59
2:D:1079:THR:HG23	2:D:1138:LYS:CG	2.23	0.59
1:E:405:PHE:CZ	1:E:408:GLU:HG3	2.37	0.59
1:A:337:VAL:CG2	5:A:2001:NAG:O7	2.49	0.59
1:E:290:PRO:O	1:E:291:ASP:HB2	2.01	0.59
2:F:971:HIS:HB2	2:F:1042:ILE:HD12	1.84	0.59
2:F:954:HIS:CD2	2:F:954:HIS:N	2.70	0.59
1:C:320:ASN:HB3	1:C:328:LEU:HG	1.83	0.59
1:A:320:ASN:HB3	1:A:328:LEU:HG	1.83	0.59
2:B:990:LEU:HD12	2:B:1035:PHE:CE2	2.39	0.58
1:E:218:GLY:O	1:E:249:THR:HG23	2.03	0.58
1:A:405:PHE:CZ	1:A:408:GLU:HG3	2.37	0.58
2:F:1148:ILE:HG22	2:F:1149:ASP:N	2.18	0.58
2:F:948:HIS:CG	2:F:949:PRO:HA	2.39	0.58
2:B:1296:TYR:CD2	2:B:1297:PRO:HA	2.39	0.58
2:B:948:HIS:CG	2:B:949:PRO:HA	2.39	0.58
2:D:1296:TYR:CD2	2:D:1297:PRO:HA	2.39	0.58
2:D:948:HIS:CG	2:D:949:PRO:HA	2.39	0.58
2:F:942:THR:CG2	2:F:1036:LEU:HD11	2.33	0.58
2:B:942:THR:CG2	2:B:1036:LEU:HD11	2.33	0.58
1:E:389:LEU:HD23	1:E:389:LEU:N	2.19	0.58
2:B:1148:ILE:HG22	2:B:1149:ASP:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1158:TRP:CD1	2:B:1158:TRP:N	2.72	0.57
2:D:942:THR:CG2	2:D:1036:LEU:HD11	2.33	0.57
2:D:1148:ILE:HG22	2:D:1149:ASP:N	2.18	0.57
2:D:1330:HIS:CE1	2:D:1332:ASN:N	2.67	0.57
2:F:978:HIS:HB2	2:F:1033:GLU:CD	2.24	0.57
2:F:1084:GLN:CG	2:F:1163:THR:H	2.15	0.57
6:A:2007:B12:H351	6:A:2007:B12:H372	1.85	0.57
1:A:389:LEU:HD23	1:A:389:LEU:N	2.19	0.57
2:B:1084:GLN:CG	2:B:1163:THR:H	2.15	0.57
1:C:389:LEU:N	1:C:389:LEU:HD23	2.19	0.57
6:E:2007:B12:H351	6:E:2007:B12:H372	1.85	0.57
2:F:990:LEU:HD12	2:F:1035:PHE:CE2	2.39	0.57
2:D:978:HIS:HB2	2:D:1033:GLU:CD	2.24	0.57
2:F:1158:TRP:CD1	2:F:1158:TRP:N	2.72	0.57
1:A:218:GLY:O	1:A:249:THR:HG23	2.03	0.57
1:A:58:LEU:HB2	1:A:75:LEU:CD2	2.35	0.57
2:D:990:LEU:HD12	2:D:1035:PHE:CE2	2.39	0.57
2:D:1158:TRP:CD1	2:D:1158:TRP:N	2.72	0.57
6:A:2007:B12:H531	6:A:2007:B12:C55	2.23	0.57
2:B:993:TYR:CD1	2:B:1000:SER:HB2	2.40	0.57
1:C:58:LEU:HB2	1:C:75:LEU:CD2	2.35	0.57
2:F:1296:TYR:CD2	2:F:1297:PRO:HA	2.39	0.57
6:C:2007:B12:H372	6:C:2007:B12:H351	1.85	0.57
1:C:218:GLY:O	1:C:249:THR:HG23	2.03	0.57
1:A:337:VAL:HG22	5:A:2001:NAG:C7	2.35	0.57
1:C:117:MET:HB3	1:C:153:ILE:HD13	1.87	0.57
2:D:1057:GLY:HA2	2:D:1158:TRP:CD1	2.40	0.57
2:D:993:TYR:CD1	2:D:1000:SER:HB2	2.40	0.57
2:F:1353:VAL:O	2:F:1353:VAL:HG22	2.05	0.57
2:B:1057:GLY:HA2	2:B:1158:TRP:CD1	2.40	0.57
2:B:978:HIS:HB2	2:B:1033:GLU:CD	2.24	0.57
2:D:1210:PHE:HD2	2:D:1211:HIS:N	2.03	0.57
2:D:1350:TYR:CE1	2:D:1356:PRO:HB3	2.40	0.57
2:F:1350:TYR:CE1	2:F:1356:PRO:HB3	2.40	0.57
2:B:1350:TYR:CE1	2:B:1356:PRO:HB3	2.40	0.56
1:E:214:ILE:HG13	1:E:220:ILE:HG23	1.87	0.56
2:F:990:LEU:HD23	2:F:991:GLU:N	2.20	0.56
1:A:94:LEU:HD22	1:A:137:LEU:HG	1.87	0.56
1:A:173:GLY:O	1:A:177:THR:CG2	2.53	0.56
2:B:1330:HIS:CE1	2:B:1332:ASN:N	2.68	0.56
1:E:29:PRO:HB2	1:E:32:GLN:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:993:TYR:CD1	2:F:1000:SER:HB2	2.40	0.56
6:C:2007:B12:O28	6:C:2007:B12:H3	2.06	0.56
2:D:1235:LEU:HD11	2:D:1237:THR:O	2.06	0.56
2:D:966:PRO:O	2:D:967:ASN:CG	2.44	0.56
1:A:117:MET:HB3	1:A:153:ILE:HD13	1.87	0.56
1:C:311:ASN:HA	1:C:338:LYS:H	1.70	0.56
2:D:1084:GLN:CG	2:D:1163:THR:H	2.15	0.56
1:E:58:LEU:HB2	1:E:75:LEU:CD2	2.35	0.56
2:B:1009:ILE:O	2:B:1009:ILE:HG23	2.06	0.56
2:B:1353:VAL:O	2:B:1353:VAL:HG22	2.05	0.56
1:E:173:GLY:O	1:E:177:THR:CG2	2.53	0.56
1:C:173:GLY:O	1:C:177:THR:CG2	2.53	0.56
2:D:1009:ILE:HG23	2:D:1009:ILE:O	2.06	0.56
2:F:1084:GLN:HG3	2:F:1162:SER:H	1.70	0.56
2:F:966:PRO:O	2:F:967:ASN:CG	2.43	0.56
1:C:29:PRO:HB2	1:C:32:GLN:CG	2.35	0.56
2:D:1210:PHE:CD2	2:D:1211:HIS:N	2.74	0.56
2:F:1057:GLY:HA2	2:F:1158:TRP:CD1	2.40	0.56
2:F:1210:PHE:HD2	2:F:1211:HIS:N	2.03	0.56
1:A:214:ILE:HG13	1:A:220:ILE:HG23	1.87	0.56
2:B:990:LEU:HD23	2:B:991:GLU:N	2.20	0.56
1:C:362:THR:CG2	1:C:371:SER:CB	2.83	0.56
2:D:990:LEU:HD23	2:D:991:GLU:N	2.20	0.56
2:F:1281:VAL:HG21	2:F:1308:TRP:CD1	2.41	0.56
2:F:956:ILE:HG22	2:F:957:ASN:N	2.21	0.56
2:B:956:ILE:HG22	2:B:957:ASN:N	2.21	0.56
6:C:2007:B12:C35	6:C:2007:B12:H362	2.36	0.56
2:D:956:ILE:HG22	2:D:957:ASN:N	2.21	0.56
1:E:311:ASN:HA	1:E:338:LYS:H	1.70	0.56
2:F:1223:LEU:HD23	2:F:1259:LEU:HB2	1.88	0.56
2:B:1210:PHE:CD2	2:B:1211:HIS:N	2.74	0.56
1:E:94:LEU:HD22	1:E:137:LEU:HG	1.87	0.56
1:E:117:MET:HB3	1:E:153:ILE:HD13	1.87	0.56
6:A:2007:B12:O28	6:A:2007:B12:H3	2.05	0.55
1:A:417:TYR:CD2	1:A:417:TYR:N	2.74	0.55
2:B:1222:TYR:HE2	2:B:1260:ARG:HD3	1.72	0.55
2:B:1281:VAL:HG21	2:B:1308:TRP:CD1	2.41	0.55
2:D:1353:VAL:HG22	2:D:1353:VAL:O	2.05	0.55
6:E:2007:B12:H362	6:E:2007:B12:C35	2.36	0.55
2:F:1210:PHE:CD2	2:F:1211:HIS:N	2.74	0.55
2:F:1366:LEU:HD13	2:F:1366:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HB2	1:A:32:GLN:CG	2.35	0.55
2:D:1281:VAL:HG21	2:D:1308:TRP:CD1	2.41	0.55
2:B:949:PRO:O	2:B:950:ASN:HB3	2.07	0.55
2:D:1222:TYR:HE2	2:D:1260:ARG:HD3	1.72	0.55
2:D:949:PRO:O	2:D:950:ASN:HB3	2.07	0.55
2:B:1235:LEU:HD11	2:B:1237:THR:O	2.06	0.55
2:B:966:PRO:O	2:B:967:ASN:CG	2.45	0.55
1:C:94:LEU:HD22	1:C:137:LEU:HG	1.87	0.55
1:C:339:SER:C	1:C:341:SER:H	2.10	0.55
2:D:1249:ARG:HG3	2:D:1250:SER:O	2.07	0.55
1:A:40:GLN:CG	1:A:272:LEU:HD11	2.30	0.55
2:B:942:THR:HG21	2:B:1036:LEU:HD11	1.89	0.55
1:C:214:ILE:HG13	1:C:220:ILE:HG23	1.87	0.55
2:D:1080:VAL:HG23	2:D:1137:ASN:HB2	1.89	0.55
1:C:417:TYR:CD2	1:C:417:TYR:N	2.74	0.55
1:E:337:VAL:HG22	5:E:2001:NAG:C7	2.37	0.55
6:A:2007:B12:H362	6:A:2007:B12:C35	2.36	0.55
2:B:1223:LEU:HD23	2:B:1259:LEU:HB2	1.88	0.55
2:F:1009:ILE:O	2:F:1009:ILE:HG23	2.06	0.55
2:F:1036:LEU:HD12	2:F:1037:ILE:H	1.72	0.55
2:F:1177:ILE:HD12	2:F:1181:TYR:CD2	2.42	0.55
1:A:311:ASN:HA	1:A:338:LYS:H	1.71	0.55
2:B:1036:LEU:HD12	2:B:1037:ILE:H	1.72	0.55
1:C:325:VAL:HG23	1:C:325:VAL:O	2.06	0.55
2:D:1366:LEU:O	2:D:1366:LEU:HD13	2.06	0.55
1:E:339:SER:C	1:E:341:SER:H	2.10	0.55
1:E:417:TYR:N	1:E:417:TYR:CD2	2.74	0.55
2:F:1080:VAL:HG23	2:F:1137:ASN:HB2	1.89	0.55
1:A:106:PRO:O	1:A:108:ASP:N	2.40	0.55
2:B:1177:ILE:HD12	2:B:1181:TYR:CD2	2.42	0.55
6:E:2007:B12:O28	6:E:2007:B12:H3	2.06	0.55
2:F:949:PRO:O	2:F:950:ASN:HB3	2.07	0.55
2:B:1210:PHE:HD2	2:B:1211:HIS:N	2.03	0.54
1:C:337:VAL:HG22	5:C:2001:NAG:C7	2.36	0.54
2:B:1366:LEU:O	2:B:1366:LEU:HD13	2.07	0.54
2:B:1387:PHE:O	2:B:1388:VAL:HG22	2.07	0.54
2:D:1036:LEU:HD12	2:D:1037:ILE:H	1.72	0.54
2:F:1387:PHE:O	2:F:1388:VAL:HG22	2.07	0.54
2:B:1170:THR:O	2:B:1170:THR:HG23	2.07	0.54
5:C:2001:NAG:C3	5:C:2001:NAG:H83	2.38	0.54
2:D:1084:GLN:HG3	2:D:1162:SER:H	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:PRO:O	1:E:108:ASP:N	2.40	0.54
6:A:2007:B12:C9B	6:A:2007:B12:N22	2.71	0.54
6:C:2007:B12:N22	6:C:2007:B12:C9B	2.71	0.54
1:E:325:VAL:O	1:E:325:VAL:HG23	2.06	0.54
2:D:1170:THR:HG23	2:D:1170:THR:O	2.07	0.54
1:E:182:CYS:HB2	1:E:281:LEU:HD21	1.90	0.54
2:F:942:THR:HG21	2:F:1036:LEU:HD11	1.89	0.54
2:B:1084:GLN:HG3	2:B:1162:SER:H	1.70	0.54
1:C:182:CYS:HB2	1:C:281:LEU:HD21	1.89	0.54
6:C:2007:B12:H8	6:C:2007:B12:O39	2.07	0.54
2:D:1387:PHE:O	2:D:1388:VAL:HG22	2.07	0.54
2:D:942:THR:HG21	2:D:1036:LEU:HD11	1.89	0.54
2:F:1235:LEU:HD11	2:F:1237:THR:O	2.06	0.54
2:F:1249:ARG:HG3	2:F:1250:SER:O	2.07	0.54
1:A:325:VAL:O	1:A:325:VAL:HG23	2.06	0.54
2:B:1192:TYR:CE1	2:B:1258:LYS:HG3	2.43	0.54
1:C:106:PRO:O	1:C:108:ASP:N	2.40	0.54
2:D:1223:LEU:HD23	2:D:1259:LEU:HB2	1.88	0.54
2:D:1377:ARG:O	2:D:1378:ARG:HB2	2.08	0.54
6:E:2007:B12:N22	6:E:2007:B12:C9B	2.71	0.54
2:F:1222:TYR:HE2	2:F:1260:ARG:HD3	1.72	0.54
2:B:1377:ARG:O	2:B:1378:ARG:HB2	2.08	0.54
1:C:337:VAL:HG13	5:C:2001:NAG:H2	1.90	0.54
2:D:999:THR:CG2	2:D:1000:SER:H	2.21	0.54
2:F:1170:THR:HG23	2:F:1170:THR:O	2.07	0.54
1:A:182:CYS:HB2	1:A:281:LEU:HD21	1.89	0.54
1:A:386:TRP:CH2	1:A:414:PHE:HB2	2.43	0.54
2:B:1080:VAL:HG23	2:B:1137:ASN:HB2	1.89	0.54
2:B:1285:ASN:O	2:B:1286:GLN:HG3	2.08	0.54
2:B:1309:THR:HG23	2:B:1367:GLN:CG	2.38	0.54
2:D:1109:ILE:HG23	2:D:1141:LEU:CD2	2.37	0.54
2:D:1177:ILE:HD12	2:D:1181:TYR:CD2	2.42	0.54
2:B:1249:ARG:HG3	2:B:1250:SER:O	2.07	0.53
2:D:1192:TYR:CE1	2:D:1258:LYS:HG3	2.43	0.53
1:E:386:TRP:CH2	1:E:414:PHE:HB2	2.43	0.53
2:F:1342:ASP:CB	2:F:1347:MET:HE2	2.34	0.53
1:A:339:SER:C	1:A:341:SER:H	2.10	0.53
1:E:40:GLN:CG	1:E:272:LEU:HD11	2.30	0.53
2:F:1109:ILE:HG23	2:F:1141:LEU:CD2	2.37	0.53
6:A:2007:B12:H8	6:A:2007:B12:O39	2.07	0.53
1:C:386:TRP:CH2	1:C:414:PHE:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1219:THR:HG23	2:F:1219:THR:O	2.07	0.53
2:F:1285:ASN:O	2:F:1286:GLN:HG3	2.08	0.53
2:F:948:HIS:CD2	2:F:949:PRO:HA	2.44	0.53
1:A:65:GLY:HA3	1:A:292:HIS:CE1	2.44	0.53
2:D:962:ILE:HG23	2:D:1020:LEU:HB2	1.91	0.53
2:D:1285:ASN:O	2:D:1286:GLN:HG3	2.08	0.53
1:E:362:THR:CG2	1:E:371:SER:CB	2.83	0.53
2:F:1377:ARG:O	2:F:1378:ARG:HB2	2.08	0.53
2:B:1219:THR:O	2:B:1219:THR:HG23	2.07	0.53
1:C:326:GLU:HG2	1:C:326:GLU:O	2.09	0.53
6:E:2007:B12:H8	6:E:2007:B12:O39	2.07	0.53
1:E:65:GLY:HA3	1:E:292:HIS:CE1	2.44	0.53
2:F:967:ASN:ND2	2:F:968:HIS:ND1	2.57	0.53
2:B:999:THR:CG2	2:B:1000:SER:H	2.21	0.53
2:B:962:ILE:HG23	2:B:1020:LEU:HB2	1.91	0.53
2:D:1219:THR:O	2:D:1219:THR:HG23	2.07	0.53
2:D:1225:VAL:HG13	2:D:1236:LEU:HB2	1.89	0.53
2:D:989:TYR:C	2:D:989:TYR:CD1	2.83	0.53
2:F:1073:GLU:HB2	2:F:1144:LYS:HD3	1.90	0.53
2:F:962:ILE:HG23	2:F:1020:LEU:HB2	1.91	0.53
2:B:1109:ILE:HG23	2:B:1141:LEU:CD2	2.37	0.53
2:B:948:HIS:CD2	2:B:949:PRO:HA	2.44	0.53
1:C:40:GLN:CG	1:C:272:LEU:HD11	2.30	0.53
1:C:65:GLY:HA3	1:C:292:HIS:CE1	2.44	0.53
2:D:948:HIS:CD2	2:D:949:PRO:HA	2.44	0.53
2:F:1330:HIS:CE1	2:F:1332:ASN:N	2.68	0.53
2:D:1197:SER:OG	2:D:1198:SER:N	2.42	0.53
2:D:1244:LYS:HG2	2:D:1244:LYS:O	2.08	0.53
2:D:993:TYR:HD1	2:D:1000:SER:HB2	1.74	0.53
2:B:1181:TYR:CG	2:B:1182:PRO:HA	2.44	0.52
2:B:1197:SER:OG	2:B:1198:SER:N	2.42	0.52
1:C:146:ASN:ND2	1:C:149:ALA:HB2	2.24	0.52
1:C:337:VAL:CG2	5:C:2001:NAG:O7	2.55	0.52
1:E:326:GLU:O	1:E:326:GLU:HG2	2.09	0.52
2:F:1225:VAL:HG13	2:F:1236:LEU:HB2	1.90	0.52
2:F:1192:TYR:CE1	2:F:1258:LYS:HG3	2.43	0.52
2:B:989:TYR:C	2:B:989:TYR:CD1	2.83	0.52
2:F:1181:TYR:CG	2:F:1182:PRO:HA	2.44	0.52
2:F:1256:PHE:O	2:F:1257:ILE:HG13	2.10	0.52
2:B:1209:ASP:OD2	2:B:1268:ARG:NH1	2.43	0.52
2:D:1073:GLU:HB2	2:D:1144:LYS:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1209:ASP:OD2	2:F:1268:ARG:NH1	2.43	0.52
2:F:1309:THR:HG23	2:F:1367:GLN:CG	2.38	0.52
1:A:326:GLU:O	1:A:326:GLU:HG2	2.09	0.52
2:B:993:TYR:HD1	2:B:1000:SER:HB2	1.75	0.52
2:B:967:ASN:ND2	2:B:968:HIS:ND1	2.57	0.52
2:B:1225:VAL:HG13	2:B:1236:LEU:HB2	1.90	0.52
2:D:1181:TYR:CG	2:D:1182:PRO:HA	2.44	0.52
2:D:967:ASN:ND2	2:D:968:HIS:ND1	2.57	0.52
2:F:1197:SER:OG	2:F:1198:SER:N	2.42	0.52
2:B:1342:ASP:CB	2:B:1347:MET:HE2	2.35	0.52
2:D:1177:ILE:CG2	2:D:1181:TYR:HB3	2.40	0.52
1:E:146:ASN:ND2	1:E:149:ALA:HB2	2.24	0.52
1:E:337:VAL:CG2	5:E:2001:NAG:O7	2.55	0.52
2:F:1035:PHE:C	2:F:1035:PHE:CD1	2.83	0.52
2:B:1328:GLU:HG3	2:B:1336:ASP:OD2	2.10	0.52
2:D:1209:ASP:OD2	2:D:1268:ARG:NH1	2.43	0.52
2:F:989:TYR:C	2:F:989:TYR:CD1	2.83	0.52
1:A:146:ASN:ND2	1:A:149:ALA:HB2	2.24	0.52
2:B:1256:PHE:O	2:B:1257:ILE:HG13	2.10	0.52
1:A:362:THR:CG2	1:A:371:SER:CB	2.83	0.52
2:B:1073:GLU:HB2	2:B:1144:LYS:HD3	1.90	0.52
5:C:2001:NAG:H83	5:C:2001:NAG:O3	2.09	0.52
2:F:1310:ILE:HD13	2:F:1386:TRP:CD2	2.45	0.52
1:C:120:TRP:O	1:C:156:ARG:NH1	2.43	0.51
2:D:1092:ASN:OD1	3:K:1:NAG:N2	2.43	0.51
2:D:1328:GLU:HG3	2:D:1336:ASP:OD2	2.10	0.51
2:B:1035:PHE:CD1	2:B:1035:PHE:C	2.83	0.51
2:B:1092:ASN:OD1	3:H:1:NAG:N2	2.43	0.51
2:D:1247:LEU:HD12	2:D:1247:LEU:C	2.31	0.51
2:F:1029:ASP:C	2:F:1030:LEU:HG	2.30	0.51
2:F:1328:GLU:HG3	2:F:1336:ASP:OD2	2.10	0.51
2:B:1177:ILE:CG2	2:B:1181:TYR:HB3	2.40	0.51
2:F:988:ASP:O	2:F:989:TYR:HB3	2.11	0.51
2:F:1244:LYS:HG2	2:F:1244:LYS:O	2.09	0.51
1:A:120:TRP:O	1:A:156:ARG:NH1	2.43	0.51
1:E:120:TRP:O	1:E:156:ARG:NH1	2.43	0.51
1:E:36:VAL:O	1:E:39:ILE:HG12	2.11	0.51
2:F:1092:ASN:OD1	3:N:1:NAG:N2	2.43	0.51
2:B:1161:SER:O	2:B:1162:SER:HB2	2.11	0.51
2:B:1247:LEU:HD12	2:B:1247:LEU:C	2.31	0.51
2:D:1029:ASP:C	2:D:1030:LEU:HG	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1256:PHE:O	2:D:1257:ILE:HG13	2.10	0.51
2:F:993:TYR:HD1	2:F:1000:SER:HB2	1.74	0.51
2:F:1247:LEU:C	2:F:1247:LEU:HD12	2.31	0.51
2:F:999:THR:CG2	2:F:1000:SER:H	2.21	0.51
2:B:1310:ILE:HD13	2:B:1386:TRP:CD2	2.45	0.51
2:D:1208:LYS:O	2:D:1209:ASP:HB2	2.11	0.51
6:E:2007:B12:C8	6:E:2007:B12:O39	2.59	0.51
1:E:312:ILE:HG22	1:E:313:THR:N	2.26	0.51
2:F:1161:SER:O	2:F:1162:SER:HB2	2.11	0.51
2:B:1029:ASP:C	2:B:1030:LEU:HG	2.30	0.51
1:C:133:TYR:HE1	6:C:2007:B12:H1P1	1.75	0.51
1:C:207:VAL:CG2	1:C:236:THR:HG21	2.41	0.51
2:D:1161:SER:O	2:D:1162:SER:HB2	2.11	0.51
1:E:215:LYS:C	1:E:217:ASN:H	2.14	0.51
1:A:133:TYR:HE1	6:A:2007:B12:H1P1	1.75	0.51
1:A:207:VAL:CG2	1:A:236:THR:HG21	2.41	0.51
1:A:405:PHE:CD1	1:A:408:GLU:HB2	2.46	0.51
1:C:29:PRO:HB2	1:C:32:GLN:HG3	1.93	0.51
2:F:1177:ILE:CG2	2:F:1181:TYR:HB3	2.40	0.51
1:A:215:LYS:C	1:A:217:ASN:H	2.14	0.50
2:B:1029:ASP:OD1	2:B:1029:ASP:N	2.42	0.50
1:C:312:ILE:HG21	1:C:406:ASN:CA	2.35	0.50
2:D:1088:VAL:HG13	2:D:1132:ILE:HB	1.93	0.50
2:B:1192:TYR:HE1	2:B:1258:LYS:CD	2.24	0.50
2:B:1332:ASN:ND2	5:B:2013:NAG:C6	2.74	0.50
1:C:215:LYS:C	1:C:217:ASN:H	2.14	0.50
1:C:405:PHE:CD1	1:C:408:GLU:HB2	2.46	0.50
2:D:1035:PHE:CD1	2:D:1035:PHE:C	2.83	0.50
2:D:1192:TYR:HE1	2:D:1258:LYS:CD	2.24	0.50
1:A:310:SER:CB	2:F:1150:THR:HB	2.41	0.50
1:A:36:VAL:O	1:A:39:ILE:HG12	2.11	0.50
2:B:988:ASP:O	2:B:989:TYR:HB3	2.11	0.50
2:D:1342:ASP:CB	2:D:1347:MET:HE2	2.37	0.50
1:E:90:GLY:HA3	6:E:2007:B12:H3P3	1.93	0.50
1:A:312:ILE:HG21	1:A:406:ASN:CA	2.35	0.50
1:A:374:ASN:O	1:A:375:ASN:HB2	2.11	0.50
2:B:1331:ILE:O	2:B:1331:ILE:HG22	2.12	0.50
2:D:1218:CYS:O	2:D:1219:THR:CB	2.59	0.50
2:B:971:HIS:O	2:B:1039:TYR:HA	2.12	0.50
1:C:36:VAL:O	1:C:39:ILE:HG12	2.11	0.50
1:C:90:GLY:HA3	6:C:2007:B12:H3P3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1296:TYR:CD2	2:D:1297:PRO:CA	2.95	0.50
1:E:374:ASN:O	1:E:375:ASN:HB2	2.11	0.50
1:E:405:PHE:CD1	1:E:408:GLU:HB2	2.46	0.50
2:F:956:ILE:HG22	2:F:957:ASN:H	1.77	0.50
1:C:374:ASN:O	1:C:375:ASN:HB2	2.11	0.50
1:C:44:GLU:HG2	1:C:61:MET:HE3	1.94	0.50
2:D:1310:ILE:HD13	2:D:1386:TRP:CD2	2.45	0.50
1:E:133:TYR:HE1	6:E:2007:B12:H1P1	1.76	0.50
1:E:207:VAL:CG2	1:E:236:THR:HG21	2.41	0.50
2:F:980:GLU:OE1	2:F:1030:LEU:HB2	2.12	0.50
2:F:1281:VAL:CG2	2:F:1308:TRP:CD1	2.95	0.50
2:B:1337:TYR:O	2:B:1370:LEU:HD12	2.11	0.50
6:C:2007:B12:C8	6:C:2007:B12:O39	2.59	0.50
2:F:1037:ILE:HG12	2:F:1037:ILE:O	2.11	0.50
2:B:980:GLU:OE1	2:B:1030:LEU:HB2	2.12	0.50
2:B:1037:ILE:O	2:B:1037:ILE:HG12	2.11	0.50
1:C:89:ILE:HG23	1:C:138:ALA:HB2	1.93	0.50
1:E:309:ALA:HB1	1:E:338:LYS:HG3	1.94	0.50
2:F:1192:TYR:HE1	2:F:1258:LYS:CD	2.24	0.50
2:F:1237:THR:CG2	2:F:1239:LEU:HD13	2.42	0.50
2:D:1237:THR:CG2	2:D:1239:LEU:HD13	2.42	0.50
2:D:1331:ILE:O	2:D:1331:ILE:HG22	2.12	0.50
2:D:988:ASP:O	2:D:989:TYR:HB3	2.11	0.50
1:E:89:ILE:HG23	1:E:138:ALA:HB2	1.93	0.50
1:E:44:GLU:HG2	1:E:61:MET:HE3	1.94	0.50
2:F:968:HIS:O	2:F:969:LEU:HD12	2.12	0.50
2:B:1332:ASN:ND2	5:B:2013:NAG:H62	2.27	0.49
1:C:124:SER:HB2	1:C:126:ASN:OD1	2.12	0.49
1:C:88:THR:O	1:C:91:HIS:HB2	2.12	0.49
2:D:1037:ILE:O	2:D:1037:ILE:HG12	2.11	0.49
2:D:1281:VAL:HG21	2:D:1308:TRP:HD1	1.77	0.49
2:D:971:HIS:O	2:D:1039:TYR:HA	2.12	0.49
1:E:29:PRO:HB2	1:E:32:GLN:HG3	1.92	0.49
2:F:1222:TYR:CD2	2:F:1222:TYR:N	2.80	0.49
2:B:1088:VAL:HG13	2:B:1132:ILE:HB	1.93	0.49
2:B:1296:TYR:CD2	2:B:1297:PRO:CA	2.95	0.49
2:B:968:HIS:O	2:B:969:LEU:HD12	2.12	0.49
2:D:956:ILE:HG22	2:D:957:ASN:H	1.77	0.49
1:E:124:SER:HB2	1:E:126:ASN:OD1	2.12	0.49
1:A:124:SER:HB2	1:A:126:ASN:OD1	2.12	0.49
1:A:89:ILE:HG23	1:A:138:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HB2	1:A:32:GLN:HG3	1.92	0.49
2:D:1302:GLU:O	2:D:1303:ASN:HB2	2.11	0.49
2:B:1222:TYR:CD2	2:B:1222:TYR:N	2.80	0.49
2:B:1237:THR:CG2	2:B:1239:LEU:HD13	2.42	0.49
2:D:1332:ASN:ND2	5:D:2013:NAG:C6	2.76	0.49
2:F:1029:ASP:OD1	2:F:1029:ASP:N	2.43	0.49
2:F:951:VAL:HB	2:F:1032:TYR:C	2.33	0.49
2:F:1079:THR:HG23	2:F:1138:LYS:CG	2.23	0.49
2:F:1332:ASN:ND2	5:F:2013:NAG:C6	2.75	0.49
2:F:1332:ASN:ND2	5:F:2013:NAG:H62	2.28	0.49
1:A:88:THR:O	1:A:91:HIS:HB2	2.12	0.49
2:B:1218:CYS:O	2:B:1219:THR:CB	2.59	0.49
2:B:1302:GLU:O	2:B:1303:ASN:HB2	2.12	0.49
2:D:968:HIS:O	2:D:969:LEU:HD12	2.12	0.49
1:E:283:VAL:HG12	1:E:284:PRO:HD3	1.94	0.49
2:F:1337:TYR:O	2:F:1370:LEU:HD12	2.11	0.49
1:A:309:ALA:HB1	1:A:338:LYS:HG3	1.94	0.49
1:A:90:GLY:HA3	6:A:2007:B12:H3P3	1.93	0.49
2:D:1337:TYR:O	2:D:1370:LEU:HD12	2.11	0.49
1:E:88:THR:O	1:E:91:HIS:HB2	2.12	0.49
2:F:1218:CYS:O	2:F:1219:THR:CB	2.59	0.49
1:C:351:GLN:OE1	1:C:358:LYS:HG3	2.13	0.49
2:D:1281:VAL:CG2	2:D:1308:TRP:CD1	2.95	0.49
2:D:1309:THR:HG23	2:D:1367:GLN:CG	2.38	0.49
2:F:971:HIS:O	2:F:1039:TYR:HA	2.12	0.49
2:F:1296:TYR:CD2	2:F:1297:PRO:CA	2.95	0.49
2:B:1281:VAL:CG2	2:B:1308:TRP:CD1	2.95	0.49
2:D:951:VAL:HB	2:D:1032:TYR:C	2.33	0.49
2:F:1008:SER:HB2	2:F:1183:MET:SD	2.53	0.49
2:F:1237:THR:HG22	2:F:1239:LEU:HD13	1.94	0.49
1:A:351:GLN:OE1	1:A:358:LYS:HG3	2.13	0.49
2:B:951:VAL:HB	2:B:1032:TYR:C	2.33	0.49
6:C:2007:B12:H253	6:C:2007:B12:H302	1.54	0.49
2:F:1088:VAL:HG13	2:F:1132:ILE:HB	1.93	0.49
2:F:1281:VAL:HG21	2:F:1308:TRP:HD1	1.77	0.49
2:B:1176:PHE:HD2	2:B:1193:TRP:CE3	2.31	0.49
2:B:1185:TYR:CZ	2:B:1266:GLN:HA	2.48	0.49
2:D:1008:SER:HB2	2:D:1183:MET:SD	2.53	0.49
2:D:980:GLU:OE1	2:D:1030:LEU:HB2	2.12	0.49
1:A:44:GLU:HG2	1:A:61:MET:HE3	1.95	0.48
2:B:1008:SER:HB2	2:B:1183:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2007:B12:H312	6:C:2007:B12:C35	2.34	0.48
2:D:1185:TYR:CZ	2:D:1266:GLN:HA	2.48	0.48
1:E:351:GLN:OE1	1:E:358:LYS:HG3	2.12	0.48
2:F:1304:GLN:HB2	2:F:1372:THR:CG2	2.43	0.48
2:B:1281:VAL:HG21	2:B:1308:TRP:HD1	1.77	0.48
1:C:148:GLU:HG3	1:C:188:PRO:CG	2.43	0.48
1:C:228:LEU:O	1:C:231:GLN:HB2	2.13	0.48
2:D:1237:THR:HG22	2:D:1239:LEU:HD13	1.94	0.48
1:E:312:ILE:HG21	1:E:406:ASN:CA	2.35	0.48
2:F:1004:TYR:CG	2:F:1009:ILE:HD12	2.48	0.48
2:F:1185:TYR:CZ	2:F:1266:GLN:HA	2.48	0.48
2:F:1302:GLU:O	2:F:1303:ASN:HB2	2.12	0.48
4:O:1:NAG:HO3	4:O:2:NAG:H2	1.76	0.48
1:A:283:VAL:HG12	1:A:284:PRO:HD3	1.94	0.48
2:D:1093:PHE:HB3	2:D:1128:LEU:HD23	1.95	0.48
2:D:1192:TYR:HE1	2:D:1258:LYS:HG3	1.78	0.48
1:E:148:GLU:HG3	1:E:188:PRO:CG	2.43	0.48
2:F:1192:TYR:HE1	2:F:1258:LYS:HG3	1.78	0.48
2:B:1004:TYR:CG	2:B:1009:ILE:HD12	2.48	0.48
2:B:1237:THR:HG22	2:B:1239:LEU:HD13	1.94	0.48
2:B:1304:GLN:HB2	2:B:1372:THR:CG2	2.43	0.48
1:C:133:TYR:CE1	6:C:2007:B12:H1P1	2.48	0.48
2:D:1222:TYR:CD2	2:D:1222:TYR:N	2.80	0.48
6:A:2007:B12:C8	6:A:2007:B12:O39	2.59	0.48
2:B:1093:PHE:HB3	2:B:1128:LEU:HD23	1.96	0.48
1:C:312:ILE:HG22	1:C:313:THR:N	2.27	0.48
2:D:1337:TYR:OH	2:D:1371:LEU:HD22	2.14	0.48
1:E:133:TYR:CE1	6:E:2007:B12:H1P1	2.49	0.48
2:F:1067:ASN:HB3	2:F:1150:THR:HG21	1.91	0.48
2:F:1093:PHE:HB3	2:F:1128:LEU:HD23	1.96	0.48
2:B:956:ILE:HG22	2:B:957:ASN:H	1.77	0.48
1:C:309:ALA:HB1	1:C:338:LYS:HG3	1.94	0.48
1:E:255:ASN:O	1:E:259:GLN:HG2	2.13	0.48
2:F:1176:PHE:HD2	2:F:1193:TRP:CE3	2.31	0.48
2:F:1218:CYS:O	2:F:1219:THR:HB	2.13	0.48
2:F:1331:ILE:HG22	2:F:1331:ILE:O	2.12	0.48
2:F:1337:TYR:OH	2:F:1371:LEU:HD22	2.14	0.48
2:B:1337:TYR:OH	2:B:1371:LEU:HD22	2.14	0.48
1:C:255:ASN:O	1:C:259:GLN:HG2	2.13	0.48
1:C:283:VAL:HG12	1:C:284:PRO:HD3	1.94	0.48
3:H:2:NAG:O3	3:H:5:MAN:H3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLU:HG3	1:A:188:PRO:CG	2.43	0.48
2:D:1004:TYR:CG	2:D:1009:ILE:HD12	2.48	0.48
2:D:1218:CYS:O	2:D:1219:THR:HB	2.13	0.48
2:F:1004:TYR:CD1	2:F:1009:ILE:HD12	2.49	0.48
2:F:1310:ILE:HB	2:F:1366:LEU:HD12	1.96	0.48
2:F:981:PHE:CD1	2:F:982:HIS:N	2.82	0.48
1:A:133:TYR:CE1	6:A:2007:B12:H1P1	2.48	0.48
1:A:255:ASN:O	1:A:259:GLN:HG2	2.13	0.48
2:D:947:GLY:HA3	2:D:951:VAL:O	2.14	0.48
1:A:228:LEU:O	1:A:231:GLN:HB2	2.13	0.48
2:B:1218:CYS:O	2:B:1219:THR:HB	2.13	0.48
2:D:1304:GLN:HB2	2:D:1372:THR:CG2	2.43	0.48
2:D:1310:ILE:HB	2:D:1366:LEU:HD12	1.96	0.48
1:E:362:THR:HG22	1:E:371:SER:CB	2.35	0.48
3:G:3:BMA:H4	3:G:5:MAN:C2	2.41	0.48
2:B:1067:ASN:HB3	2:B:1150:THR:HG21	1.91	0.47
2:B:1109:ILE:HD12	2:B:1123:PHE:CE2	2.49	0.47
2:B:1193:TRP:CD1	2:B:1193:TRP:N	2.82	0.47
2:D:1304:GLN:H	2:D:1372:THR:CG2	2.24	0.47
3:K:2:NAG:O3	3:K:5:MAN:H3	2.14	0.47
2:B:1004:TYR:CD1	2:B:1009:ILE:HD12	2.49	0.47
2:B:1187:HIS:HB3	2:B:1266:GLN:HE22	1.78	0.47
2:F:1193:TRP:CD1	2:F:1193:TRP:N	2.82	0.47
2:F:1187:HIS:CB	2:F:1266:GLN:NE2	2.75	0.47
2:F:1092:ASN:OD1	3:N:1:NAG:C2	2.61	0.47
1:A:287:THR:HG22	1:A:288:CYS:N	2.29	0.47
2:B:1192:TYR:HE1	2:B:1258:LYS:HG3	1.78	0.47
1:C:354:ASN:C	1:C:354:ASN:OD1	2.53	0.47
2:D:1004:TYR:CD1	2:D:1009:ILE:HD12	2.49	0.47
1:E:228:LEU:O	1:E:231:GLN:HB2	2.13	0.47
2:B:1092:ASN:OD1	3:H:1:NAG:C2	2.61	0.47
2:B:1294:ILE:HG13	2:B:1295:GLY:H	1.79	0.47
2:B:1310:ILE:HB	2:B:1366:LEU:HD12	1.96	0.47
2:B:947:GLY:HA3	2:B:951:VAL:O	2.14	0.47
2:D:1294:ILE:HG13	2:D:1295:GLY:H	1.79	0.47
1:E:389:LEU:CD2	1:E:389:LEU:N	2.76	0.47
1:A:312:ILE:HG22	1:A:313:THR:N	2.27	0.47
1:A:354:ASN:OD1	1:A:354:ASN:C	2.53	0.47
1:A:389:LEU:CD2	1:A:389:LEU:N	2.76	0.47
2:B:1128:LEU:HA	2:B:1128:LEU:HD23	1.65	0.47
2:B:1314:THR:HG22	2:B:1315:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:LEU:CD2	1:C:389:LEU:N	2.76	0.47
2:D:1035:PHE:HD1	2:D:1035:PHE:C	2.17	0.47
2:D:1176:PHE:HD2	2:D:1193:TRP:CE3	2.31	0.47
2:D:1225:VAL:HG23	2:D:1257:ILE:HG12	1.96	0.47
2:D:981:PHE:CD1	2:D:982:HIS:N	2.82	0.47
2:B:981:PHE:CD1	2:B:982:HIS:N	2.82	0.47
2:D:1193:TRP:CD1	2:D:1193:TRP:N	2.82	0.47
1:E:287:THR:HG22	1:E:288:CYS:N	2.29	0.47
2:F:1294:ILE:HG13	2:F:1295:GLY:H	1.79	0.47
2:B:1225:VAL:HG23	2:B:1257:ILE:HG12	1.96	0.47
2:D:1109:ILE:HD12	2:D:1123:PHE:CE2	2.49	0.47
1:E:135:PRO:O	1:E:139:ILE:HG13	2.14	0.47
2:F:1060:THR:HG21	2:F:1064:PHE:HB3	1.96	0.47
2:F:947:GLY:HA3	2:F:951:VAL:O	2.14	0.47
1:C:320:ASN:O	1:C:327:LEU:HB2	2.15	0.47
2:F:1314:THR:HG22	2:F:1315:GLY:N	2.29	0.47
1:A:320:ASN:O	1:A:327:LEU:HB2	2.15	0.47
1:C:287:THR:HG22	1:C:288:CYS:N	2.29	0.47
2:D:1060:THR:HG21	2:D:1064:PHE:HB3	1.96	0.47
1:E:354:ASN:C	1:E:354:ASN:OD1	2.53	0.47
3:N:2:NAG:O3	3:N:5:MAN:H3	2.14	0.47
1:A:318:ILE:O	1:A:318:ILE:CG1	2.63	0.47
2:B:1140:TRP:O	2:B:1141:LEU:HD23	2.15	0.47
2:B:1208:LYS:O	2:B:1209:ASP:HB2	2.13	0.47
1:C:318:ILE:CG1	1:C:318:ILE:O	2.63	0.47
2:D:1140:TRP:O	2:D:1141:LEU:HD23	2.15	0.47
2:D:1067:ASN:ND2	2:D:1150:THR:HG22	2.29	0.47
2:D:1229:PRO:HG3	2:D:1254:SER:OG	2.15	0.47
2:D:1092:ASN:OD1	3:K:1:NAG:C2	2.61	0.47
1:C:135:PRO:O	1:C:139:ILE:HG13	2.14	0.47
6:A:2007:B12:H312	6:A:2007:B12:C35	2.34	0.46
2:B:1045:ALA:C	2:B:1047:ALA:H	2.19	0.46
1:E:308:SER:O	1:E:309:ALA:CB	2.64	0.46
2:F:1140:TRP:O	2:F:1141:LEU:HD23	2.15	0.46
2:F:1162:SER:C	2:F:1164:GLY:H	2.18	0.46
1:A:135:PRO:O	1:A:139:ILE:HG13	2.14	0.46
2:D:1314:THR:HG22	2:D:1315:GLY:N	2.29	0.46
2:D:1332:ASN:ND2	5:D:2013:NAG:H62	2.30	0.46
1:E:318:ILE:O	1:E:318:ILE:CG1	2.63	0.46
2:F:1045:ALA:C	2:F:1047:ALA:H	2.19	0.46
3:M:3:BMA:H4	3:M:5:MAN:C2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:ASN:HA	1:E:355:PRO:HD3	1.71	0.46
2:F:1061:SER:HB3	2:F:1154:PHE:CD2	2.51	0.46
2:F:1109:ILE:HD12	2:F:1123:PHE:CE2	2.49	0.46
4:L:1:NAG:HO3	4:L:2:NAG:H2	1.80	0.46
2:D:1215:HIS:HB2	2:D:1220:LEU:CD1	2.45	0.46
1:E:283:VAL:O	1:E:286:VAL:HG23	2.16	0.46
1:E:320:ASN:O	1:E:327:LEU:HB2	2.15	0.46
2:F:1225:VAL:HG23	2:F:1257:ILE:HG12	1.96	0.46
4:L:1:NAG:H2	4:L:1:NAG:H82	1.65	0.46
1:A:283:VAL:O	1:A:286:VAL:HG23	2.16	0.46
2:B:1035:PHE:C	2:B:1035:PHE:HD1	2.17	0.46
2:B:1061:SER:HB3	2:B:1154:PHE:CD2	2.51	0.46
2:B:1217:ASN:HB2	5:B:2008:NAG:H61	1.98	0.46
2:B:982:HIS:CD2	2:B:987:ASN:HB2	2.51	0.46
1:E:228:LEU:HA	1:E:228:LEU:HD23	1.66	0.46
2:F:1084:GLN:HG2	2:F:1161:SER:CA	2.46	0.46
2:D:1081:ARG:NH2	2:D:1084:GLN:HE22	2.14	0.46
2:F:952:TYR:HA	2:F:953:PRO:HD3	1.78	0.46
2:B:1067:ASN:ND2	2:B:1150:THR:HG22	2.29	0.46
2:B:1176:PHE:N	2:B:1176:PHE:CD1	2.84	0.46
2:B:1243:GLU:O	2:B:1245:PRO:HD3	2.16	0.46
2:B:1187:HIS:CB	2:B:1266:GLN:NE2	2.75	0.46
1:C:308:SER:O	1:C:309:ALA:CB	2.64	0.46
2:F:1067:ASN:ND2	2:F:1150:THR:HG22	2.30	0.46
2:F:1215:HIS:HB2	2:F:1220:LEU:CD1	2.45	0.46
2:F:1229:PRO:HG3	2:F:1254:SER:OG	2.15	0.46
2:F:982:HIS:CD2	2:F:987:ASN:HB2	2.51	0.46
1:A:403:ILE:HA	1:A:404:PRO:HD3	1.70	0.46
2:B:1215:HIS:HB2	2:B:1220:LEU:CD1	2.45	0.46
2:B:1229:PRO:HG3	2:B:1254:SER:OG	2.15	0.46
1:C:281:LEU:HA	1:C:281:LEU:HD23	1.80	0.46
2:D:1045:ALA:C	2:D:1047:ALA:H	2.19	0.46
2:D:1187:HIS:HB3	2:D:1266:GLN:HE22	1.78	0.46
6:E:2007:B12:H312	6:E:2007:B12:C35	2.35	0.46
2:F:1178:SER:HB3	2:F:1270:PHE:CE2	2.51	0.46
2:F:1205:LEU:HB2	2:F:1248:ILE:HB	1.98	0.46
3:M:3:BMA:C4	3:M:5:MAN:H2	2.42	0.46
2:B:1081:ARG:NH2	2:B:1084:GLN:HE22	2.14	0.46
1:C:283:VAL:O	1:C:286:VAL:HG23	2.16	0.46
2:D:1061:SER:HB3	2:D:1154:PHE:CD2	2.51	0.46
2:D:1176:PHE:CD1	2:D:1176:PHE:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:2007:B12:H253	6:E:2007:B12:H302	1.54	0.46
2:B:1178:SER:HB3	2:B:1270:PHE:CE2	2.51	0.45
1:C:180:LEU:HA	1:C:180:LEU:HD12	1.49	0.45
2:D:1205:LEU:HB2	2:D:1248:ILE:HB	1.98	0.45
2:F:1208:LYS:O	2:F:1209:ASP:HB2	2.14	0.45
4:I:1:NAG:HO3	4:I:2:NAG:H2	1.78	0.45
1:A:308:SER:O	1:A:309:ALA:CB	2.64	0.45
2:B:1084:GLN:HG2	2:B:1161:SER:CA	2.46	0.45
2:B:1338:LEU:C	2:B:1338:LEU:HD23	2.37	0.45
2:D:982:HIS:CD2	2:D:987:ASN:HB2	2.51	0.45
1:E:86:ASP:OD1	1:E:86:ASP:N	2.49	0.45
4:O:1:NAG:H82	4:O:1:NAG:H2	1.65	0.45
2:B:1056:LEU:O	2:B:1158:TRP:CZ2	2.70	0.45
2:D:1243:GLU:O	2:D:1245:PRO:HD3	2.16	0.45
2:D:1338:LEU:C	2:D:1338:LEU:HD23	2.37	0.45
2:F:1035:PHE:C	2:F:1035:PHE:HD1	2.17	0.45
2:B:999:THR:CG2	2:B:1000:SER:N	2.78	0.45
2:D:1162:SER:C	2:D:1164:GLY:H	2.19	0.45
1:E:180:LEU:HD12	1:E:180:LEU:HA	1.49	0.45
2:F:1081:ARG:NH2	2:F:1084:GLN:HE22	2.14	0.45
2:F:1243:GLU:O	2:F:1245:PRO:HD3	2.16	0.45
1:A:335:VAL:CG2	5:A:2001:NAG:H5	2.46	0.45
1:A:335:VAL:HG23	5:A:2001:NAG:H5	1.99	0.45
2:B:1196:LYS:HA	2:B:1203:PHE:HE1	1.82	0.45
2:B:982:HIS:HB3	2:B:985:CYS:HA	1.98	0.45
2:D:1067:ASN:HB3	2:D:1150:THR:HG21	1.91	0.45
2:D:1056:LEU:O	2:D:1158:TRP:CZ2	2.70	0.45
2:D:1260:ARG:HG2	2:D:1261:THR:N	2.31	0.45
5:E:2001:NAG:C3	5:E:2001:NAG:H83	2.46	0.45
2:F:1196:LYS:HA	2:F:1203:PHE:HE1	1.82	0.45
2:F:1338:LEU:HD23	2:F:1338:LEU:C	2.37	0.45
2:B:1060:THR:HG21	2:B:1064:PHE:HB3	1.96	0.45
2:B:1169:LEU:HD12	2:B:1169:LEU:H	1.82	0.45
2:B:1196:LYS:HA	2:B:1203:PHE:CE1	2.52	0.45
2:B:1304:GLN:H	2:B:1372:THR:CG2	2.24	0.45
2:B:952:TYR:HE1	2:B:988:ASP:OD2	2.00	0.45
2:D:1245:PRO:HA	2:D:1246:PRO:HD3	1.67	0.45
1:A:362:THR:HG22	1:A:371:SER:CB	2.35	0.45
2:B:1317:THR:O	2:B:1388:VAL:HA	2.17	0.45
2:F:1169:LEU:H	2:F:1169:LEU:HD12	1.82	0.45
3:J:3:BMA:H4	3:J:5:MAN:C2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD13	1:A:94:LEU:HA	1.78	0.45
1:A:201:GLN:HE22	2:B:1147:GLN:HG2	1.82	0.45
2:F:999:THR:CG2	2:F:1000:SER:N	2.78	0.45
2:F:992:VAL:HG13	2:F:1001:LEU:HB2	1.98	0.45
2:F:1196:LYS:HA	2:F:1203:PHE:CE1	2.52	0.45
2:F:1217:ASN:HB2	5:F:2008:NAG:H61	1.98	0.45
2:F:1304:GLN:H	2:F:1372:THR:CG2	2.24	0.45
3:G:3:BMA:C4	3:G:5:MAN:H2	2.42	0.45
1:A:281:LEU:HA	1:A:281:LEU:HD23	1.80	0.45
2:B:1205:LEU:HB2	2:B:1248:ILE:HB	1.98	0.45
2:D:1196:LYS:HA	2:D:1203:PHE:CE1	2.52	0.45
2:D:1350:TYR:CD1	2:D:1356:PRO:HB3	2.52	0.45
1:E:58:LEU:HB2	1:E:75:LEU:HD23	1.98	0.45
1:A:310:SER:HB2	2:F:1150:THR:HB	1.98	0.45
2:F:1245:PRO:HA	2:F:1246:PRO:HD3	1.67	0.45
1:A:146:ASN:ND2	1:A:149:ALA:CB	2.80	0.45
2:B:1013:LEU:HD23	2:B:1013:LEU:HA	1.81	0.45
1:C:58:LEU:HB2	1:C:75:LEU:HD23	1.99	0.45
2:D:1084:GLN:HG2	2:D:1161:SER:CA	2.46	0.45
2:F:1260:ARG:HG2	2:F:1261:THR:N	2.31	0.45
1:A:58:LEU:HB2	1:A:75:LEU:HD23	1.98	0.44
1:A:86:ASP:OD1	1:A:86:ASP:N	2.49	0.44
1:A:89:ILE:HG22	1:A:90:GLY:N	2.32	0.44
2:B:1162:SER:C	2:B:1164:GLY:H	2.19	0.44
2:D:1338:LEU:HA	2:D:1369:LEU:O	2.17	0.44
1:E:146:ASN:ND2	1:E:149:ALA:CB	2.80	0.44
2:F:1056:LEU:O	2:F:1158:TRP:CZ2	2.70	0.44
1:E:201:GLN:HE22	2:F:1147:GLN:HG2	1.82	0.44
2:B:1043:SER:O	2:B:1047:ALA:HB2	2.17	0.44
1:C:146:ASN:ND2	1:C:149:ALA:CB	2.81	0.44
1:C:29:PRO:HB2	1:C:32:GLN:HG2	1.99	0.44
2:D:992:VAL:HG13	2:D:1001:LEU:HB2	1.99	0.44
2:D:1095:LEU:HD21	2:D:1143:PHE:HE1	1.82	0.44
1:C:201:GLN:HE22	2:D:1147:GLN:HG2	1.82	0.44
2:D:1178:SER:HB3	2:D:1270:PHE:CE2	2.51	0.44
2:D:1317:THR:O	2:D:1388:VAL:HA	2.17	0.44
2:D:982:HIS:HB3	2:D:985:CYS:HA	1.99	0.44
2:F:1317:THR:O	2:F:1388:VAL:HA	2.17	0.44
2:F:952:TYR:HE1	2:F:988:ASP:OD2	1.99	0.44
2:F:982:HIS:HB3	2:F:985:CYS:HA	1.99	0.44
1:A:180:LEU:HA	1:A:180:LEU:HD12	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2007:B12:H253	6:A:2007:B12:H302	1.54	0.44
1:C:298:LEU:N	1:C:299:PRO:HD3	2.32	0.44
2:D:1043:SER:O	2:D:1047:ALA:HB2	2.17	0.44
2:D:1093:PHE:C	2:D:1093:PHE:CD2	2.90	0.44
2:D:1169:LEU:HD12	2:D:1169:LEU:H	1.82	0.44
2:D:1217:ASN:HB2	5:D:2008:NAG:H61	1.98	0.44
1:E:281:LEU:HD23	1:E:281:LEU:HA	1.80	0.44
2:F:1176:PHE:CD1	2:F:1176:PHE:N	2.84	0.44
1:A:369:VAL:HG13	6:A:2007:B12:O44	2.17	0.44
2:B:1093:PHE:C	2:B:1093:PHE:CD2	2.91	0.44
2:B:1146:ASP:HB2	2:B:1147:GLN:OE1	2.17	0.44
1:C:369:VAL:HG13	6:C:2007:B12:O44	2.17	0.44
1:C:89:ILE:HG22	1:C:90:GLY:N	2.32	0.44
2:D:1146:ASP:HB2	2:D:1147:GLN:OE1	2.17	0.44
2:F:1067:ASN:HB3	2:F:1150:THR:HG22	1.98	0.44
3:J:3:BMA:C4	3:J:5:MAN:H2	2.42	0.44
6:A:2007:B12:H18	6:A:2007:B12:H562	1.87	0.44
1:C:403:ILE:HA	1:C:404:PRO:HD3	1.70	0.44
1:E:142:LEU:HA	1:E:142:LEU:HD12	1.82	0.44
1:E:369:VAL:HG13	6:E:2007:B12:O44	2.17	0.44
1:E:379:ASN:ND2	1:E:382:HIS:ND1	2.66	0.44
2:F:1338:LEU:HA	2:F:1369:LEU:O	2.17	0.44
2:B:992:VAL:HG13	2:B:1001:LEU:HB2	1.99	0.44
2:B:1260:ARG:HG2	2:B:1261:THR:N	2.31	0.44
2:D:1196:LYS:HA	2:D:1203:PHE:HE1	1.82	0.44
2:D:1291:LEU:HA	2:D:1291:LEU:HD23	1.64	0.44
2:D:952:TYR:HE1	2:D:988:ASP:OD2	2.00	0.44
1:E:54:ASN:HB3	1:E:57:ILE:HD12	2.00	0.44
2:F:1043:SER:O	2:F:1047:ALA:HB2	2.17	0.44
2:F:1093:PHE:CD2	2:F:1093:PHE:C	2.90	0.44
1:A:390:SER:O	1:A:392:VAL:N	2.47	0.44
2:B:1243:GLU:CA	2:B:1243:GLU:OE1	2.65	0.44
2:B:1338:LEU:HA	2:B:1369:LEU:O	2.17	0.44
2:B:978:HIS:CE1	2:B:1007:LYS:NZ	2.85	0.44
1:C:86:ASP:N	1:C:86:ASP:OD1	2.49	0.44
1:A:298:LEU:N	1:A:299:PRO:HD3	2.32	0.44
1:C:151:LEU:HD22	1:C:195:TYR:CD2	2.53	0.44
1:C:379:ASN:ND2	1:C:382:HIS:ND1	2.66	0.44
2:D:1190:GLU:HG2	2:D:1260:ARG:HB2	2.00	0.44
1:E:151:LEU:HD22	1:E:195:TYR:CD2	2.53	0.44
2:F:989:TYR:CZ	2:F:1025:VAL:HG12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1190:GLU:HG2	2:B:1260:ARG:HB2	2.00	0.44
2:B:1291:LEU:HA	2:B:1291:LEU:HD23	1.64	0.44
2:D:989:TYR:CZ	2:D:1025:VAL:HG12	2.53	0.44
2:F:1146:ASP:HB2	2:F:1147:GLN:OE1	2.17	0.44
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.78	0.43
2:D:967:ASN:ND2	2:D:968:HIS:CE1	2.87	0.43
1:E:405:PHE:CE1	1:E:408:GLU:HB2	2.53	0.43
2:F:1190:GLU:HG2	2:F:1260:ARG:HB2	2.00	0.43
2:F:1289:GLY:O	2:F:1290:ILE:HD13	2.18	0.43
2:F:1350:TYR:CD1	2:F:1356:PRO:HB3	2.52	0.43
2:B:1022:LEU:HD23	2:B:1022:LEU:HA	1.66	0.43
2:F:1176:PHE:CD2	2:F:1193:TRP:CE3	3.07	0.43
2:B:1046:THR:HG22	2:B:1046:THR:O	2.18	0.43
2:D:1187:HIS:CB	2:D:1266:GLN:NE2	2.75	0.43
1:E:298:LEU:N	1:E:299:PRO:HD3	2.32	0.43
2:F:1022:LEU:HD23	2:F:1022:LEU:HA	1.66	0.43
2:F:1089:HIS:HB2	2:F:1157:TYR:CZ	2.53	0.43
2:F:1178:SER:HB3	2:F:1270:PHE:CD2	2.53	0.43
6:A:2007:B12:H363	6:A:2007:B12:H411	1.48	0.43
1:A:29:PRO:HB2	1:A:32:GLN:HG2	2.00	0.43
1:A:379:ASN:ND2	1:A:382:HIS:ND1	2.66	0.43
2:B:989:TYR:CZ	2:B:1025:VAL:HG12	2.53	0.43
6:C:2007:B12:H251	6:C:2007:B12:N29	2.32	0.43
1:C:405:PHE:CE1	1:C:408:GLU:HB2	2.53	0.43
2:D:1046:THR:HG22	2:D:1046:THR:O	2.18	0.43
2:D:1128:LEU:HD23	2:D:1128:LEU:HA	1.65	0.43
1:E:352:ARG:CG	1:E:352:ARG:NH1	2.72	0.43
6:A:2007:B12:H251	6:A:2007:B12:N29	2.32	0.43
2:B:1095:LEU:HD21	2:B:1143:PHE:HE1	1.83	0.43
2:B:1176:PHE:CD2	2:B:1193:TRP:CE3	3.07	0.43
1:C:177:THR:CG2	1:C:206:ILE:HG21	2.42	0.43
1:C:317:THR:HB	1:C:411:THR:HG23	2.01	0.43
2:F:1387:PHE:C	2:F:1388:VAL:CG2	2.87	0.43
1:A:317:THR:HB	1:A:411:THR:HG23	2.01	0.43
2:B:942:THR:HG22	2:B:1036:LEU:HD11	1.99	0.43
2:B:1289:GLY:O	2:B:1290:ILE:HD13	2.18	0.43
2:B:967:ASN:ND2	2:B:968:HIS:CE1	2.87	0.43
2:D:1219:THR:O	2:D:1219:THR:CG2	2.66	0.43
2:D:948:HIS:HA	2:D:950:ASN:N	2.34	0.43
1:E:369:VAL:HG12	1:E:370:VAL:N	2.34	0.43
1:E:89:ILE:HG22	1:E:90:GLY:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1084:GLN:N	2:F:1084:GLN:OE1	2.51	0.43
2:F:1177:ILE:HG23	2:F:1181:TYR:CB	2.47	0.43
2:F:942:THR:HG22	2:F:1036:LEU:HD11	1.99	0.43
2:F:948:HIS:HA	2:F:950:ASN:N	2.34	0.43
6:A:2007:B12:C48	6:A:2007:B12:H533	2.49	0.43
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.66	0.43
1:A:54:ASN:HB3	1:A:57:ILE:HD12	2.00	0.43
2:B:1350:TYR:CD1	2:B:1356:PRO:HB3	2.53	0.43
2:B:948:HIS:HA	2:B:950:ASN:N	2.34	0.43
2:D:988:ASP:OD2	2:D:1026:THR:HB	2.19	0.43
2:D:1061:SER:HB3	2:D:1154:PHE:H	1.84	0.43
2:D:1387:PHE:C	2:D:1388:VAL:CG2	2.87	0.43
1:E:279:THR:C	1:E:281:LEU:N	2.72	0.43
2:F:1046:THR:HG22	2:F:1046:THR:O	2.18	0.43
2:F:954:HIS:HD2	2:F:954:HIS:H	1.59	0.43
2:F:967:ASN:ND2	2:F:968:HIS:CE1	2.86	0.43
1:A:405:PHE:CE1	1:A:408:GLU:HB2	2.53	0.43
2:B:1089:HIS:HB2	2:B:1157:TYR:CZ	2.53	0.43
2:B:1248:ILE:HG22	2:B:1248:ILE:O	2.19	0.43
2:D:1289:GLY:O	2:D:1290:ILE:HD13	2.19	0.43
2:F:1179:PRO:C	2:F:1181:TYR:H	2.22	0.43
2:F:1312:ALA:O	2:F:1364:SER:HB2	2.19	0.43
2:F:1313:THR:HG22	5:F:2009:NAG:C8	2.41	0.43
2:F:988:ASP:OD2	2:F:1026:THR:HB	2.19	0.43
4:I:1:NAG:H2	4:I:1:NAG:H82	1.65	0.43
1:A:151:LEU:HD22	1:A:195:TYR:CD2	2.53	0.43
2:B:1219:THR:O	2:B:1219:THR:CG2	2.66	0.43
2:B:1312:ALA:O	2:B:1364:SER:HB2	2.19	0.43
2:B:952:TYR:HA	2:B:953:PRO:HD3	1.78	0.43
2:B:964:VAL:CG2	2:B:965:GLN:N	2.82	0.43
1:C:130:SER:HA	1:C:172:THR:OG1	2.19	0.43
2:D:1057:GLY:HA3	2:D:1157:TYR:CA	2.48	0.43
2:D:1302:GLU:HB3	2:D:1374:GLY:HA2	2.01	0.43
1:E:29:PRO:HB2	1:E:32:GLN:HG2	1.99	0.43
1:E:336:SER:O	1:E:337:VAL:C	2.58	0.43
2:F:1139:LEU:HD23	2:F:1139:LEU:HA	1.87	0.43
2:B:1178:SER:HB3	2:B:1270:PHE:CD2	2.53	0.43
1:C:389:LEU:CB	1:C:394:PRO:HA	2.45	0.43
1:C:54:ASN:HB3	1:C:57:ILE:HD12	2.00	0.43
2:D:978:HIS:CE1	2:D:1007:LYS:NZ	2.87	0.43
2:D:1089:HIS:HB2	2:D:1157:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1243:GLU:CA	2:D:1243:GLU:OE1	2.65	0.43
2:D:1248:ILE:HG22	2:D:1248:ILE:O	2.19	0.43
2:D:1304:GLN:HG3	2:D:1372:THR:HG21	2.01	0.43
2:D:1355:LEU:HA	2:D:1356:PRO:HD3	1.92	0.43
6:E:2007:B12:N29	6:E:2007:B12:H251	2.32	0.43
2:F:978:HIS:CE1	2:F:1007:LYS:NZ	2.86	0.43
2:F:1302:GLU:HB3	2:F:1374:GLY:HA2	2.01	0.43
1:A:130:SER:HA	1:A:172:THR:OG1	2.19	0.42
1:A:279:THR:C	1:A:281:LEU:N	2.72	0.42
2:B:1320:TYR:OH	2:B:1366:LEU:CD2	2.66	0.42
2:B:1387:PHE:C	2:B:1388:VAL:CG2	2.87	0.42
2:D:1190:GLU:CG	2:D:1260:ARG:HG3	2.49	0.42
2:D:1178:SER:HB3	2:D:1270:PHE:CD2	2.53	0.42
1:E:297:THR:HG22	1:E:299:PRO:CD	2.46	0.42
2:F:1331:ILE:HG22	2:F:1334:SER:OG	2.19	0.42
2:F:1379:GLU:CD	2:F:1379:GLU:H	2.23	0.42
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.51	0.42
2:B:1205:LEU:CD2	2:B:1255:MET:SD	3.07	0.42
2:B:1330:HIS:CD2	2:B:1331:ILE:H	2.35	0.42
1:C:374:ASN:O	1:C:375:ASN:CB	2.67	0.42
1:C:393:THR:HA	1:C:394:PRO:HD3	1.91	0.42
1:C:58:LEU:HB2	1:C:75:LEU:HD21	2.01	0.42
2:D:1084:GLN:OE1	2:D:1084:GLN:N	2.51	0.42
2:D:1120:LEU:HA	2:D:1120:LEU:HD23	1.90	0.42
2:D:1205:LEU:CD2	2:D:1255:MET:SD	3.07	0.42
2:D:942:THR:HG22	2:D:1036:LEU:HD11	1.99	0.42
2:F:1057:GLY:HA3	2:F:1157:TYR:CA	2.48	0.42
2:F:1330:HIS:ND1	2:F:1332:ASN:N	2.55	0.42
2:F:964:VAL:CG2	2:F:965:GLN:N	2.82	0.42
2:B:1343:GLY:HA3	2:B:1344:PRO:HD3	1.88	0.42
1:C:336:SER:O	1:C:337:VAL:C	2.58	0.42
2:D:1161:SER:O	2:D:1162:SER:CB	2.67	0.42
1:E:337:VAL:C	1:E:338:LYS:O	2.57	0.42
1:E:374:ASN:O	1:E:375:ASN:CB	2.67	0.42
2:F:1084:GLN:HG2	2:F:1160:GLY:O	2.19	0.42
2:F:1161:SER:O	2:F:1162:SER:CB	2.67	0.42
2:B:988:ASP:OD2	2:B:1026:THR:HB	2.19	0.42
2:B:1061:SER:HB3	2:B:1154:PHE:H	1.84	0.42
2:B:1179:PRO:C	2:B:1181:TYR:H	2.22	0.42
2:B:1379:GLU:CD	2:B:1379:GLU:H	2.23	0.42
2:B:978:HIS:HB3	2:B:1032:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:VAL:HG12	1:C:370:VAL:N	2.34	0.42
2:D:1084:GLN:HG2	2:D:1160:GLY:O	2.19	0.42
2:D:1176:PHE:CD2	2:D:1193:TRP:CE3	3.07	0.42
2:D:1387:PHE:O	2:D:1388:VAL:CG2	2.68	0.42
2:D:980:GLU:OE2	2:D:987:ASN:ND2	2.52	0.42
6:E:2007:B12:H533	6:E:2007:B12:C48	2.49	0.42
1:E:317:THR:HB	1:E:411:THR:HG23	2.01	0.42
2:F:1190:GLU:CG	2:F:1260:ARG:HG3	2.50	0.42
2:F:1330:HIS:CD2	2:F:1331:ILE:H	2.36	0.42
1:A:369:VAL:HG12	1:A:370:VAL:N	2.34	0.42
1:C:335:VAL:CG2	5:C:2001:NAG:H5	2.50	0.42
2:D:1179:PRO:C	2:D:1181:TYR:H	2.22	0.42
2:D:1335:THR:HG23	2:D:1336:ASP:N	2.29	0.42
2:F:1205:LEU:CD2	2:F:1255:MET:SD	3.07	0.42
2:F:1248:ILE:O	2:F:1248:ILE:HG22	2.19	0.42
2:F:1320:TYR:OH	2:F:1366:LEU:CD2	2.68	0.42
2:F:1340:LEU:HA	2:F:1340:LEU:HD23	1.82	0.42
2:F:1387:PHE:O	2:F:1388:VAL:CG2	2.68	0.42
5:A:2001:NAG:C3	5:A:2001:NAG:H83	2.50	0.42
1:A:294:VAL:O	1:A:294:VAL:HG23	2.20	0.42
2:B:1304:GLN:HG3	2:B:1372:THR:HG21	2.01	0.42
2:B:980:GLU:OE2	2:B:987:ASN:ND2	2.52	0.42
6:C:2007:B12:C48	6:C:2007:B12:H533	2.49	0.42
1:C:386:TRP:CZ3	1:C:414:PHE:HB2	2.55	0.42
1:C:74:LEU:O	1:C:78:GLN:HG3	2.20	0.42
2:B:1190:GLU:CG	2:B:1260:ARG:HG3	2.50	0.42
2:B:1331:ILE:HG22	2:B:1334:SER:OG	2.19	0.42
2:B:1355:LEU:HA	2:B:1356:PRO:HD3	1.92	0.42
2:B:1291:LEU:HD11	2:B:1368:VAL:HG21	2.01	0.42
2:B:974:PHE:O	2:B:975:GLU:C	2.57	0.42
1:C:215:LYS:C	1:C:217:ASN:N	2.73	0.42
1:C:219:ILE:HG12	1:C:252:MET:CE	2.50	0.42
1:C:228:LEU:HA	1:C:228:LEU:HD23	1.66	0.42
1:C:87:LEU:HA	1:C:91:HIS:CD2	2.55	0.42
2:D:1330:HIS:CD2	2:D:1331:ILE:H	2.35	0.42
2:D:1331:ILE:HG22	2:D:1334:SER:OG	2.19	0.42
1:E:130:SER:HA	1:E:172:THR:OG1	2.19	0.42
1:E:294:VAL:HG23	1:E:294:VAL:O	2.20	0.42
2:F:1095:LEU:HD21	2:F:1143:PHE:HE1	1.82	0.42
2:F:1219:THR:CG2	2:F:1219:THR:O	2.66	0.42
2:F:980:GLU:OE2	2:F:987:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:SER:O	1:A:337:VAL:C	2.58	0.42
1:A:389:LEU:CB	1:A:394:PRO:HA	2.45	0.42
2:B:1161:SER:O	2:B:1162:SER:CB	2.67	0.42
6:C:2007:B12:H482	6:C:2007:B12:H533	2.02	0.42
1:C:181:THR:HG21	1:C:235:VAL:HG13	2.02	0.42
1:C:362:THR:HG22	1:C:371:SER:CB	2.35	0.42
2:D:1068:TYR:C	2:D:1068:TYR:CD1	2.93	0.42
2:D:1205:LEU:HD23	2:D:1255:MET:SD	2.60	0.42
2:F:1085:LEU:HD21	2:F:1165:CYS:HA	2.01	0.42
2:F:1291:LEU:HD23	2:F:1291:LEU:HA	1.64	0.42
1:A:279:THR:C	1:A:281:LEU:H	2.23	0.42
2:B:1205:LEU:HD23	2:B:1255:MET:SD	2.60	0.42
2:B:1302:GLU:HB3	2:B:1374:GLY:HA2	2.01	0.42
1:C:36:VAL:C	1:C:38:GLY:N	2.73	0.42
2:D:1060:THR:HG23	2:D:1064:PHE:CB	2.46	0.42
2:D:1085:LEU:HD21	2:D:1165:CYS:HA	2.01	0.42
2:F:1060:THR:HG23	2:F:1064:PHE:CB	2.46	0.42
2:F:1068:TYR:CD1	2:F:1068:TYR:C	2.93	0.42
2:F:1119:LEU:HA	2:F:1119:LEU:HD12	1.79	0.42
2:F:1187:HIS:HB3	2:F:1266:GLN:HE22	1.78	0.42
2:F:1226:TYR:CE1	2:F:1235:LEU:HB2	2.55	0.42
2:F:975:GLU:HG3	2:F:1036:LEU:HD23	2.02	0.42
6:A:2007:B12:H533	6:A:2007:B12:H482	2.02	0.42
1:A:215:LYS:C	1:A:217:ASN:N	2.73	0.42
1:A:219:ILE:HG12	1:A:252:MET:CE	2.50	0.42
1:A:203:LEU:HD22	1:A:236:THR:HG22	2.02	0.42
1:A:74:LEU:O	1:A:78:GLN:HG3	2.20	0.42
1:C:185:ASN:HB3	1:E:287:THR:HG23	2.02	0.42
1:C:337:VAL:C	1:C:338:LYS:O	2.57	0.42
2:D:964:VAL:CG2	2:D:965:GLN:N	2.82	0.42
1:E:386:TRP:CZ3	1:E:414:PHE:HB2	2.55	0.42
1:E:389:LEU:CB	1:E:394:PRO:HA	2.45	0.42
2:F:1061:SER:HB3	2:F:1154:PHE:H	1.84	0.42
2:F:1304:GLN:HG3	2:F:1372:THR:HG21	2.01	0.42
2:F:1217:ASN:HB2	5:F:2008:NAG:C6	2.50	0.42
1:A:148:GLU:HG3	1:A:188:PRO:HG2	2.02	0.41
1:A:275:LEU:HA	1:A:275:LEU:HD23	1.88	0.41
2:B:1084:GLN:HG2	2:B:1160:GLY:O	2.20	0.41
2:B:1217:ASN:HB2	5:B:2008:NAG:C6	2.50	0.41
1:C:148:GLU:HG3	1:C:188:PRO:HG2	2.02	0.41
1:C:279:THR:C	1:C:281:LEU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1217:ASN:HB2	5:D:2008:NAG:C6	2.50	0.41
2:D:1226:TYR:CE1	2:D:1235:LEU:HB2	2.55	0.41
2:D:1312:ALA:O	2:D:1364:SER:HB2	2.19	0.41
1:E:335:VAL:CG2	5:E:2001:NAG:H5	2.50	0.41
2:F:1205:LEU:HD23	2:F:1255:MET:SD	2.60	0.41
2:F:974:PHE:O	2:F:975:GLU:C	2.57	0.41
2:B:1387:PHE:O	2:B:1388:VAL:CG2	2.68	0.41
1:C:89:ILE:HG21	1:C:89:ILE:HD13	1.66	0.41
2:D:974:PHE:O	2:D:975:GLU:C	2.57	0.41
2:D:978:HIS:HB3	2:D:1032:TYR:HB2	2.02	0.41
1:E:203:LEU:HD22	1:E:236:THR:HG22	2.02	0.41
2:F:1062:PRO:O	2:F:1063:ASN:HB2	2.21	0.41
2:F:1314:THR:HG22	2:F:1315:GLY:H	1.84	0.41
1:A:363:MET:HG3	1:A:364:THR:N	2.36	0.41
1:A:374:ASN:O	1:A:375:ASN:CB	2.67	0.41
1:C:65:GLY:CA	1:C:292:HIS:CE1	3.03	0.41
2:D:1177:ILE:HG22	2:D:1178:SER:O	2.21	0.41
1:A:58:LEU:HB2	1:A:75:LEU:HD21	2.01	0.41
2:B:1177:ILE:HG22	2:B:1178:SER:O	2.21	0.41
2:B:1220:LEU:HG	2:B:1220:LEU:H	1.67	0.41
2:B:950:ASN:HA	2:B:951:VAL:HA	1.76	0.41
1:C:335:VAL:HG23	5:C:2001:NAG:H5	2.02	0.41
1:C:294:VAL:O	1:C:294:VAL:HG23	2.20	0.41
2:D:1062:PRO:O	2:D:1063:ASN:HB2	2.20	0.41
2:D:1067:ASN:HB3	2:D:1150:THR:HG22	1.98	0.41
2:D:1220:LEU:O	2:D:1260:ARG:NH1	2.54	0.41
2:D:1314:THR:HG22	2:D:1315:GLY:H	1.85	0.41
2:D:1330:HIS:ND1	2:D:1332:ASN:N	2.55	0.41
1:E:177:THR:CG2	1:E:206:ILE:HG21	2.42	0.41
1:E:219:ILE:HG12	1:E:252:MET:CE	2.50	0.41
2:F:1086:ILE:H	2:F:1134:SER:HG	1.67	0.41
2:F:1120:LEU:HD13	2:F:1132:ILE:CG2	2.51	0.41
2:F:1192:TYR:HE1	2:F:1258:LYS:CG	2.33	0.41
2:F:952:TYR:CE1	2:F:988:ASP:OD2	2.73	0.41
3:M:3:BMA:H61	3:M:5:MAN:H2	1.78	0.41
1:A:123:SER:O	2:B:1101:ASN:HB2	2.20	0.41
1:A:386:TRP:CZ3	1:A:414:PHE:HB2	2.55	0.41
2:D:1291:LEU:HD11	2:D:1368:VAL:HG21	2.01	0.41
2:D:1343:GLY:HA3	2:D:1344:PRO:HD3	1.88	0.41
2:D:963:LEU:HD12	2:D:964:VAL:N	2.35	0.41
2:F:1220:LEU:O	2:F:1260:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1343:GLY:HA3	2:F:1344:PRO:HD3	1.88	0.41
2:F:1291:LEU:HD11	2:F:1368:VAL:HG21	2.01	0.41
1:A:297:THR:HG22	1:A:299:PRO:CD	2.47	0.41
1:A:87:LEU:HA	1:A:91:HIS:CD2	2.55	0.41
2:B:1062:PRO:O	2:B:1063:ASN:HB2	2.20	0.41
2:B:1068:TYR:C	2:B:1068:TYR:CD1	2.93	0.41
2:B:1120:LEU:HD13	2:B:1132:ILE:CG2	2.51	0.41
2:B:1148:ILE:CG2	2:B:1149:ASP:N	2.83	0.41
2:B:1177:ILE:HD13	2:B:1177:ILE:HA	1.85	0.41
1:C:339:SER:C	1:C:341:SER:N	2.74	0.41
1:C:94:LEU:HA	1:C:94:LEU:HD13	1.78	0.41
2:D:989:TYR:CZ	2:D:1025:VAL:CG1	3.04	0.41
2:D:952:TYR:CE1	2:D:988:ASP:OD2	2.73	0.41
1:E:331:GLU:N	1:E:331:GLU:OE1	2.52	0.41
2:F:1148:ILE:CG2	2:F:1149:ASP:N	2.83	0.41
5:F:2001:NAG:C7	5:F:2001:NAG:O3	2.69	0.41
1:A:181:THR:HG21	1:A:235:VAL:HG13	2.02	0.41
1:A:289:SER:N	1:A:290:PRO:HD3	2.36	0.41
2:B:1192:TYR:HE1	2:B:1258:LYS:CG	2.33	0.41
2:B:1335:THR:HG23	2:B:1336:ASP:N	2.29	0.41
1:C:252:MET:HE3	1:C:253:ILE:HG12	2.02	0.41
2:D:1379:GLU:H	2:D:1379:GLU:CD	2.22	0.41
1:E:198:LEU:C	1:E:198:LEU:HD22	2.41	0.41
1:E:181:THR:HG21	1:E:235:VAL:HG13	2.02	0.41
1:E:363:MET:HG3	1:E:364:THR:N	2.35	0.41
2:F:1177:ILE:HG22	2:F:1178:SER:O	2.21	0.41
2:F:978:HIS:HB3	2:F:1032:TYR:HB2	2.03	0.41
1:A:406:ASN:OD1	1:A:407:HIS:N	2.54	0.41
1:A:58:LEU:HD23	1:A:79:LEU:HD12	2.03	0.41
2:B:1060:THR:HG23	2:B:1064:PHE:CB	2.46	0.41
2:B:1085:LEU:HD21	2:B:1165:CYS:HA	2.01	0.41
2:B:1226:TYR:CE1	2:B:1235:LEU:HB2	2.55	0.41
2:B:954:HIS:ND1	2:B:1028:SER:O	2.54	0.41
1:C:198:LEU:C	1:C:198:LEU:CD2	2.89	0.41
1:C:203:LEU:HD22	1:C:236:THR:HG22	2.02	0.41
2:D:1120:LEU:HD13	2:D:1132:ILE:CG2	2.51	0.41
2:D:1148:ILE:CG2	2:D:1149:ASP:N	2.83	0.41
1:E:148:GLU:HG3	1:E:188:PRO:HG2	2.02	0.41
1:E:159:LYS:HD3	2:F:1104:THR:HG22	2.02	0.41
1:E:74:LEU:O	1:E:78:GLN:HG3	2.20	0.41
1:E:87:LEU:HA	1:E:91:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:964:VAL:O	2:F:1018:ASN:HB2	2.21	0.41
2:F:954:HIS:ND1	2:F:1028:SER:O	2.54	0.41
1:A:331:GLU:N	1:A:331:GLU:OE1	2.52	0.41
1:A:36:VAL:C	1:A:38:GLY:N	2.73	0.41
2:B:1288:TYR:CD2	2:B:1288:TYR:N	2.89	0.41
2:B:954:HIS:H	2:B:954:HIS:HD2	1.59	0.41
2:B:963:LEU:HD12	2:B:964:VAL:N	2.35	0.41
1:C:123:SER:O	2:D:1101:ASN:HB2	2.20	0.41
1:C:198:LEU:C	1:C:198:LEU:HD22	2.41	0.41
1:C:317:THR:CG2	1:C:331:GLU:HG3	2.42	0.41
2:D:954:HIS:ND1	2:D:1028:SER:O	2.54	0.41
2:D:1288:TYR:CD2	2:D:1288:TYR:N	2.89	0.41
2:D:962:ILE:O	2:D:1019:SER:HA	2.21	0.41
6:E:2007:B12:H482	6:E:2007:B12:H533	2.02	0.41
1:E:36:VAL:C	1:E:38:GLY:N	2.73	0.41
1:E:403:ILE:HA	1:E:404:PRO:HD3	1.70	0.41
1:A:267:SER:HB3	1:A:366:TRP:CH2	2.56	0.41
2:B:989:TYR:CZ	2:B:1025:VAL:CG1	3.04	0.41
2:B:1177:ILE:HG23	2:B:1181:TYR:CB	2.48	0.41
2:B:975:GLU:HG3	2:B:1036:LEU:HD23	2.02	0.41
1:C:279:THR:C	1:C:281:LEU:N	2.72	0.41
2:D:948:HIS:HA	2:D:949:PRO:C	2.41	0.41
1:E:215:LYS:C	1:E:217:ASN:N	2.73	0.41
1:E:58:LEU:HB2	1:E:75:LEU:HD21	2.01	0.41
2:F:1128:LEU:HA	2:F:1128:LEU:HD23	1.65	0.41
6:A:2007:B12:C20	6:A:2007:B12:H302	2.45	0.41
1:A:252:MET:HE3	1:A:253:ILE:HG12	2.03	0.41
1:A:339:SER:C	1:A:341:SER:N	2.74	0.41
2:B:1051:ASP:OD1	2:B:1077:ARG:HD2	2.21	0.41
2:B:1089:HIS:HB2	2:B:1157:TYR:CE2	2.56	0.41
1:C:289:SER:N	1:C:290:PRO:HD3	2.36	0.41
2:D:1051:ASP:OD1	2:D:1077:ARG:HD2	2.21	0.41
2:D:1089:HIS:HB2	2:D:1157:TYR:CE2	2.56	0.41
1:E:289:SER:N	1:E:290:PRO:HD3	2.36	0.41
1:E:406:ASN:OD1	1:E:407:HIS:N	2.54	0.41
1:E:58:LEU:HD23	1:E:79:LEU:HD12	2.03	0.41
1:E:89:ILE:HD11	1:E:117:MET:SD	2.61	0.41
1:A:406:ASN:ND2	2:F:1066:ASN:HA	2.36	0.41
1:A:65:GLY:CA	1:A:292:HIS:CE1	3.03	0.40
2:B:962:ILE:O	2:B:1019:SER:HA	2.21	0.40
2:B:1220:LEU:O	2:B:1260:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2007:B12:H562	6:C:2007:B12:H18	1.87	0.40
1:C:331:GLU:OE1	1:C:331:GLU:N	2.52	0.40
2:D:1342:ASP:CA	2:D:1347:MET:HE2	2.51	0.40
1:E:65:GLY:CA	1:E:292:HIS:CE1	3.03	0.40
2:F:964:VAL:HG21	2:F:1041:ALA:HB2	2.03	0.40
2:F:963:LEU:HD12	2:F:964:VAL:N	2.35	0.40
1:A:170:VAL:O	1:A:171:ASP:C	2.59	0.40
2:B:1084:GLN:HG3	2:B:1163:THR:N	2.21	0.40
2:B:1274:TYR:O	2:B:1274:TYR:CG	2.74	0.40
2:B:1330:HIS:ND1	2:B:1332:ASN:N	2.55	0.40
1:C:214:ILE:HG12	1:C:220:ILE:HG12	2.03	0.40
1:C:363:MET:HG3	1:C:364:THR:N	2.36	0.40
1:C:159:LYS:HD3	2:D:1104:THR:HG22	2.02	0.40
2:D:1177:ILE:HG23	2:D:1181:TYR:CB	2.47	0.40
2:D:1320:TYR:OH	2:D:1366:LEU:CD2	2.68	0.40
2:D:993:TYR:HB3	2:D:1021:MET:CB	2.51	0.40
1:E:279:THR:C	1:E:281:LEU:H	2.23	0.40
1:E:334:ASN:N	1:E:334:ASN:OD1	2.54	0.40
1:E:123:SER:O	2:F:1101:ASN:HB2	2.20	0.40
2:F:1274:TYR:CG	2:F:1274:TYR:O	2.73	0.40
1:A:89:ILE:HD11	1:A:117:MET:SD	2.61	0.40
1:A:142:LEU:HA	1:A:142:LEU:HD12	1.82	0.40
1:A:214:ILE:HG12	1:A:220:ILE:HG12	2.04	0.40
2:B:947:GLY:O	2:B:948:HIS:C	2.60	0.40
2:B:952:TYR:CE1	2:B:988:ASP:OD2	2.73	0.40
2:D:1274:TYR:O	2:D:1274:TYR:CG	2.74	0.40
5:D:2001:NAG:C7	5:D:2001:NAG:O3	2.69	0.40
2:F:1051:ASP:OD1	2:F:1077:ARG:HD2	2.21	0.40
1:A:198:LEU:CD2	1:A:198:LEU:C	2.89	0.40
2:B:1244:LYS:HG2	2:B:1244:LYS:O	2.22	0.40
2:B:1314:THR:HG22	2:B:1315:GLY:H	1.84	0.40
5:B:2001:NAG:O3	5:B:2001:NAG:C7	2.69	0.40
1:C:267:SER:HB3	1:C:366:TRP:CH2	2.56	0.40
1:C:363:MET:C	1:C:364:THR:CG2	2.90	0.40
2:D:1022:LEU:HA	2:D:1022:LEU:HD23	1.66	0.40
2:D:1192:TYR:HE1	2:D:1258:LYS:CG	2.33	0.40
2:D:975:GLU:HG3	2:D:1036:LEU:HD23	2.02	0.40
1:E:214:ILE:HG12	1:E:220:ILE:HG12	2.03	0.40
1:E:335:VAL:HG23	5:E:2001:NAG:H5	2.03	0.40
2:F:962:ILE:O	2:F:1019:SER:HA	2.21	0.40
2:F:964:VAL:HG22	2:F:965:GLN:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2007:B12:H473	6:A:2007:B12:H481	1.14	0.40
2:B:1099:ILE:O	2:B:1102:TYR:HB2	2.22	0.40
2:B:1297:PRO:O	2:B:1380:LYS:CD	2.63	0.40
2:B:1342:ASP:CA	2:B:1347:MET:HE2	2.52	0.40
1:C:170:VAL:O	1:C:171:ASP:C	2.59	0.40
2:D:1235:LEU:O	2:D:1235:LEU:HG	2.22	0.40
2:D:1221:ASP:OD2	2:D:1262:ASP:OD1	2.40	0.40
2:D:950:ASN:HA	2:D:951:VAL:HA	1.76	0.40
2:F:1089:HIS:HB2	2:F:1157:TYR:CE2	2.56	0.40
2:F:1288:TYR:N	2:F:1288:TYR:CD2	2.89	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	381/393 (97%)	334 (88%)	37 (10%)	10 (3%)	5	27
1	C	381/393 (97%)	334 (88%)	37 (10%)	10 (3%)	5	27
1	E	381/393 (97%)	334 (88%)	37 (10%)	10 (3%)	5	27
2	B	455/457 (100%)	376 (83%)	52 (11%)	27 (6%)	1	10
2	D	455/457 (100%)	376 (83%)	52 (11%)	27 (6%)	1	10
2	F	455/457 (100%)	376 (83%)	52 (11%)	27 (6%)	1	10
All	All	2508/2550 (98%)	2130 (85%)	267 (11%)	111 (4%)	2	16

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLY
1	A	309	ALA

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Mol	Chain	Res	Type
2	B	1105	ASP
2	B	1162	SER
2	B	1219	THR
1	C	107	GLY
1	C	309	ALA
2	D	1105	ASP
2	D	1162	SER
2	D	1219	THR
1	E	107	GLY
1	E	309	ALA
2	F	1105	ASP
2	F	1162	SER
2	F	1219	THR
1	A	291	ASP
2	B	950	ASN
2	B	987	ASN
2	B	1046	THR
2	B	1169	LEU
2	B	1179	PRO
2	B	1218	CYS
2	B	1227	ASP
2	B	1265	GLN
2	B	1294	ILE
1	C	291	ASP
2	D	950	ASN
2	D	987	ASN
2	D	1046	THR
2	D	1169	LEU
2	D	1179	PRO
2	D	1209	ASP
2	D	1218	CYS
2	D	1227	ASP
2	D	1265	GLN
2	D	1294	ILE
1	E	291	ASP
2	F	950	ASN
2	F	987	ASN
2	F	1046	THR
2	F	1169	LEU
2	F	1179	PRO
2	F	1218	CYS
2	F	1227	ASP

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Mol	Chain	Res	Type
2	F	1265	GLN
2	F	1294	ILE
1	A	241	LYS
1	A	338	LYS
2	B	1054	ASP
2	B	1209	ASP
2	B	1328	GLU
2	B	1378	ARG
1	C	241	LYS
1	C	338	LYS
2	D	1054	ASP
2	D	1328	GLU
2	D	1378	ARG
1	E	338	LYS
2	F	1054	ASP
2	F	1209	ASP
2	F	1328	GLU
2	F	1378	ARG
1	A	217	ASN
1	A	339	SER
2	B	1030	LEU
2	B	1180	ASN
2	B	1330	HIS
1	C	217	ASN
1	C	339	SER
2	D	1030	LEU
2	D	1180	ASN
2	D	1330	HIS
1	E	217	ASN
1	E	241	LYS
1	E	339	SER
2	F	1030	LEU
2	F	1180	ASN
2	F	1330	HIS
2	B	977	PHE
2	B	1009	ILE
2	B	1037	ILE
2	D	977	PHE
2	D	1009	ILE
2	D	1037	ILE
2	F	977	PHE
2	F	1009	ILE

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Mol	Chain	Res	Type
2	F	1037	ILE
2	B	1149	ASP
2	B	1326	ASP
2	D	1149	ASP
2	D	1326	ASP
2	F	1149	ASP
2	F	1326	ASP
1	A	38	GLY
2	B	1080	VAL
2	B	1358	PRO
1	C	38	GLY
2	D	1080	VAL
2	D	1358	PRO
1	E	38	GLY
2	F	1080	VAL
2	F	1358	PRO
1	C	391	GLY
1	A	391	GLY
1	E	391	GLY
1	A	392	VAL
2	B	1264	GLY
1	C	392	VAL
2	D	1264	GLY
1	E	392	VAL
2	F	1264	GLY

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	337/343 (98%)	283 (84%)	54 (16%)	2 11
1	C	337/343 (98%)	283 (84%)	54 (16%)	2 11
1	E	337/343 (98%)	282 (84%)	55 (16%)	2 10
2	B	406/406 (100%)	334 (82%)	72 (18%)	2 8
2	D	406/406 (100%)	334 (82%)	72 (18%)	2 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	406/406 (100%)	335 (82%)	71 (18%)	2 8
All	All	2229/2247 (99%)	1851 (83%)	378 (17%)	2 9

All (378) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	39	ILE
1	A	40	GLN
1	A	42	LEU
1	A	52	TYR
1	A	56	SER
1	A	63	LEU
1	A	86	ASP
1	A	89	ILE
1	A	91	HIS
1	A	94	LEU
1	A	115	ARG
1	A	124	SER
1	A	137	LEU
1	A	143	CYS
1	A	147	SER
1	A	177	THR
1	A	180	LEU
1	A	191	SER
1	A	198	LEU
1	A	206	ILE
1	A	215	LYS
1	A	223	ILE
1	A	225	SER
1	A	236	THR
1	A	238	GLU
1	A	251	ASP
1	A	271	ILE
1	A	272	LEU
1	A	310	SER
1	A	311	ASN
1	A	312	ILE
1	A	313	THR
1	A	322	LEU
1	A	323	ARG
1	A	327	LEU

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Mol	Chain	Res	Type
1	A	328	LEU
1	A	332	THR
1	A	333	ILE
1	A	334	ASN
1	A	335	VAL
1	A	337	VAL
1	A	341	SER
1	A	347	LEU
1	A	352	ARG
1	A	361	THR
1	A	362	THR
1	A	368	LEU
1	A	371	SER
1	A	380	VAL
1	A	384	THR
1	A	389	LEU
1	A	393	THR
1	A	417	TYR
2	B	935	ILE
2	B	937	THR
2	B	939	SER
2	B	940	THR
2	B	942	THR
2	B	945	SER
2	B	954	HIS
2	B	964	VAL
2	B	973	MET
2	B	976	THR
2	B	978	HIS
2	B	980	GLU
2	B	981	PHE
2	B	985	CYS
2	B	988	ASP
2	B	997	SER
2	B	1000	SER
2	B	1021	MET
2	B	1025	VAL
2	B	1029	ASP
2	B	1035	PHE
2	B	1037	ILE
2	B	1048	CYS
2	B	1050	GLN

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Mol	Chain	Res	Type
2	B	1059	PHE
2	B	1060	THR
2	B	1077	ARG
2	B	1078	ILE
2	B	1079	THR
2	B	1080	VAL
2	B	1088	VAL
2	B	1091	THR
2	B	1095	LEU
2	B	1115	GLU
2	B	1144	LYS
2	B	1149	ASP
2	B	1158	TRP
2	B	1161	SER
2	B	1165	CYS
2	B	1170	THR
2	B	1173	SER
2	B	1176	PHE
2	B	1183	MET
2	B	1193	TRP
2	B	1205	LEU
2	B	1219	THR
2	B	1221	ASP
2	B	1223	LEU
2	B	1225	VAL
2	B	1231	SER
2	B	1239	LEU
2	B	1242	ASP
2	B	1254	SER
2	B	1259	LEU
2	B	1263	GLU
2	B	1275	ARG
2	B	1277	THR
2	B	1278	CYS
2	B	1284	VAL
2	B	1287	THR
2	B	1291	LEU
2	B	1301	SER
2	B	1309	THR
2	B	1335	THR
2	B	1364	SER
2	B	1365	LYS

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Mol	Chain	Res	Type
2	B	1366	LEU
2	B	1368	VAL
2	B	1377	ARG
2	B	1378	ARG
2	B	1384	MET
2	B	1386	TRP
1	C	25	SER
1	C	39	ILE
1	C	40	GLN
1	C	42	LEU
1	C	52	TYR
1	C	56	SER
1	C	63	LEU
1	C	86	ASP
1	C	89	ILE
1	C	91	HIS
1	C	94	LEU
1	C	115	ARG
1	C	124	SER
1	C	137	LEU
1	C	143	CYS
1	C	147	SER
1	C	177	THR
1	C	180	LEU
1	C	191	SER
1	C	198	LEU
1	C	206	ILE
1	C	215	LYS
1	C	223	ILE
1	C	225	SER
1	C	236	THR
1	C	238	GLU
1	C	251	ASP
1	C	271	ILE
1	C	272	LEU
1	C	310	SER
1	C	311	ASN
1	C	312	ILE
1	C	313	THR
1	C	322	LEU
1	C	323	ARG
1	C	327	LEU

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Mol	Chain	Res	Type
1	C	328	LEU
1	C	332	THR
1	C	333	ILE
1	C	334	ASN
1	C	335	VAL
1	C	337	VAL
1	C	341	SER
1	C	347	LEU
1	C	352	ARG
1	C	361	THR
1	C	362	THR
1	C	368	LEU
1	C	371	SER
1	C	380	VAL
1	C	384	THR
1	C	389	LEU
1	C	393	THR
1	C	417	TYR
2	D	935	ILE
2	D	937	THR
2	D	939	SER
2	D	940	THR
2	D	942	THR
2	D	945	SER
2	D	954	HIS
2	D	964	VAL
2	D	973	MET
2	D	976	THR
2	D	978	HIS
2	D	980	GLU
2	D	981	PHE
2	D	985	CYS
2	D	988	ASP
2	D	997	SER
2	D	1000	SER
2	D	1021	MET
2	D	1025	VAL
2	D	1029	ASP
2	D	1035	PHE
2	D	1037	ILE
2	D	1048	CYS
2	D	1050	GLN

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Mol	Chain	Res	Type
2	D	1059	PHE
2	D	1060	THR
2	D	1077	ARG
2	D	1078	ILE
2	D	1079	THR
2	D	1080	VAL
2	D	1088	VAL
2	D	1091	THR
2	D	1095	LEU
2	D	1115	GLU
2	D	1144	LYS
2	D	1149	ASP
2	D	1158	TRP
2	D	1161	SER
2	D	1165	CYS
2	D	1170	THR
2	D	1173	SER
2	D	1176	PHE
2	D	1183	MET
2	D	1193	TRP
2	D	1205	LEU
2	D	1219	THR
2	D	1221	ASP
2	D	1223	LEU
2	D	1225	VAL
2	D	1231	SER
2	D	1239	LEU
2	D	1242	ASP
2	D	1254	SER
2	D	1259	LEU
2	D	1263	GLU
2	D	1275	ARG
2	D	1277	THR
2	D	1278	CYS
2	D	1284	VAL
2	D	1287	THR
2	D	1291	LEU
2	D	1301	SER
2	D	1309	THR
2	D	1335	THR
2	D	1364	SER
2	D	1365	LYS

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Mol	Chain	Res	Type
2	D	1366	LEU
2	D	1368	VAL
2	D	1377	ARG
2	D	1378	ARG
2	D	1384	MET
2	D	1386	TRP
1	E	25	SER
1	E	39	ILE
1	E	40	GLN
1	E	42	LEU
1	E	52	TYR
1	E	56	SER
1	E	63	LEU
1	E	86	ASP
1	E	89	ILE
1	E	91	HIS
1	E	94	LEU
1	E	115	ARG
1	E	124	SER
1	E	137	LEU
1	E	143	CYS
1	E	147	SER
1	E	177	THR
1	E	180	LEU
1	E	191	SER
1	E	198	LEU
1	E	206	ILE
1	E	215	LYS
1	E	223	ILE
1	E	225	SER
1	E	236	THR
1	E	238	GLU
1	E	251	ASP
1	E	271	ILE
1	E	272	LEU
1	E	310	SER
1	E	311	ASN
1	E	312	ILE
1	E	313	THR
1	E	322	LEU
1	E	323	ARG
1	E	325	VAL

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Mol	Chain	Res	Type
1	E	327	LEU
1	E	328	LEU
1	E	332	THR
1	E	333	ILE
1	E	334	ASN
1	E	335	VAL
1	E	337	VAL
1	E	341	SER
1	E	347	LEU
1	E	352	ARG
1	E	361	THR
1	E	362	THR
1	E	368	LEU
1	E	371	SER
1	E	380	VAL
1	E	384	THR
1	E	389	LEU
1	E	393	THR
1	E	417	TYR
2	F	935	ILE
2	F	937	THR
2	F	939	SER
2	F	940	THR
2	F	942	THR
2	F	945	SER
2	F	954	HIS
2	F	964	VAL
2	F	973	MET
2	F	976	THR
2	F	978	HIS
2	F	980	GLU
2	F	985	CYS
2	F	988	ASP
2	F	997	SER
2	F	1000	SER
2	F	1021	MET
2	F	1025	VAL
2	F	1029	ASP
2	F	1035	PHE
2	F	1037	ILE
2	F	1048	CYS
2	F	1050	GLN

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Mol	Chain	Res	Type
2	F	1059	PHE
2	F	1060	THR
2	F	1077	ARG
2	F	1078	ILE
2	F	1079	THR
2	F	1080	VAL
2	F	1088	VAL
2	F	1091	THR
2	F	1095	LEU
2	F	1115	GLU
2	F	1144	LYS
2	F	1149	ASP
2	F	1158	TRP
2	F	1161	SER
2	F	1165	CYS
2	F	1170	THR
2	F	1173	SER
2	F	1176	PHE
2	F	1183	MET
2	F	1193	TRP
2	F	1205	LEU
2	F	1219	THR
2	F	1221	ASP
2	F	1223	LEU
2	F	1225	VAL
2	F	1231	SER
2	F	1239	LEU
2	F	1242	ASP
2	F	1254	SER
2	F	1259	LEU
2	F	1263	GLU
2	F	1275	ARG
2	F	1277	THR
2	F	1278	CYS
2	F	1284	VAL
2	F	1287	THR
2	F	1291	LEU
2	F	1301	SER
2	F	1309	THR
2	F	1335	THR
2	F	1364	SER
2	F	1365	LYS

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Mol	Chain	Res	Type
2	F	1366	LEU
2	F	1368	VAL
2	F	1377	ARG
2	F	1378	ARG
2	F	1384	MET
2	F	1386	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	295	GLN
2	B	954	HIS
2	B	965	GLN
2	B	967	ASN
2	B	978	HIS
2	B	982	HIS
2	B	1232	ASN
2	B	1265	GLN
2	B	1266	GLN
2	B	1280	ASN
1	C	85	ASN
1	C	295	GLN
2	D	954	HIS
2	D	965	GLN
2	D	967	ASN
2	D	978	HIS
2	D	982	HIS
2	D	1232	ASN
2	D	1265	GLN
2	D	1266	GLN
2	D	1280	ASN
1	E	85	ASN
1	E	295	GLN
2	F	954	HIS
2	F	965	GLN
2	F	967	ASN
2	F	978	HIS
2	F	982	HIS
2	F	1232	ASN
2	F	1265	GLN
2	F	1266	GLN

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Mol	Chain	Res	Type
2	F	1280	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	0.78	0	17,19,21	2.64	5 (29%)
3	NAG	G	2	3	14,14,15	0.98	1 (7%)	17,19,21	2.66	10 (58%)
3	BMA	G	3	3	11,11,12	0.85	0	15,15,17	1.31	2 (13%)
3	MAN	G	4	3	11,11,12	1.30	2 (18%)	15,15,17	2.33	8 (53%)
3	MAN	G	5	3	11,11,12	1.32	2 (18%)	15,15,17	2.20	6 (40%)
3	NAG	H	1	3,2	14,14,15	0.76	0	17,19,21	3.28	10 (58%)
3	NAG	H	2	3	14,14,15	0.37	0	17,19,21	1.23	2 (11%)
3	BMA	H	3	3	11,11,12	0.62	0	15,15,17	2.37	4 (26%)
3	MAN	H	4	3	11,11,12	1.24	2 (18%)	15,15,17	3.22	11 (73%)
3	MAN	H	5	3	11,11,12	1.16	1 (9%)	15,15,17	1.96	4 (26%)
4	NAG	I	1	2,4	14,14,15	0.57	0	17,19,21	2.09	3 (17%)
4	NAG	I	2	4	14,14,15	0.95	1 (7%)	17,19,21	1.66	3 (17%)
3	NAG	J	1	1,3	14,14,15	0.79	0	17,19,21	2.64	5 (29%)
3	NAG	J	2	3	14,14,15	0.98	1 (7%)	17,19,21	2.66	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	J	3	3	11,11,12	0.84	0	15,15,17	1.31	2 (13%)
3	MAN	J	4	3	11,11,12	1.30	2 (18%)	15,15,17	2.32	8 (53%)
3	MAN	J	5	3	11,11,12	1.33	2 (18%)	15,15,17	2.19	6 (40%)
3	NAG	K	1	3,2	14,14,15	0.76	0	17,19,21	3.28	10 (58%)
3	NAG	K	2	3	14,14,15	0.37	0	17,19,21	1.23	2 (11%)
3	BMA	K	3	3	11,11,12	0.62	0	15,15,17	2.37	4 (26%)
3	MAN	K	4	3	11,11,12	1.24	2 (18%)	15,15,17	3.22	11 (73%)
3	MAN	K	5	3	11,11,12	1.16	1 (9%)	15,15,17	1.95	4 (26%)
4	NAG	L	1	2,4	14,14,15	0.57	0	17,19,21	2.10	3 (17%)
4	NAG	L	2	4	14,14,15	0.95	1 (7%)	17,19,21	1.66	3 (17%)
3	NAG	M	1	1,3	14,14,15	0.78	0	17,19,21	2.64	5 (29%)
3	NAG	M	2	3	14,14,15	0.97	1 (7%)	17,19,21	2.65	10 (58%)
3	BMA	M	3	3	11,11,12	0.85	0	15,15,17	1.31	2 (13%)
3	MAN	M	4	3	11,11,12	1.30	2 (18%)	15,15,17	2.33	8 (53%)
3	MAN	M	5	3	11,11,12	1.32	2 (18%)	15,15,17	2.20	6 (40%)
3	NAG	N	1	3,2	14,14,15	0.76	0	17,19,21	3.28	10 (58%)
3	NAG	N	2	3	14,14,15	0.36	0	17,19,21	1.23	2 (11%)
3	BMA	N	3	3	11,11,12	0.62	0	15,15,17	2.38	4 (26%)
3	MAN	N	4	3	11,11,12	1.24	2 (18%)	15,15,17	3.22	11 (73%)
3	MAN	N	5	3	11,11,12	1.17	1 (9%)	15,15,17	1.95	4 (26%)
4	NAG	O	1	2,4	14,14,15	0.58	0	17,19,21	2.09	3 (17%)
4	NAG	O	2	4	14,14,15	0.95	1 (7%)	17,19,21	1.66	3 (17%)

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

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

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

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	5	MAN	C1-C2	3.00	1.59	1.52
3	G	5	MAN	C1-C2	2.99	1.59	1.52
3	M	5	MAN	C1-C2	2.97	1.59	1.52
3	J	2	NAG	C1-C2	2.84	1.56	1.52
3	G	2	NAG	C1-C2	2.83	1.56	1.52
3	M	2	NAG	C1-C2	2.79	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	4	MAN	O5-C1	2.64	1.47	1.43
3	J	4	MAN	O5-C1	2.63	1.47	1.43
3	G	4	MAN	O5-C1	2.63	1.47	1.43
3	G	4	MAN	C1-C2	2.55	1.58	1.52
3	M	4	MAN	C1-C2	2.55	1.58	1.52
3	J	4	MAN	C1-C2	2.54	1.58	1.52
3	N	4	MAN	O5-C1	2.41	1.47	1.43
3	H	4	MAN	O5-C1	2.38	1.47	1.43
3	K	4	MAN	O5-C1	2.37	1.47	1.43
3	M	5	MAN	O5-C1	2.19	1.47	1.43
3	N	5	MAN	C1-C2	2.19	1.57	1.52
3	J	5	MAN	O5-C1	2.19	1.47	1.43
3	G	5	MAN	O5-C1	2.18	1.47	1.43
3	H	5	MAN	C1-C2	2.18	1.57	1.52
3	K	5	MAN	C1-C2	2.17	1.57	1.52
3	K	4	MAN	C1-C2	2.16	1.57	1.52
3	N	4	MAN	C1-C2	2.16	1.57	1.52
3	H	4	MAN	C1-C2	2.15	1.57	1.52
4	L	2	NAG	C1-C2	2.10	1.55	1.52
4	I	2	NAG	C1-C2	2.08	1.55	1.52
4	O	2	NAG	C1-C2	2.04	1.55	1.52

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	1	NAG	C1-O5-C5	8.60	123.84	112.19
3	H	1	NAG	C1-O5-C5	8.59	123.83	112.19
3	N	1	NAG	C1-O5-C5	8.59	123.83	112.19
3	J	1	NAG	C1-O5-C5	6.98	121.65	112.19
3	G	1	NAG	C1-O5-C5	6.98	121.65	112.19
3	M	1	NAG	C1-O5-C5	6.96	121.62	112.19
3	H	4	MAN	C1-O5-C5	6.88	121.51	112.19
3	N	4	MAN	C1-O5-C5	6.86	121.49	112.19
3	K	4	MAN	C1-O5-C5	6.86	121.49	112.19
3	N	3	BMA	C1-C2-C3	6.46	117.60	109.67
3	K	3	BMA	C1-C2-C3	6.42	117.56	109.67
3	H	3	BMA	C1-C2-C3	6.41	117.55	109.67
4	L	1	NAG	O5-C1-C2	-5.37	102.81	111.29
4	O	1	NAG	O5-C1-C2	-5.37	102.81	111.29
4	I	1	NAG	O5-C1-C2	-5.36	102.83	111.29
3	H	4	MAN	O5-C5-C6	5.12	115.22	107.20
3	N	4	MAN	O5-C5-C6	5.09	115.19	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	4	MAN	O5-C5-C6	5.09	115.19	107.20
3	J	2	NAG	C2-N2-C7	4.98	129.99	122.90
3	G	2	NAG	C2-N2-C7	4.97	129.98	122.90
3	M	2	NAG	C2-N2-C7	4.93	129.92	122.90
4	L	1	NAG	C2-N2-C7	-4.89	115.94	122.90
4	O	1	NAG	C2-N2-C7	-4.87	115.97	122.90
4	I	1	NAG	C2-N2-C7	-4.86	115.98	122.90
3	M	1	NAG	O5-C5-C6	-4.84	99.62	107.20
3	G	1	NAG	O5-C5-C6	-4.81	99.66	107.20
3	J	1	NAG	O5-C5-C6	-4.81	99.66	107.20
3	J	2	NAG	O5-C1-C2	-4.63	103.97	111.29
3	G	2	NAG	O5-C1-C2	-4.62	104.00	111.29
3	M	2	NAG	O5-C1-C2	-4.61	104.00	111.29
4	I	2	NAG	C4-C3-C2	4.41	117.48	111.02
4	L	2	NAG	C4-C3-C2	4.41	117.48	111.02
4	O	2	NAG	C4-C3-C2	4.39	117.45	111.02
3	H	3	BMA	O5-C5-C6	4.37	114.05	107.20
3	K	3	BMA	O5-C5-C6	4.37	114.05	107.20
3	N	3	BMA	O5-C5-C6	4.36	114.04	107.20
3	H	1	NAG	C3-C4-C5	4.26	117.83	110.24
3	N	1	NAG	C3-C4-C5	4.25	117.82	110.24
3	K	1	NAG	C3-C4-C5	4.24	117.80	110.24
3	H	5	MAN	C1-O5-C5	4.22	117.92	112.19
3	N	5	MAN	C1-O5-C5	4.21	117.90	112.19
3	K	5	MAN	C1-O5-C5	4.21	117.89	112.19
3	M	4	MAN	C1-O5-C5	4.10	117.75	112.19
3	G	4	MAN	C1-O5-C5	4.08	117.72	112.19
3	J	4	MAN	C1-O5-C5	4.06	117.69	112.19
3	K	1	NAG	O4-C4-C3	-3.91	101.30	110.35
3	H	1	NAG	O4-C4-C3	-3.91	101.31	110.35
3	M	4	MAN	O5-C5-C6	3.91	113.33	107.20
3	N	1	NAG	O4-C4-C3	-3.91	101.32	110.35
3	G	4	MAN	O5-C5-C6	3.90	113.31	107.20
3	J	4	MAN	O5-C5-C6	3.88	113.29	107.20
3	G	5	MAN	O2-C2-C1	3.88	117.08	109.15
3	M	5	MAN	O2-C2-C1	3.87	117.08	109.15
3	J	5	MAN	O2-C2-C1	3.87	117.08	109.15
3	M	2	NAG	C1-C2-N2	3.85	117.06	110.49
3	G	2	NAG	C1-C2-N2	3.83	117.03	110.49
3	H	4	MAN	C2-C3-C4	-3.83	104.27	110.89
3	K	1	NAG	C2-N2-C7	3.82	128.35	122.90
3	K	4	MAN	C2-C3-C4	-3.82	104.28	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	2	NAG	C1-C2-N2	3.82	117.01	110.49
3	N	4	MAN	C2-C3-C4	-3.82	104.29	110.89
3	H	1	NAG	C2-N2-C7	3.81	128.33	122.90
3	H	1	NAG	C4-C3-C2	3.81	116.59	111.02
3	K	1	NAG	C4-C3-C2	3.80	116.59	111.02
3	N	1	NAG	C4-C3-C2	3.80	116.59	111.02
3	N	1	NAG	C2-N2-C7	3.79	128.29	122.90
3	G	1	NAG	O4-C4-C3	3.71	118.94	110.35
3	J	1	NAG	O4-C4-C3	3.71	118.92	110.35
3	M	1	NAG	O4-C4-C3	3.69	118.89	110.35
3	G	3	BMA	C1-O5-C5	-3.46	107.51	112.19
3	K	4	MAN	O5-C1-C2	3.45	116.09	110.77
3	J	3	BMA	C1-O5-C5	-3.45	107.52	112.19
3	M	3	BMA	C1-O5-C5	-3.45	107.52	112.19
3	K	4	MAN	O3-C3-C2	3.44	116.58	109.99
3	H	4	MAN	O3-C3-C2	3.43	116.57	109.99
3	H	4	MAN	O5-C1-C2	3.43	116.06	110.77
3	N	4	MAN	O5-C1-C2	3.43	116.06	110.77
3	N	4	MAN	O3-C3-C2	3.43	116.56	109.99
3	J	2	NAG	O5-C5-C4	3.38	119.04	110.83
3	G	2	NAG	O5-C5-C4	3.38	119.04	110.83
3	M	2	NAG	O5-C5-C4	3.37	119.03	110.83
3	M	5	MAN	C1-O5-C5	3.32	116.69	112.19
3	J	5	MAN	C1-O5-C5	3.30	116.66	112.19
3	G	5	MAN	C1-O5-C5	3.30	116.66	112.19
3	M	1	NAG	O5-C5-C4	3.24	118.70	110.83
3	J	1	NAG	O5-C5-C4	3.24	118.70	110.83
3	G	1	NAG	O5-C5-C4	3.23	118.70	110.83
3	M	5	MAN	O5-C5-C6	3.14	112.12	107.20
3	G	5	MAN	O5-C5-C6	3.13	112.12	107.20
3	J	5	MAN	O5-C5-C6	3.13	112.11	107.20
3	H	5	MAN	O5-C5-C6	3.11	112.09	107.20
3	N	5	MAN	O5-C5-C6	3.11	112.08	107.20
3	K	5	MAN	O5-C5-C6	3.10	112.07	107.20
4	L	2	NAG	C2-N2-C7	3.07	127.28	122.90
4	O	2	NAG	C2-N2-C7	3.06	127.26	122.90
4	I	2	NAG	C2-N2-C7	3.05	127.25	122.90
3	N	2	NAG	C1-C2-N2	-2.99	105.38	110.49
3	H	2	NAG	C1-C2-N2	-2.98	105.39	110.49
3	K	2	NAG	C1-C2-N2	-2.97	105.41	110.49
3	N	4	MAN	O2-C2-C1	2.97	115.23	109.15
3	K	4	MAN	O2-C2-C1	2.97	115.23	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	4	MAN	O2-C2-C1	2.96	115.22	109.15
3	J	2	NAG	O3-C3-C2	2.95	115.56	109.47
3	M	2	NAG	O3-C3-C2	2.93	115.54	109.47
3	G	2	NAG	O3-C3-C2	2.93	115.53	109.47
3	G	4	MAN	O3-C3-C2	2.93	115.60	109.99
3	J	4	MAN	O3-C3-C2	2.92	115.59	109.99
3	M	4	MAN	O3-C3-C2	2.92	115.59	109.99
3	H	5	MAN	O2-C2-C1	2.83	114.95	109.15
3	K	5	MAN	O2-C2-C1	2.83	114.94	109.15
3	N	5	MAN	O2-C2-C1	2.82	114.93	109.15
3	K	1	NAG	C6-C5-C4	-2.80	106.44	113.00
3	H	1	NAG	C6-C5-C4	-2.79	106.46	113.00
3	N	1	NAG	C6-C5-C4	-2.79	106.47	113.00
3	N	4	MAN	O2-C2-C3	2.72	115.59	110.14
3	H	4	MAN	O2-C2-C3	2.70	115.55	110.14
3	K	4	MAN	O2-C2-C3	2.69	115.53	110.14
3	M	5	MAN	C2-C3-C4	-2.69	106.24	110.89
3	G	5	MAN	C2-C3-C4	-2.68	106.26	110.89
3	J	5	MAN	C2-C3-C4	-2.68	106.26	110.89
3	H	1	NAG	O7-C7-N2	2.68	126.87	121.95
3	N	1	NAG	O7-C7-N2	2.67	126.87	121.95
3	M	5	MAN	O3-C3-C2	2.67	115.11	109.99
3	G	5	MAN	O3-C3-C2	2.67	115.10	109.99
3	J	5	MAN	O3-C3-C2	2.66	115.09	109.99
3	K	1	NAG	O7-C7-N2	2.66	126.83	121.95
3	K	1	NAG	O5-C5-C6	2.57	111.24	107.20
3	H	1	NAG	O5-C5-C6	2.55	111.21	107.20
3	N	1	NAG	O5-C5-C6	2.55	111.20	107.20
4	O	1	NAG	O5-C5-C4	2.54	117.00	110.83
4	I	1	NAG	O5-C5-C4	2.53	116.98	110.83
4	L	1	NAG	O5-C5-C4	2.53	116.98	110.83
3	K	3	BMA	O2-C2-C3	-2.50	105.13	110.14
3	N	3	BMA	O2-C2-C3	-2.50	105.14	110.14
3	H	3	BMA	O2-C2-C3	-2.49	105.15	110.14
3	G	4	MAN	O2-C2-C1	2.45	114.16	109.15
3	M	2	NAG	C3-C4-C5	2.45	114.61	110.24
3	G	2	NAG	O3-C3-C4	-2.45	104.69	110.35
3	J	2	NAG	O3-C3-C4	-2.44	104.70	110.35
3	H	2	NAG	O4-C4-C5	2.44	115.36	109.30
3	N	2	NAG	O4-C4-C5	2.44	115.35	109.30
3	K	2	NAG	O4-C4-C5	2.43	115.34	109.30
3	J	4	MAN	O2-C2-C1	2.43	114.13	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	2	NAG	O3-C3-C4	-2.43	104.73	110.35
3	M	4	MAN	O2-C2-C1	2.43	114.12	109.15
3	J	2	NAG	C3-C4-C5	2.43	114.57	110.24
3	G	2	NAG	C3-C4-C5	2.42	114.56	110.24
3	J	5	MAN	O4-C4-C5	2.42	115.31	109.30
3	G	5	MAN	O4-C4-C5	2.42	115.30	109.30
3	M	4	MAN	O4-C4-C3	2.41	115.93	110.35
3	J	4	MAN	O4-C4-C3	2.41	115.91	110.35
3	M	5	MAN	O4-C4-C5	2.40	115.27	109.30
3	G	4	MAN	O4-C4-C3	2.40	115.90	110.35
3	J	4	MAN	O5-C1-C2	2.36	114.41	110.77
3	M	4	MAN	O4-C4-C5	2.35	115.14	109.30
3	G	4	MAN	O5-C1-C2	2.35	114.39	110.77
3	G	4	MAN	O4-C4-C5	2.35	115.12	109.30
3	M	4	MAN	O5-C1-C2	2.34	114.39	110.77
3	H	4	MAN	O3-C3-C4	2.34	115.75	110.35
3	K	4	MAN	O3-C3-C4	2.34	115.75	110.35
3	J	4	MAN	O4-C4-C5	2.33	115.08	109.30
3	N	4	MAN	O3-C3-C4	2.32	115.70	110.35
3	M	1	NAG	C3-C4-C5	-2.32	106.11	110.24
3	G	1	NAG	C3-C4-C5	-2.31	106.11	110.24
3	J	1	NAG	C3-C4-C5	-2.31	106.11	110.24
3	J	2	NAG	O7-C7-C8	-2.31	117.77	122.06
3	G	2	NAG	O7-C7-C8	-2.31	117.77	122.06
3	M	2	NAG	O7-C7-C8	-2.29	117.80	122.06
3	G	2	NAG	C6-C5-C4	-2.26	107.72	113.00
3	J	2	NAG	C6-C5-C4	-2.24	107.75	113.00
3	M	2	NAG	C6-C5-C4	-2.24	107.75	113.00
3	N	4	MAN	O4-C4-C3	2.24	115.52	110.35
3	H	4	MAN	O4-C4-C3	2.23	115.50	110.35
3	K	4	MAN	O4-C4-C3	2.23	115.50	110.35
3	N	1	NAG	O6-C6-C5	2.20	118.85	111.29
3	H	1	NAG	O6-C6-C5	2.20	118.83	111.29
3	K	1	NAG	O6-C6-C5	2.20	118.83	111.29
3	K	3	BMA	C2-C3-C4	2.18	114.67	110.89
3	H	3	BMA	C2-C3-C4	2.18	114.66	110.89
3	G	2	NAG	O4-C4-C5	2.17	114.68	109.30
3	J	2	NAG	O4-C4-C5	2.17	114.68	109.30
3	M	2	NAG	O4-C4-C5	2.16	114.67	109.30
3	M	4	MAN	O3-C3-C4	2.16	115.34	110.35
3	N	3	BMA	C2-C3-C4	2.15	114.62	110.89
3	M	3	BMA	O4-C4-C5	2.15	114.64	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	4	MAN	O3-C3-C4	2.15	115.31	110.35
3	N	4	MAN	O5-C5-C4	2.14	116.03	110.83
3	J	4	MAN	O3-C3-C4	2.14	115.29	110.35
3	G	3	BMA	O4-C4-C5	2.14	114.61	109.30
3	K	4	MAN	O5-C5-C4	2.14	116.03	110.83
3	J	3	BMA	O4-C4-C5	2.13	114.58	109.30
3	H	4	MAN	O5-C5-C4	2.13	116.00	110.83
3	N	4	MAN	O4-C4-C5	2.10	114.51	109.30
3	H	4	MAN	O4-C4-C5	2.09	114.49	109.30
3	K	4	MAN	O4-C4-C5	2.09	114.48	109.30
3	N	1	NAG	C1-C2-N2	2.08	114.04	110.49
3	H	1	NAG	C1-C2-N2	2.08	114.04	110.49
4	I	2	NAG	O7-C7-C8	-2.06	118.24	122.06
3	K	1	NAG	C1-C2-N2	2.05	113.99	110.49
4	L	2	NAG	O7-C7-C8	-2.05	118.25	122.06
4	O	2	NAG	O7-C7-C8	-2.04	118.27	122.06
3	K	5	MAN	O4-C4-C5	2.04	114.35	109.30
3	H	5	MAN	O4-C4-C5	2.03	114.35	109.30
3	N	5	MAN	O4-C4-C5	2.02	114.31	109.30

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2

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

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Mol	Chain	Res	Type	Atoms
3	K	5	MAN	C4-C5-C6-O6
3	N	5	MAN	C4-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6

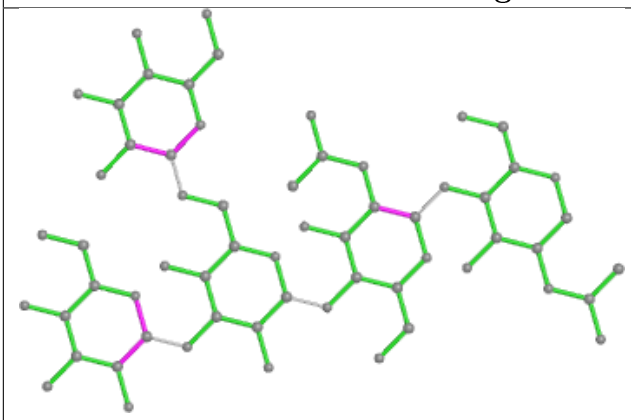
There are no ring outliers.

24 monomers are involved in 34 short contacts:

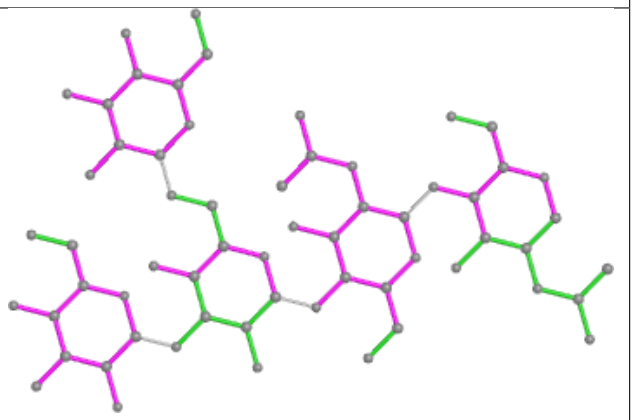
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	3	BMA	2	0
4	L	1	NAG	3	0
3	N	3	BMA	2	0
3	K	5	MAN	3	0
4	I	2	NAG	2	0
4	O	2	NAG	2	0
4	I	1	NAG	3	0
3	K	1	NAG	2	0
3	H	3	BMA	2	0
3	G	5	MAN	3	0
3	J	5	MAN	3	0
3	H	5	MAN	3	0
3	K	2	NAG	1	0
4	O	1	NAG	3	0
3	H	1	NAG	2	0
4	L	2	NAG	2	0
3	N	1	NAG	2	0
3	M	5	MAN	4	0
3	J	3	BMA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

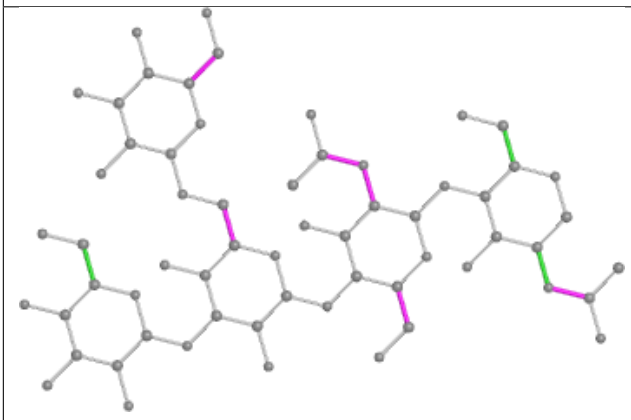
Oligosaccharide Chain G



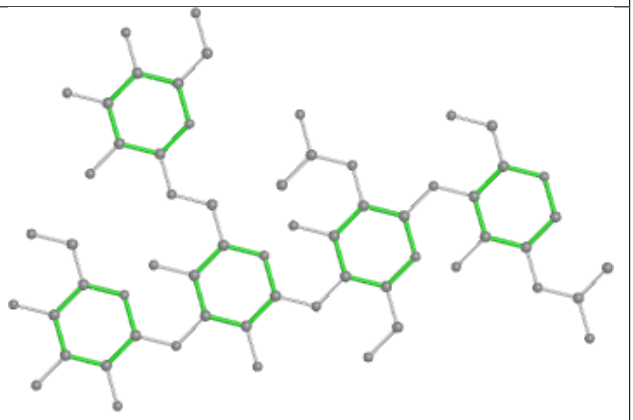
Bond lengths



Bond angles

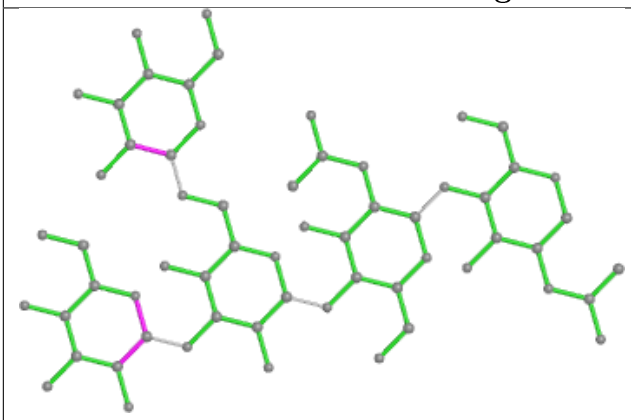


Torsions

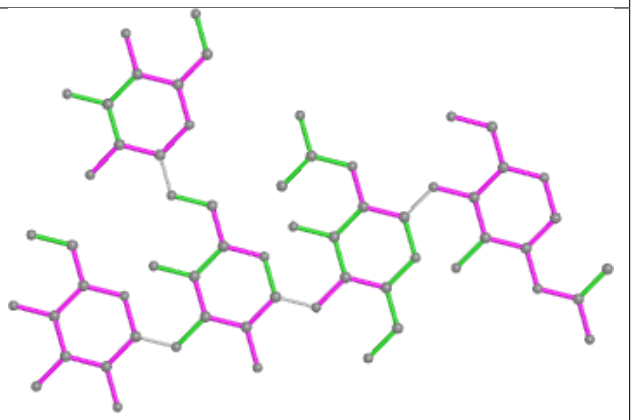


Rings

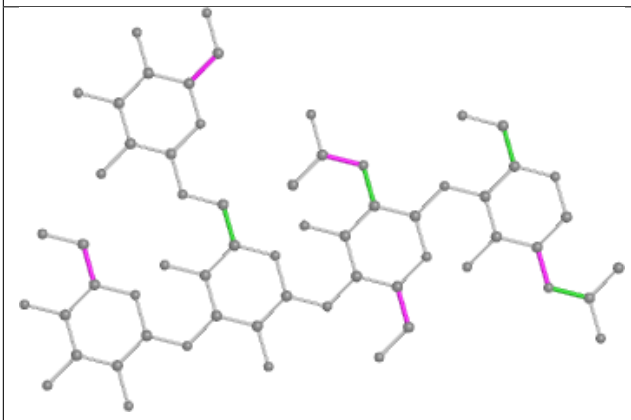
Oligosaccharide Chain H



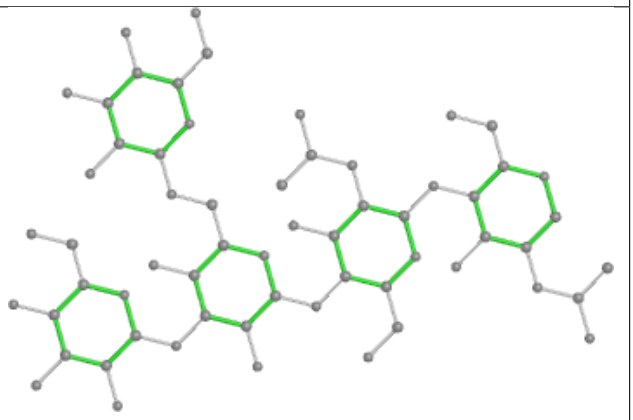
Bond lengths



Bond angles

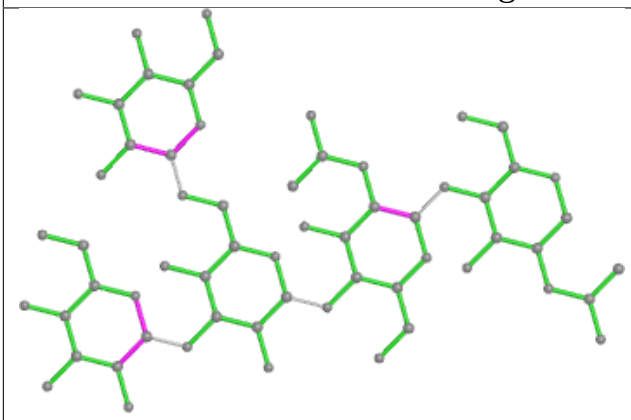


Torsions

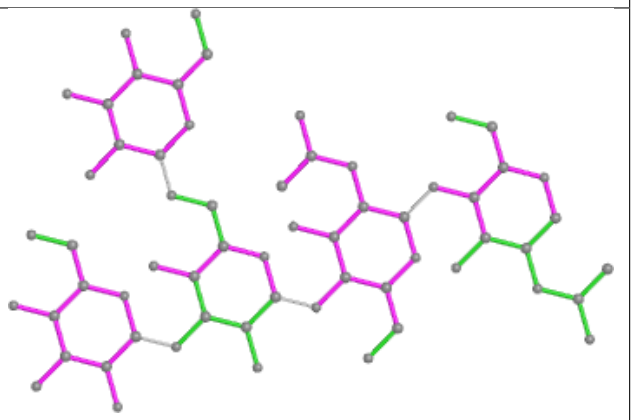


Rings

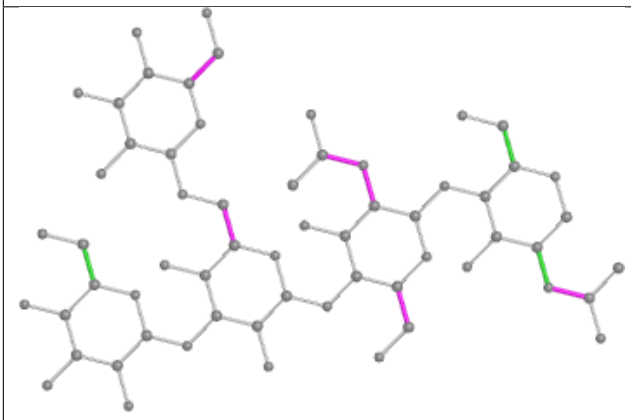
Oligosaccharide Chain J



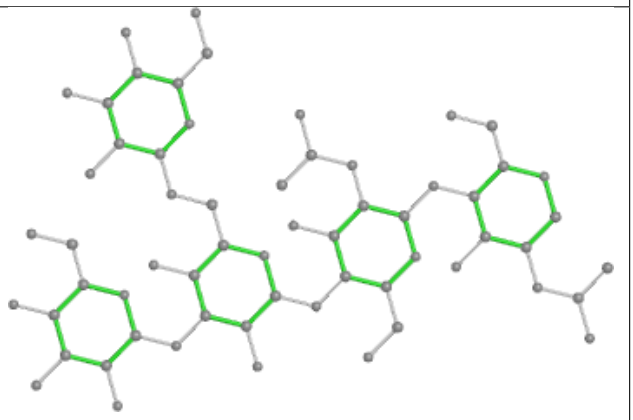
Bond lengths



Bond angles

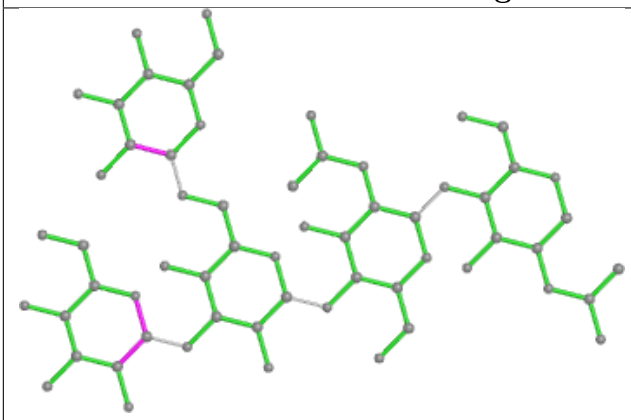


Torsions

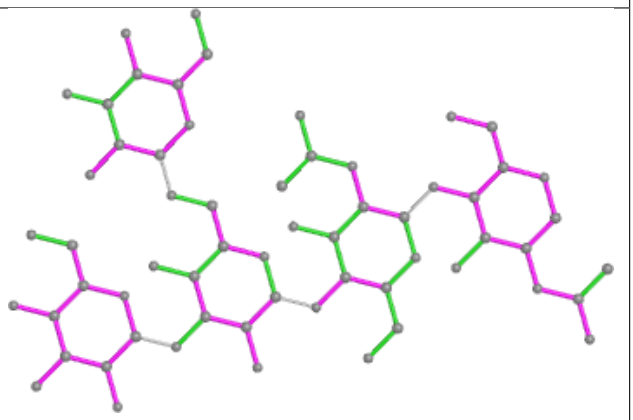


Rings

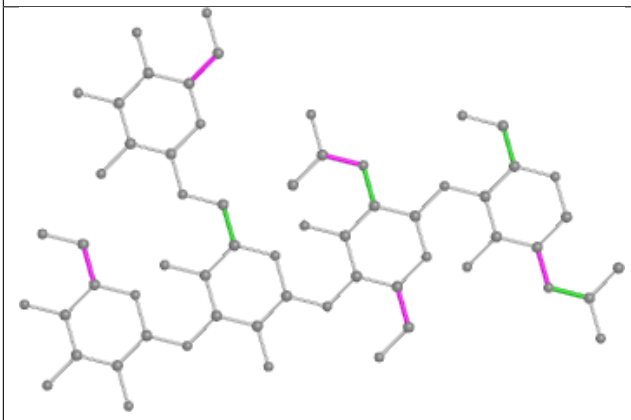
Oligosaccharide Chain K



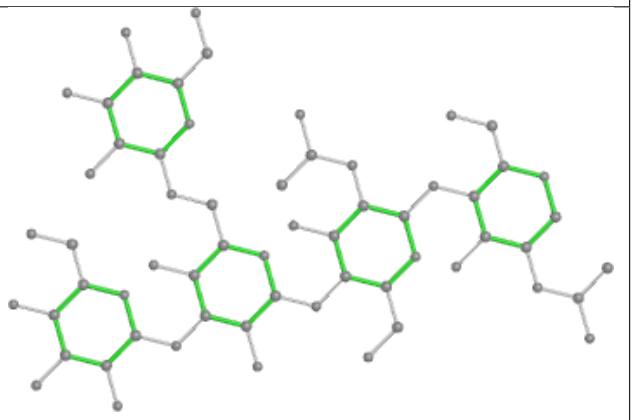
Bond lengths



Bond angles

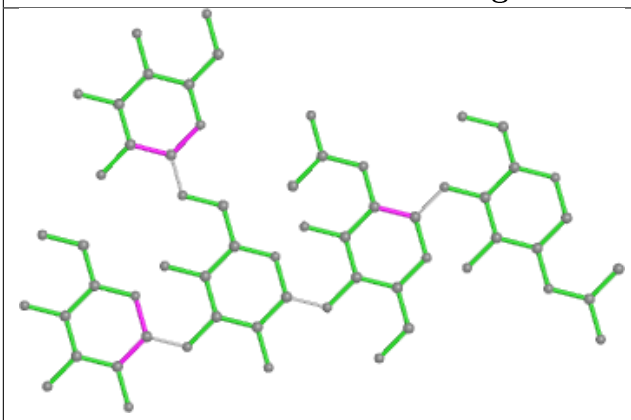


Torsions

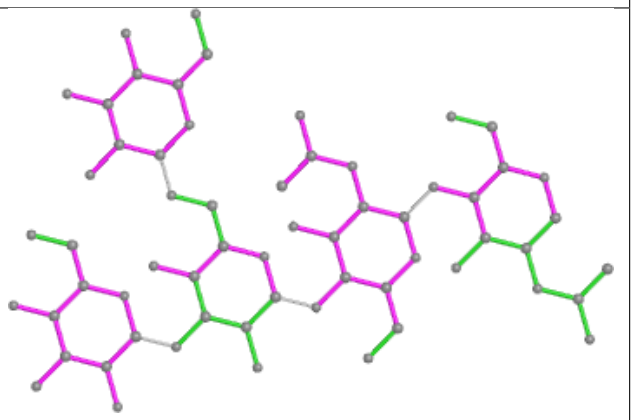


Rings

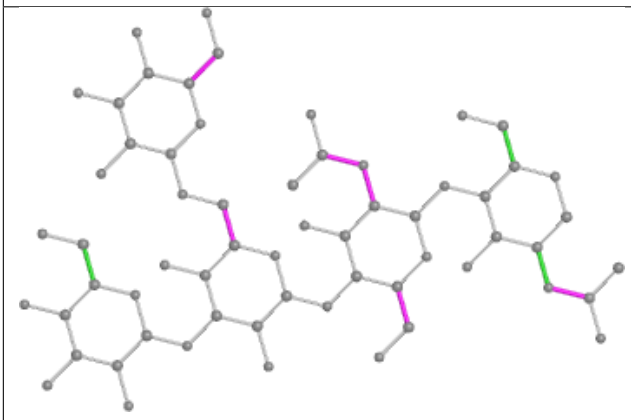
Oligosaccharide Chain M



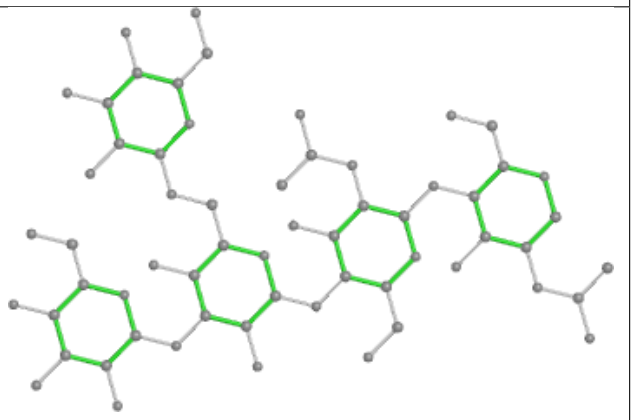
Bond lengths



Bond angles

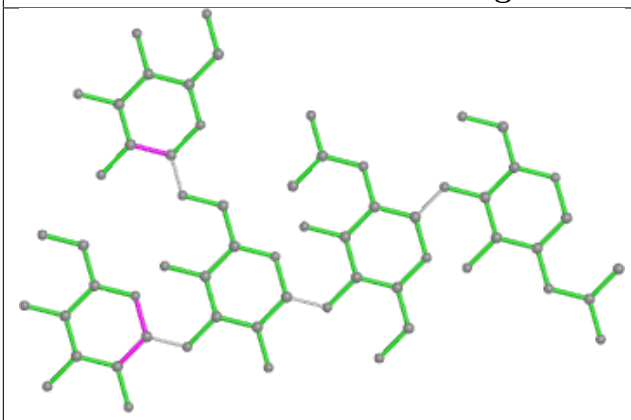


Torsions

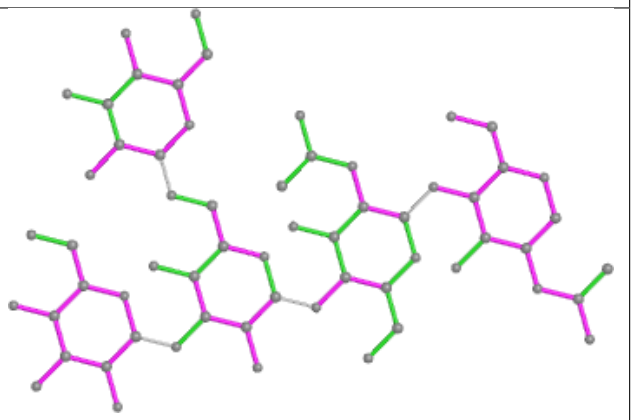


Rings

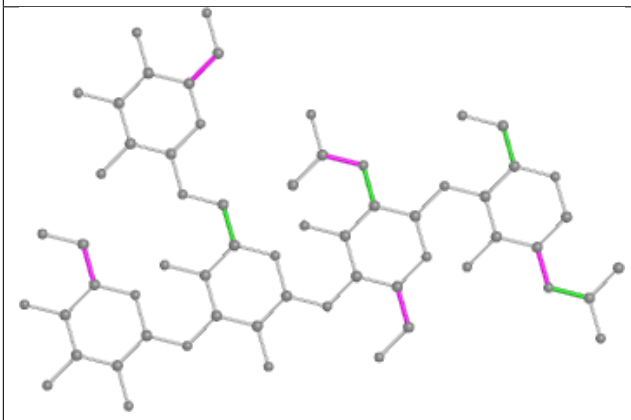
Oligosaccharide Chain N



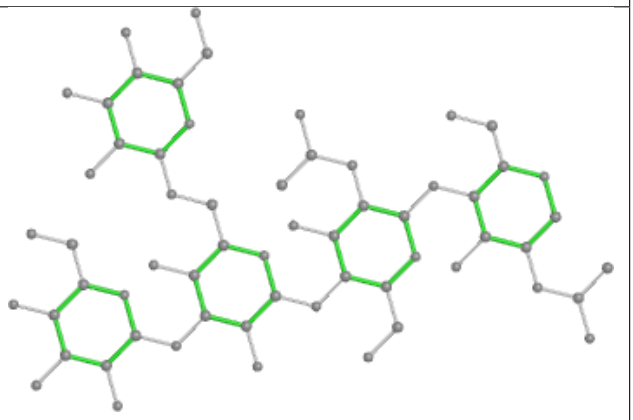
Bond lengths



Bond angles

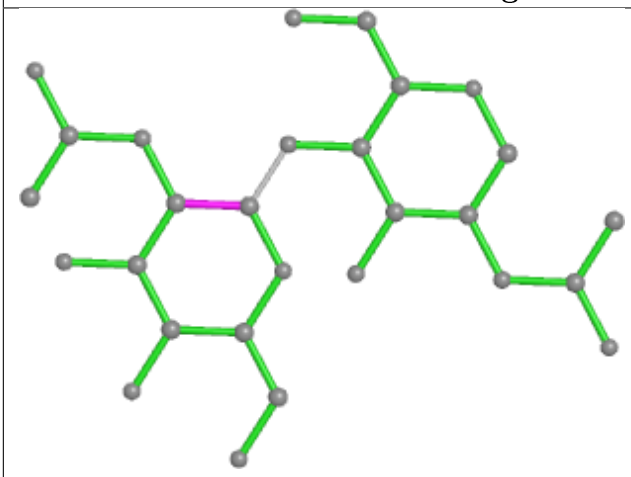


Torsions

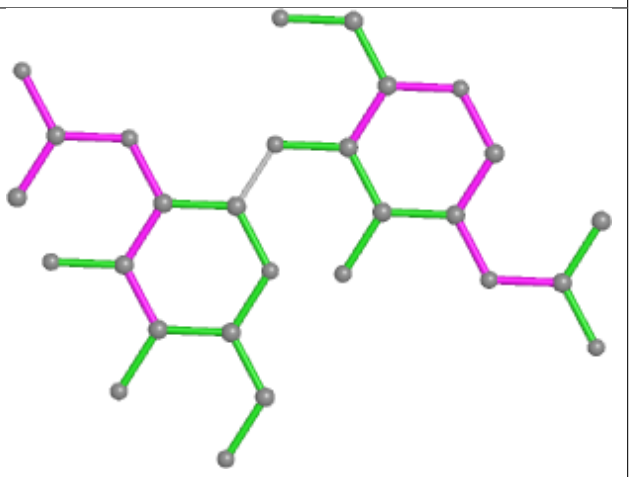


Rings

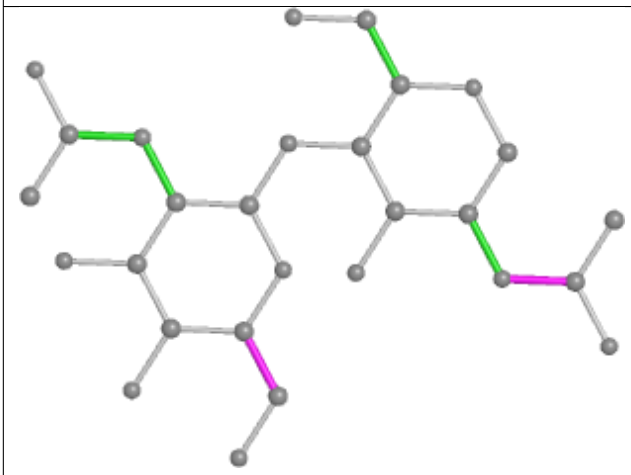
Oligosaccharide Chain I



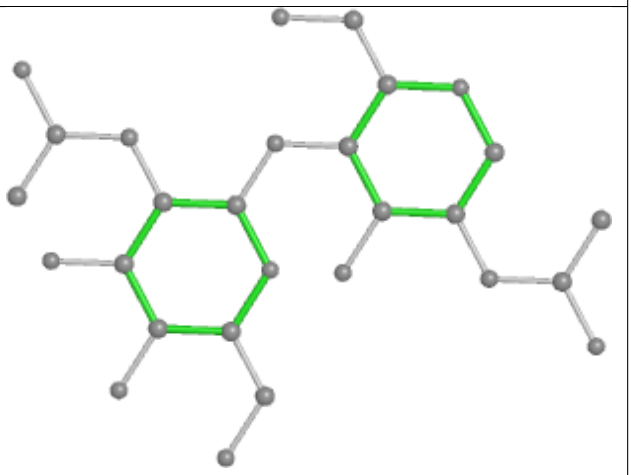
Bond lengths



Bond angles

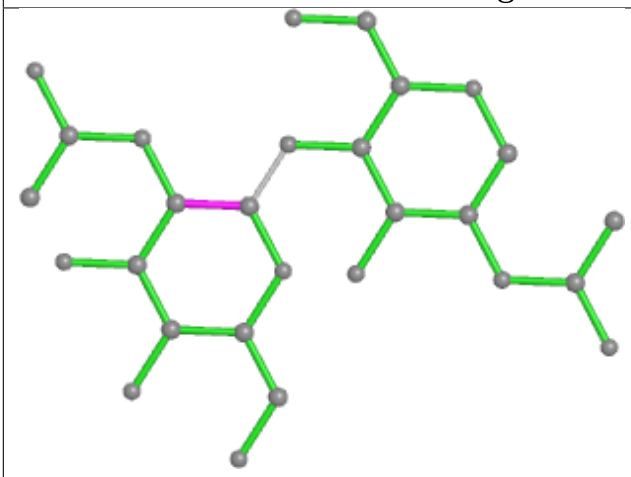


Torsions

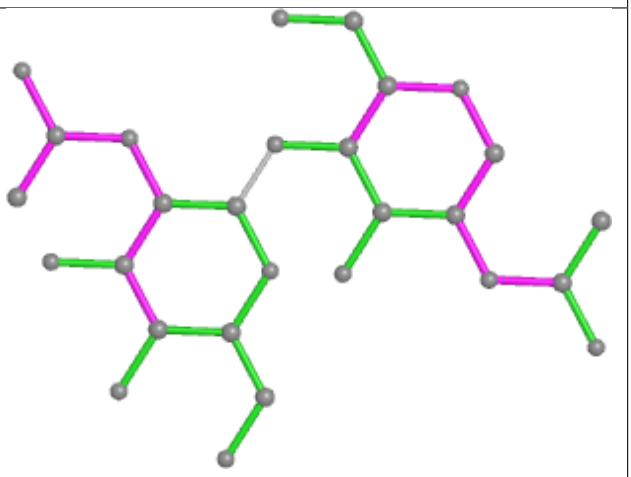


Rings

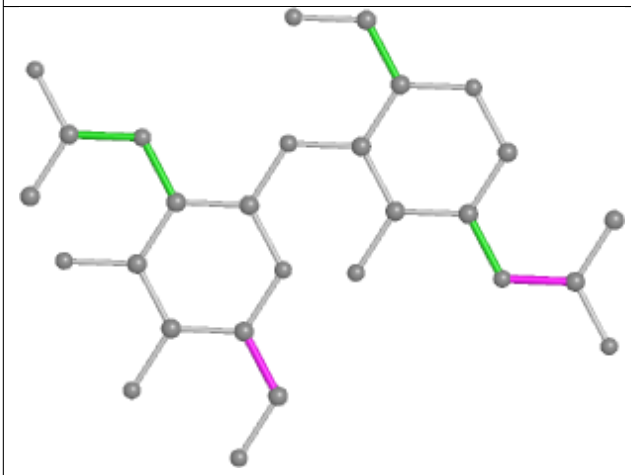
Oligosaccharide Chain L



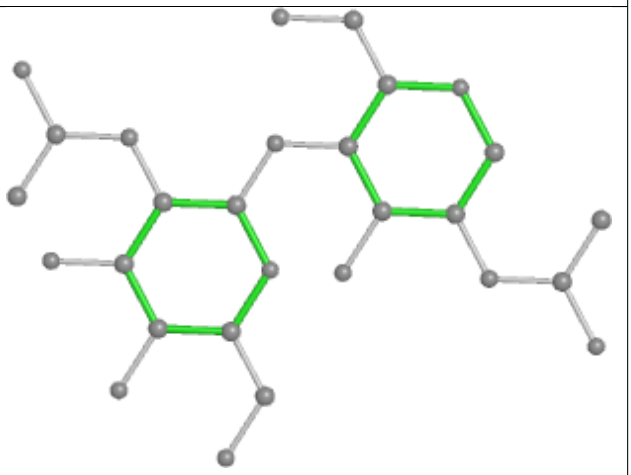
Bond lengths



Bond angles

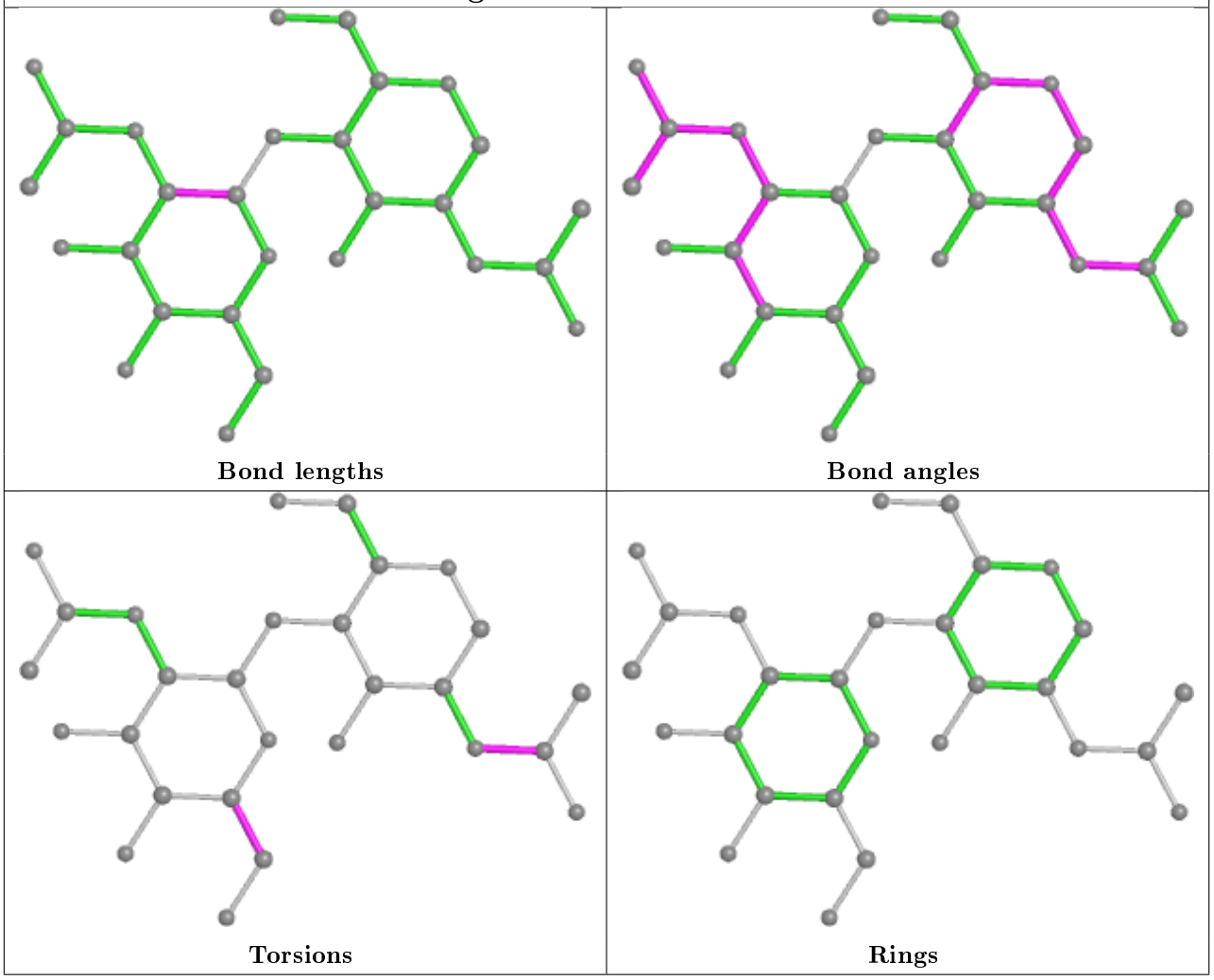


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

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	$\#\|Z\| > 2$
5	NAG	F	2009	2	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
5	NAG	F	2012	2	14,14,15	0.59	0	17,19,21	2.05	6 (35%)
5	NAG	D	2012	2	14,14,15	0.61	0	17,19,21	1.70	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	D	2013	2	14,14,15	0.62	0	17,19,21	2.07	5 (29%)
5	NAG	B	2007	2	14,14,15	0.54	0	17,19,21	1.12	3 (17%)
5	NAG	B	2008	2	14,14,15	0.58	0	17,19,21	1.12	2 (11%)
5	NAG	B	2001	2	14,14,15	0.94	1 (7%)	17,19,21	1.89	5 (29%)
6	B12	A	2007	-	80,101,101	1.23	7 (8%)	101,166,166	2.36	25 (24%)
5	NAG	B	2013	2	14,14,15	0.66	0	17,19,21	2.01	4 (23%)
5	NAG	F	2013	2	14,14,15	0.64	0	17,19,21	1.86	4 (23%)
5	NAG	E	2001	1	14,14,15	1.11	2 (14%)	17,19,21	2.39	7 (41%)
5	NAG	D	2009	2	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
6	B12	E	2007	-	80,101,101	1.23	7 (8%)	101,166,166	2.36	26 (25%)
5	NAG	F	2008	2	14,14,15	0.57	0	17,19,21	1.12	2 (11%)
6	B12	C	2007	-	80,101,101	1.24	7 (8%)	101,166,166	2.36	25 (24%)
5	NAG	F	2001	2	14,14,15	0.96	1 (7%)	17,19,21	1.90	5 (29%)
5	NAG	D	2001	2	14,14,15	0.93	1 (7%)	17,19,21	1.90	5 (29%)
5	NAG	D	2008	2	14,14,15	0.57	0	17,19,21	1.13	2 (11%)
5	NAG	B	2012	2	14,14,15	0.65	0	17,19,21	2.19	3 (17%)
5	NAG	B	2009	2	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
5	NAG	A	2001	1	14,14,15	1.10	2 (14%)	17,19,21	2.36	7 (41%)
5	NAG	D	2007	2	14,14,15	0.53	0	17,19,21	1.12	3 (17%)
5	NAG	F	2007	2	14,14,15	0.54	0	17,19,21	1.12	3 (17%)
5	NAG	C	2001	1	14,14,15	1.09	1 (7%)	17,19,21	2.37	7 (41%)

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
5	NAG	F	2009	2	-	0/6/23/26	0/1/1/1
5	NAG	F	2012	2	-	4/6/23/26	0/1/1/1
5	NAG	D	2012	2	-	4/6/23/26	0/1/1/1
5	NAG	D	2013	2	-	3/6/23/26	0/1/1/1
5	NAG	B	2007	2	-	2/6/23/26	0/1/1/1
5	NAG	B	2008	2	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	B	2001	2	1/1/5/7	5/6/23/26	0/1/1/1
6	B12	A	2007	-	1/1/36/38	10/51/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	2013	2	-	3/6/23/26	0/1/1/1
5	NAG	F	2013	2	-	3/6/23/26	0/1/1/1
5	NAG	E	2001	1	1/1/5/7	6/6/23/26	0/1/1/1
5	NAG	D	2009	2	-	0/6/23/26	0/1/1/1
6	B12	E	2007	-	1/1/36/38	10/51/223/223	0/3/11/11
5	NAG	F	2008	2	1/1/5/7	5/6/23/26	0/1/1/1
6	B12	C	2007	-	1/1/36/38	10/51/223/223	0/3/11/11
5	NAG	F	2001	2	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	D	2001	2	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	D	2008	2	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	B	2012	2	-	4/6/23/26	0/1/1/1
5	NAG	B	2009	2	-	0/6/23/26	0/1/1/1
5	NAG	A	2001	1	1/1/5/7	6/6/23/26	0/1/1/1
5	NAG	D	2007	2	-	2/6/23/26	0/1/1/1
5	NAG	F	2007	2	-	2/6/23/26	0/1/1/1
5	NAG	C	2001	1	1/1/5/7	6/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	2007	B12	C11-C10	-4.72	1.33	1.40
6	A	2007	B12	C11-C10	-4.71	1.33	1.40
6	C	2007	B12	C11-C10	-4.70	1.33	1.40
6	C	2007	B12	C2-C3	-4.09	1.51	1.58
6	A	2007	B12	C2-C3	-4.08	1.51	1.58
6	E	2007	B12	C2-C3	-4.05	1.51	1.58
6	A	2007	B12	C8B-C9B	3.54	1.47	1.40
6	E	2007	B12	C8B-C9B	3.53	1.47	1.40
6	C	2007	B12	C8B-C9B	3.49	1.47	1.40
6	C	2007	B12	C6B-C5B	2.97	1.48	1.40
6	E	2007	B12	C6B-C5B	2.96	1.48	1.40
6	A	2007	B12	C6B-C5B	2.96	1.48	1.40
5	C	2001	NAG	C1-C2	2.75	1.56	1.52
5	F	2001	NAG	C1-C2	2.67	1.56	1.52
5	A	2001	NAG	C1-C2	2.64	1.56	1.52
5	B	2001	NAG	C1-C2	2.62	1.56	1.52
5	D	2001	NAG	C1-C2	2.57	1.56	1.52
5	E	2001	NAG	C1-C2	2.41	1.55	1.52
6	C	2007	B12	C1-C19	-2.35	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2007	B12	C1-C19	-2.32	1.50	1.55
6	E	2007	B12	C1-C19	-2.31	1.50	1.55
5	A	2001	NAG	C2-N2	2.21	1.50	1.46
6	C	2007	B12	C16-C15	-2.20	1.33	1.41
6	A	2007	B12	C16-C15	-2.19	1.33	1.41
6	E	2007	B12	C16-C15	-2.19	1.33	1.41
6	E	2007	B12	C1-C2	-2.15	1.53	1.58
6	C	2007	B12	C1-C2	-2.13	1.53	1.58
6	A	2007	B12	C1-C2	-2.13	1.53	1.58
5	E	2001	NAG	C2-N2	2.13	1.49	1.46

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	2007	B12	C1-C19-N24	9.01	116.38	106.24
6	A	2007	B12	C1-C19-N24	8.99	116.36	106.24
6	C	2007	B12	C1-C19-N24	8.99	116.35	106.24
6	C	2007	B12	C20-C1-C19	-6.61	102.98	109.36
6	C	2007	B12	C12-C11-C10	-6.61	113.43	124.64
6	A	2007	B12	C12-C11-C10	-6.61	113.43	124.64
6	E	2007	B12	C12-C11-C10	-6.58	113.48	124.64
6	E	2007	B12	C20-C1-C19	-6.57	103.03	109.36
6	A	2007	B12	C20-C1-C19	-6.56	103.03	109.36
6	C	2007	B12	C1-C19-C18	6.01	131.87	121.93
6	A	2007	B12	C1-C19-C18	5.99	131.84	121.93
6	E	2007	B12	C1-C19-C18	5.99	131.84	121.93
6	C	2007	B12	C47-C12-C46	5.98	122.26	109.73
6	A	2007	B12	C47-C12-C46	5.95	122.20	109.73
6	E	2007	B12	C47-C12-C46	5.95	122.19	109.73
6	E	2007	B12	C25-C2-C3	-5.67	106.94	115.58
6	A	2007	B12	C25-C2-C3	-5.66	106.94	115.58
6	C	2007	B12	C25-C2-C3	-5.65	106.96	115.58
5	B	2012	NAG	C1-O5-C5	5.46	119.58	112.19
5	B	2012	NAG	O5-C1-C2	-5.34	102.85	111.29
6	C	2007	B12	C30-C3-C2	-5.19	108.12	119.13
6	A	2007	B12	C30-C3-C2	-5.19	108.14	119.13
6	E	2007	B12	C30-C3-C2	-5.19	108.14	119.13
5	F	2012	NAG	O5-C1-C2	-5.03	103.35	111.29
5	F	2001	NAG	O5-C1-C2	-5.00	103.39	111.29
5	D	2001	NAG	O5-C1-C2	-5.00	103.40	111.29
5	B	2001	NAG	O5-C1-C2	-4.95	103.48	111.29
6	C	2007	B12	C2-C1-C19	4.73	126.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	2007	B12	C2-C1-C19	4.73	126.06	118.60
6	A	2007	B12	C2-C1-C19	4.71	126.03	118.60
5	A	2001	NAG	C1-C2-N2	4.65	118.43	110.49
5	D	2013	NAG	O5-C1-C2	-4.65	103.95	111.29
5	E	2001	NAG	C1-C2-N2	4.60	118.35	110.49
5	C	2001	NAG	C1-C2-N2	4.52	118.20	110.49
5	C	2001	NAG	O5-C1-C2	4.46	118.34	111.29
5	E	2001	NAG	O5-C1-C2	4.45	118.31	111.29
5	B	2013	NAG	O5-C1-C2	-4.41	104.32	111.29
6	A	2007	B12	O3-C2P-C1P	4.39	115.68	106.92
6	C	2007	B12	O3-C2P-C1P	4.38	115.66	106.92
6	E	2007	B12	O3-C2P-C1P	4.38	115.65	106.92
5	B	2013	NAG	O5-C5-C6	4.23	113.84	107.20
5	A	2001	NAG	O5-C1-C2	4.20	117.92	111.29
5	D	2013	NAG	O5-C5-C6	4.19	113.77	107.20
6	C	2007	B12	C4B-C9B-C8B	-4.01	116.99	121.10
6	A	2007	B12	C4B-C9B-C8B	-4.00	117.00	121.10
5	F	2013	NAG	O5-C5-C6	4.00	113.48	107.20
5	A	2001	NAG	O7-C7-C8	-3.96	114.71	122.06
6	E	2007	B12	C4B-C9B-C8B	-3.95	117.05	121.10
6	E	2007	B12	C20-C1-C2	-3.83	106.99	113.32
5	F	2013	NAG	O5-C1-C2	-3.82	105.25	111.29
6	C	2007	B12	C2-C26-C27	-3.82	104.48	115.22
6	A	2007	B12	C20-C1-C2	-3.82	107.00	113.32
6	A	2007	B12	C2-C26-C27	-3.82	104.49	115.22
6	E	2007	B12	C2-C26-C27	-3.81	104.50	115.22
6	C	2007	B12	C20-C1-C2	-3.81	107.01	113.32
5	E	2001	NAG	O7-C7-C8	-3.75	115.10	122.06
6	E	2007	B12	C54-C17-C18	-3.70	107.52	112.98
6	C	2007	B12	C54-C17-C18	-3.70	107.53	112.98
6	A	2007	B12	C54-C17-C18	-3.69	107.54	112.98
5	F	2012	NAG	C1-O5-C5	3.66	117.14	112.19
5	D	2012	NAG	C1-O5-C5	3.58	117.04	112.19
5	D	2012	NAG	O5-C1-C2	-3.38	105.95	111.29
5	E	2001	NAG	O7-C7-N2	3.36	128.12	121.95
5	C	2001	NAG	O6-C6-C5	-3.24	100.19	111.29
5	C	2001	NAG	O7-C7-N2	3.22	127.88	121.95
5	C	2001	NAG	O3-C3-C4	-3.19	102.97	110.35
5	E	2001	NAG	O6-C6-C5	-3.17	100.41	111.29
5	D	2013	NAG	C1-O5-C5	3.16	116.47	112.19
6	E	2007	B12	O6R-C4R-C5R	-3.10	102.51	109.21
5	A	2001	NAG	O7-C7-N2	3.10	127.65	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2012	NAG	O3-C3-C2	3.10	115.87	109.47
6	A	2007	B12	O6R-C4R-C5R	-3.09	102.53	109.21
6	C	2007	B12	O6R-C4R-C5R	-3.09	102.54	109.21
5	F	2013	NAG	C1-O5-C5	3.03	116.29	112.19
5	C	2001	NAG	O7-C7-C8	-2.97	116.55	122.06
5	B	2013	NAG	C1-O5-C5	2.95	116.19	112.19
6	A	2007	B12	C26-C2-C1	2.94	114.59	110.02
6	E	2007	B12	C26-C2-C1	2.93	114.58	110.02
5	F	2001	NAG	C1-O5-C5	2.93	116.16	112.19
5	D	2001	NAG	C1-O5-C5	2.93	116.16	112.19
6	C	2007	B12	C26-C2-C1	2.92	114.56	110.02
5	B	2001	NAG	C1-O5-C5	2.91	116.13	112.19
6	C	2007	B12	C9-C10-C11	-2.90	120.78	130.91
6	E	2007	B12	C9-C10-C11	-2.90	120.79	130.91
6	A	2007	B12	C9-C10-C11	-2.90	120.79	130.91
6	A	2007	B12	O8R-C5R-C4R	-2.84	101.56	111.29
6	C	2007	B12	O8R-C5R-C4R	-2.83	101.58	111.29
6	E	2007	B12	O8R-C5R-C4R	-2.82	101.61	111.29
6	C	2007	B12	C16-C15-C14	-2.81	119.88	124.27
6	A	2007	B12	C16-C15-C14	-2.81	119.88	124.27
6	E	2007	B12	C16-C15-C14	-2.80	119.90	124.27
5	A	2001	NAG	O6-C6-C5	-2.78	101.74	111.29
5	E	2001	NAG	O3-C3-C4	-2.74	104.01	110.35
6	C	2007	B12	C8-C9-N22	2.72	114.51	111.12
6	A	2007	B12	C8-C9-N22	2.71	114.51	111.12
6	E	2007	B12	C8-C9-N22	2.71	114.50	111.12
5	A	2001	NAG	C4-C3-C2	2.59	114.82	111.02
5	A	2001	NAG	O3-C3-C4	-2.55	104.45	110.35
5	B	2013	NAG	C1-C2-N2	2.49	114.74	110.49
6	C	2007	B12	C1-C2-C3	2.46	104.67	101.59
6	A	2007	B12	C1-C2-C3	2.46	104.66	101.59
5	E	2001	NAG	C4-C3-C2	2.45	114.61	111.02
5	D	2007	NAG	C2-N2-C7	-2.44	119.42	122.90
6	E	2007	B12	C1-C2-C3	2.44	104.65	101.59
6	A	2007	B12	C13-C14-C15	-2.44	122.83	131.68
6	C	2007	B12	C13-C14-C15	-2.44	122.84	131.68
5	F	2007	NAG	C2-N2-C7	-2.44	119.43	122.90
6	E	2007	B12	C13-C14-C15	-2.44	122.84	131.68
5	B	2007	NAG	C2-N2-C7	-2.43	119.45	122.90
5	F	2012	NAG	O5-C5-C6	2.40	110.97	107.20
5	D	2001	NAG	O5-C5-C6	2.36	110.90	107.20
5	F	2001	NAG	O5-C5-C6	2.35	110.89	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2001	NAG	O5-C5-C6	2.34	110.87	107.20
6	C	2007	B12	C3-C4-C5	-2.33	123.22	131.68
6	E	2007	B12	C3-C4-C5	-2.33	123.22	131.68
6	A	2007	B12	C3-C4-C5	-2.33	123.25	131.68
5	B	2001	NAG	O7-C7-C8	-2.33	117.74	122.06
5	F	2001	NAG	O7-C7-C8	-2.32	117.74	122.06
6	C	2007	B12	C6-C5-C4	-2.31	120.67	124.27
5	D	2001	NAG	O7-C7-C8	-2.31	117.77	122.06
5	F	2012	NAG	O3-C3-C2	2.30	114.22	109.47
6	A	2007	B12	C6-C5-C4	-2.29	120.70	124.27
5	D	2008	NAG	C1-C2-N2	2.29	114.40	110.49
6	E	2007	B12	C6-C5-C4	-2.28	120.71	124.27
5	F	2013	NAG	C1-C2-N2	2.27	114.36	110.49
5	B	2008	NAG	C1-C2-N2	2.26	114.36	110.49
5	F	2008	NAG	C1-C2-N2	2.25	114.33	110.49
5	D	2012	NAG	O4-C4-C3	-2.23	105.20	110.35
5	F	2012	NAG	C1-C2-N2	-2.22	106.69	110.49
5	F	2007	NAG	C1-O5-C5	2.21	115.19	112.19
5	B	2007	NAG	C1-O5-C5	2.20	115.17	112.19
5	D	2007	NAG	C1-O5-C5	2.19	115.16	112.19
5	F	2012	NAG	O3-C3-C4	-2.18	105.30	110.35
5	B	2009	NAG	C4-C3-C2	-2.17	107.84	111.02
6	E	2007	B12	C36-C7-C8	-2.16	108.21	112.11
5	D	2012	NAG	O3-C3-C2	2.15	113.92	109.47
5	D	2009	NAG	C4-C3-C2	-2.15	107.86	111.02
5	F	2009	NAG	C4-C3-C2	-2.15	107.86	111.02
5	D	2013	NAG	C2-N2-C7	-2.14	119.85	122.90
5	D	2008	NAG	O5-C1-C2	-2.14	107.91	111.29
6	A	2007	B12	C36-C7-C8	-2.13	108.26	112.11
5	B	2008	NAG	O5-C1-C2	-2.13	107.93	111.29
6	C	2007	B12	C36-C7-C8	-2.13	108.27	112.11
5	F	2008	NAG	O5-C1-C2	-2.12	107.94	111.29
5	B	2001	NAG	C1-C2-N2	2.11	114.09	110.49
5	F	2007	NAG	O5-C5-C6	2.10	110.50	107.20
5	D	2007	NAG	O5-C5-C6	2.10	110.49	107.20
5	D	2001	NAG	C1-C2-N2	2.09	114.06	110.49
5	B	2007	NAG	O5-C5-C6	2.09	110.48	107.20
5	D	2013	NAG	C1-C2-N2	2.08	114.04	110.49
5	C	2001	NAG	C1-O5-C5	2.08	115.01	112.19
5	F	2001	NAG	C1-C2-N2	2.07	114.02	110.49
6	A	2007	B12	C4B-C9B-N3B	2.01	136.27	130.88
6	C	2007	B12	C4B-C9B-N3B	2.01	136.25	130.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	2007	B12	C55-C17-C18	2.00	115.01	111.14
6	E	2007	B12	C4B-C9B-N3B	2.00	136.24	130.88

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	2008	NAG	C1
5	B	2001	NAG	C1
6	A	2007	B12	C19
5	E	2001	NAG	C1
6	E	2007	B12	C19
5	F	2008	NAG	C1
6	C	2007	B12	C19
5	F	2001	NAG	C1
5	D	2001	NAG	C1
5	D	2008	NAG	C1
5	A	2001	NAG	C1
5	C	2001	NAG	C1

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2012	NAG	O7-C7-N2-C2
5	D	2012	NAG	C8-C7-N2-C2
5	D	2012	NAG	O7-C7-N2-C2
5	D	2013	NAG	C8-C7-N2-C2
5	D	2013	NAG	O7-C7-N2-C2
5	B	2008	NAG	C8-C7-N2-C2
5	B	2008	NAG	O7-C7-N2-C2
5	B	2001	NAG	C3-C2-N2-C7
5	B	2001	NAG	C8-C7-N2-C2
5	B	2001	NAG	O7-C7-N2-C2
6	A	2007	B12	C42-C41-C8-C7
6	A	2007	B12	C16-C17-C55-C56
6	A	2007	B12	C18-C17-C55-C56
5	B	2013	NAG	C8-C7-N2-C2
5	B	2013	NAG	O7-C7-N2-C2
5	F	2013	NAG	C8-C7-N2-C2
5	F	2013	NAG	O7-C7-N2-C2
5	E	2001	NAG	C8-C7-N2-C2
5	E	2001	NAG	O7-C7-N2-C2
6	E	2007	B12	C42-C41-C8-C7

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Mol	Chain	Res	Type	Atoms
6	E	2007	B12	C16-C17-C55-C56
6	E	2007	B12	C18-C17-C55-C56
5	F	2008	NAG	C8-C7-N2-C2
5	F	2008	NAG	O7-C7-N2-C2
6	C	2007	B12	C42-C41-C8-C7
6	C	2007	B12	C16-C17-C55-C56
6	C	2007	B12	C18-C17-C55-C56
5	F	2001	NAG	C3-C2-N2-C7
5	F	2001	NAG	C8-C7-N2-C2
5	F	2001	NAG	O7-C7-N2-C2
5	D	2001	NAG	C3-C2-N2-C7
5	D	2001	NAG	C8-C7-N2-C2
5	D	2001	NAG	O7-C7-N2-C2
5	D	2008	NAG	C8-C7-N2-C2
5	D	2008	NAG	O7-C7-N2-C2
5	B	2012	NAG	C8-C7-N2-C2
5	B	2012	NAG	O7-C7-N2-C2
5	A	2001	NAG	C8-C7-N2-C2
5	A	2001	NAG	O7-C7-N2-C2
5	C	2001	NAG	C8-C7-N2-C2
5	C	2001	NAG	O7-C7-N2-C2
5	F	2012	NAG	C8-C7-N2-C2
5	B	2007	NAG	C8-C7-N2-C2
5	B	2007	NAG	O7-C7-N2-C2
5	D	2007	NAG	C8-C7-N2-C2
5	D	2007	NAG	O7-C7-N2-C2
5	F	2007	NAG	C8-C7-N2-C2
5	F	2007	NAG	O7-C7-N2-C2
5	B	2008	NAG	O5-C5-C6-O6
5	F	2008	NAG	O5-C5-C6-O6
5	D	2008	NAG	O5-C5-C6-O6
5	B	2001	NAG	O5-C5-C6-O6
5	F	2001	NAG	O5-C5-C6-O6
5	D	2001	NAG	O5-C5-C6-O6
5	E	2001	NAG	C1-C2-N2-C7
5	D	2012	NAG	O5-C5-C6-O6
5	B	2008	NAG	C4-C5-C6-O6
5	F	2008	NAG	C4-C5-C6-O6
5	D	2008	NAG	C4-C5-C6-O6
5	F	2012	NAG	O5-C5-C6-O6
5	B	2001	NAG	C4-C5-C6-O6
5	F	2001	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	2001	NAG	C4-C5-C6-O6
5	B	2012	NAG	O5-C5-C6-O6
5	C	2001	NAG	O5-C5-C6-O6
5	A	2001	NAG	C1-C2-N2-C7
5	C	2001	NAG	C1-C2-N2-C7
5	B	2008	NAG	C1-C2-N2-C7
5	F	2008	NAG	C1-C2-N2-C7
5	D	2008	NAG	C1-C2-N2-C7
5	E	2001	NAG	O5-C5-C6-O6
5	C	2001	NAG	C4-C5-C6-O6
5	E	2001	NAG	C4-C5-C6-O6
6	C	2007	B12	O58-C57-N59-C1P
6	A	2007	B12	O58-C57-N59-C1P
6	E	2007	B12	O58-C57-N59-C1P
5	D	2013	NAG	O5-C5-C6-O6
5	B	2013	NAG	O5-C5-C6-O6
5	F	2013	NAG	O5-C5-C6-O6
6	A	2007	B12	C56-C57-N59-C1P
6	E	2007	B12	C56-C57-N59-C1P
6	C	2007	B12	C56-C57-N59-C1P
5	A	2001	NAG	O5-C5-C6-O6
5	B	2012	NAG	C4-C5-C6-O6
6	A	2007	B12	N59-C1P-C2P-C3P
6	E	2007	B12	N59-C1P-C2P-C3P
6	C	2007	B12	N59-C1P-C2P-C3P
6	A	2007	B12	N59-C1P-C2P-O3
6	E	2007	B12	N59-C1P-C2P-O3
6	C	2007	B12	N59-C1P-C2P-O3
5	E	2001	NAG	C3-C2-N2-C7
5	A	2001	NAG	C3-C2-N2-C7
5	C	2001	NAG	C3-C2-N2-C7
5	D	2012	NAG	C4-C5-C6-O6
5	A	2001	NAG	C4-C5-C6-O6
5	F	2012	NAG	C4-C5-C6-O6
6	A	2007	B12	C18-C60-C61-O63
6	E	2007	B12	C18-C60-C61-O63
6	C	2007	B12	C18-C60-C61-O63
6	A	2007	B12	C42-C41-C8-C9
6	A	2007	B12	C14-C13-C48-C49
6	E	2007	B12	C42-C41-C8-C9
6	E	2007	B12	C14-C13-C48-C49
6	C	2007	B12	C42-C41-C8-C9

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Mol	Chain	Res	Type	Atoms
6	C	2007	B12	C14-C13-C48-C49

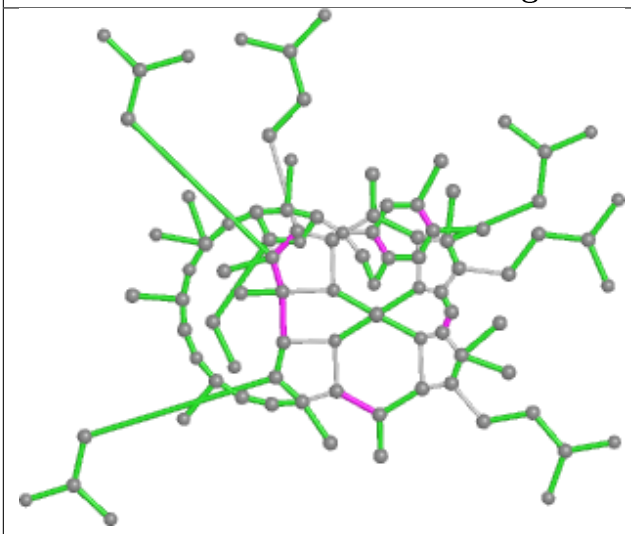
There are no ring outliers.

18 monomers are involved in 124 short contacts:

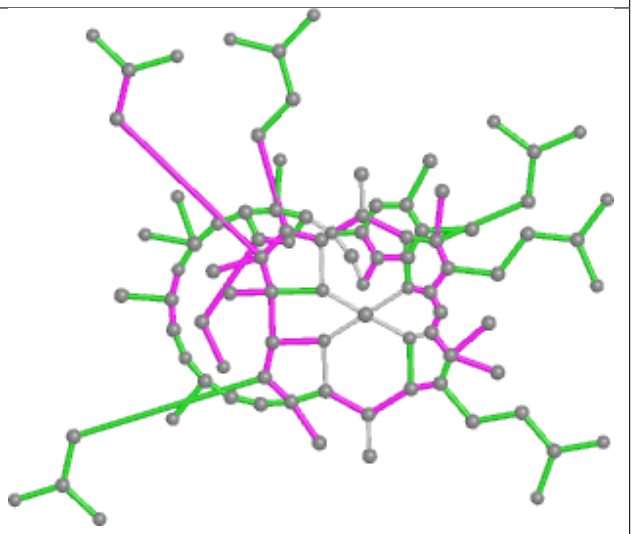
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2009	NAG	3	0
5	D	2013	NAG	2	0
5	B	2008	NAG	2	0
5	B	2001	NAG	1	0
6	A	2007	B12	29	0
5	B	2013	NAG	2	0
5	F	2013	NAG	2	0
5	E	2001	NAG	7	0
5	D	2009	NAG	2	0
6	E	2007	B12	25	0
5	F	2008	NAG	2	0
6	C	2007	B12	26	0
5	F	2001	NAG	1	0
5	D	2001	NAG	1	0
5	D	2008	NAG	2	0
5	B	2009	NAG	2	0
5	A	2001	NAG	7	0
5	C	2001	NAG	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

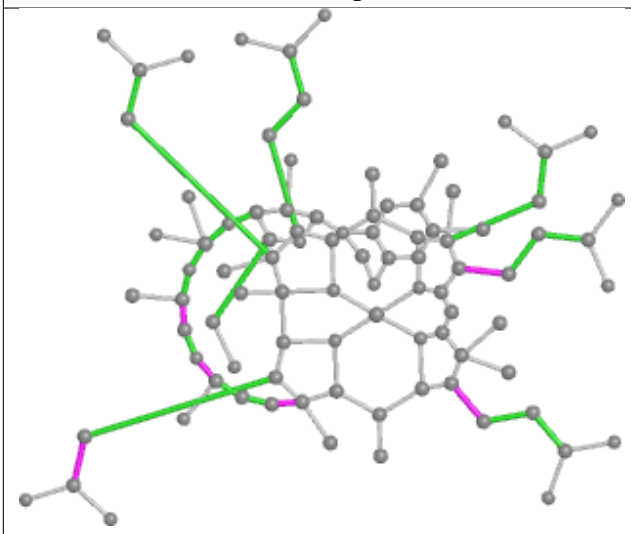
Ligand B12 A 2007



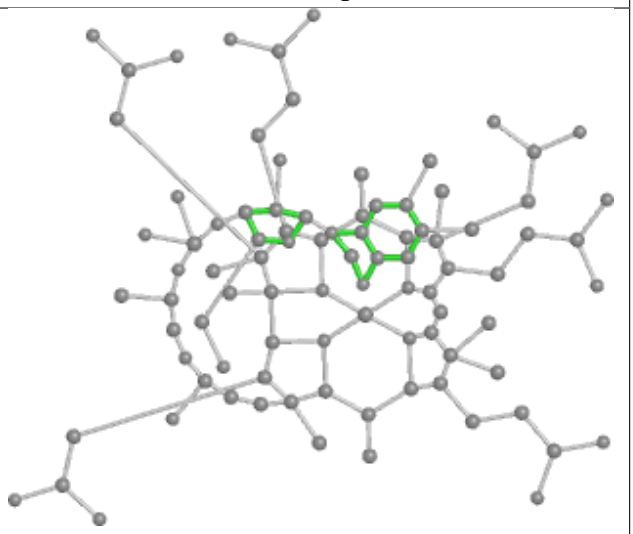
Bond lengths



Bond angles

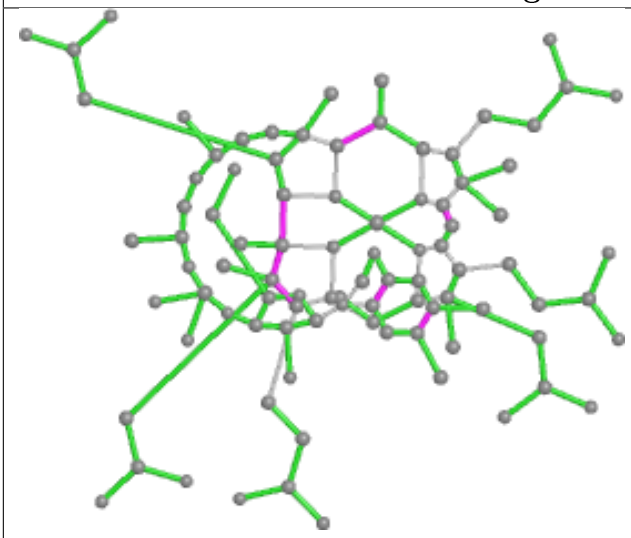


Torsions

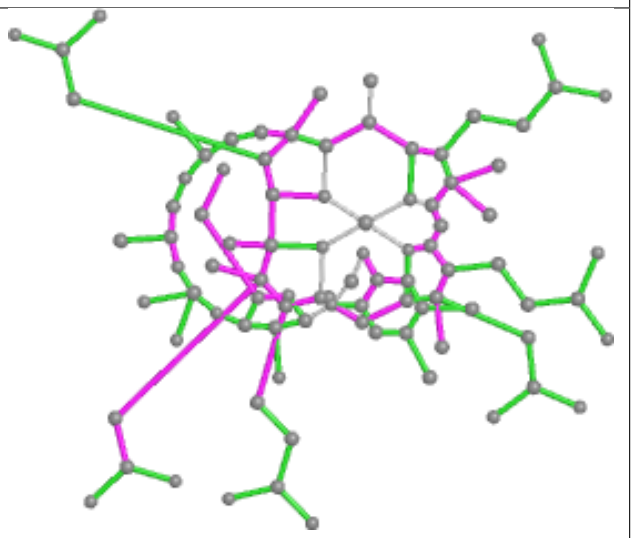


Rings

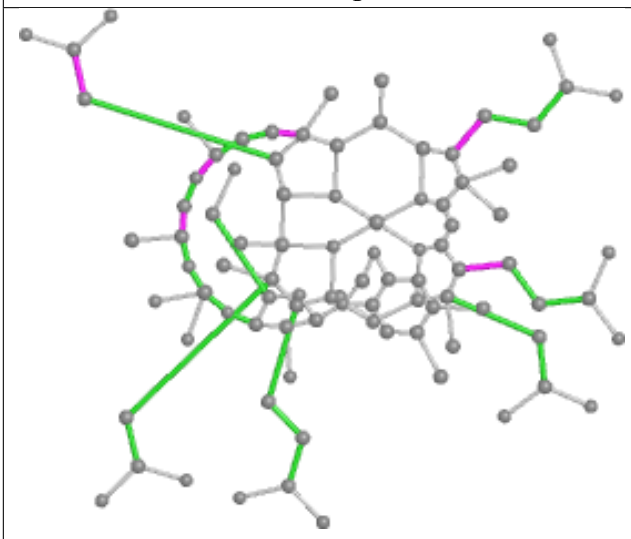
Ligand B12 E 2007



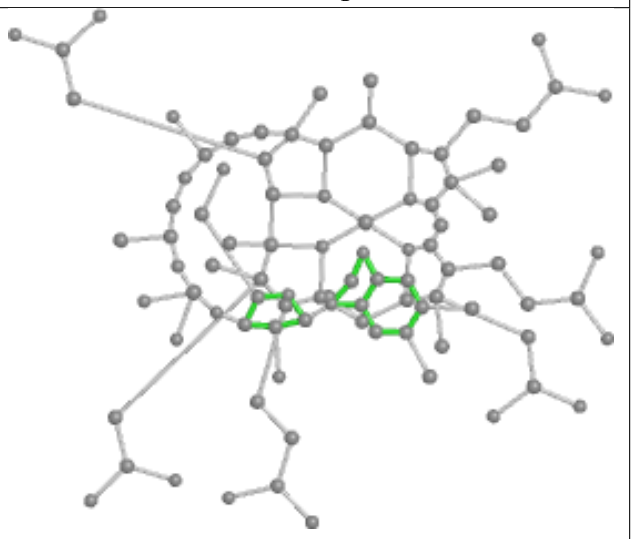
Bond lengths



Bond angles

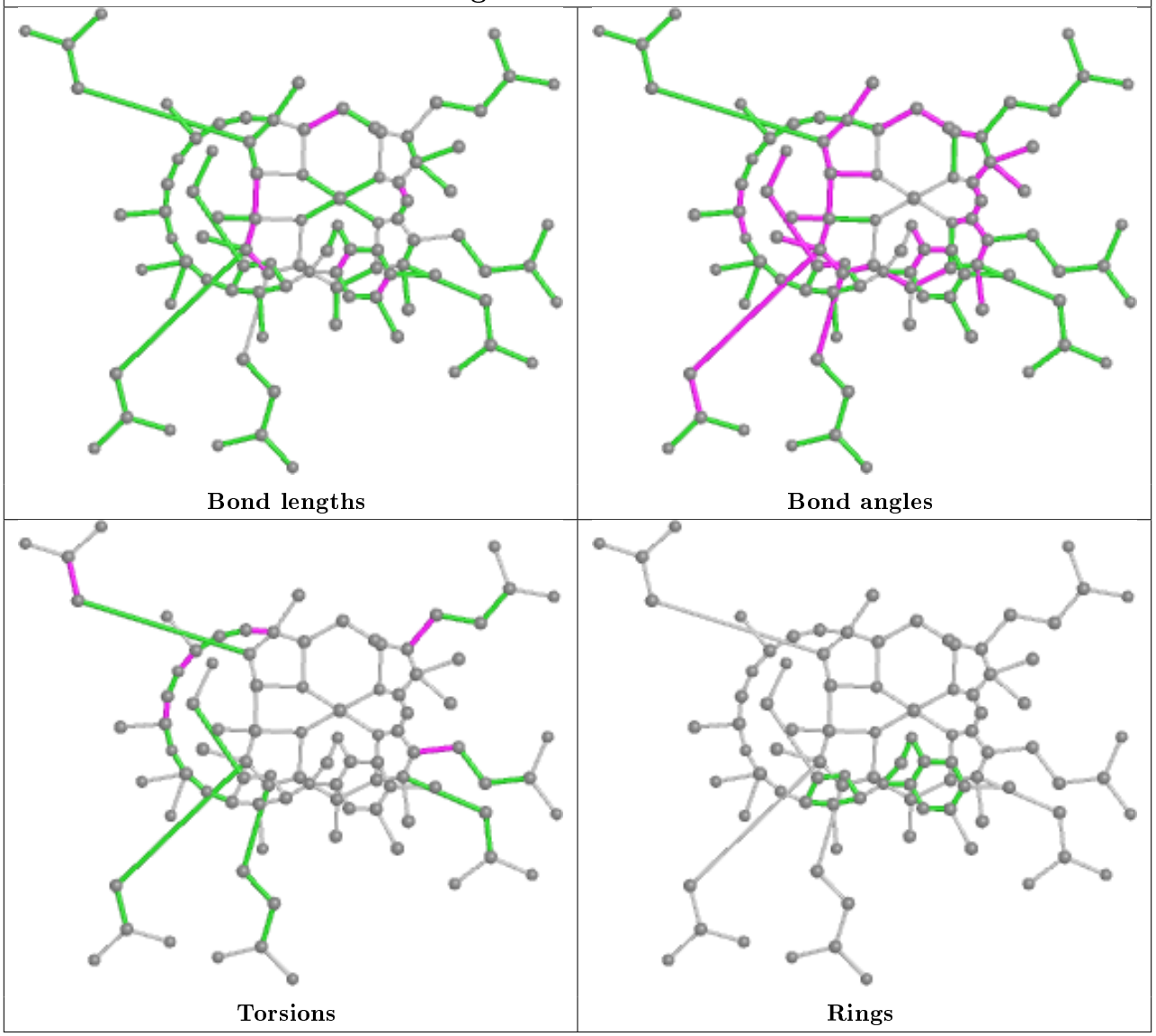


Torsions



Rings

Ligand B12 C 2007



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	385/393 (97%)	0.24	8 (2%)	63	62	47, 77, 133, 281	1 (0%)
1	C	385/393 (97%)	0.15	4 (1%)	82	82	47, 76, 139, 284	1 (0%)
1	E	385/393 (97%)	0.24	6 (1%)	72	70	50, 77, 140, 256	1 (0%)
2	B	457/457 (100%)	0.28	21 (4%)	32	30	59, 111, 172, 219	0
2	D	457/457 (100%)	0.22	18 (3%)	39	37	59, 110, 176, 228	0
2	F	457/457 (100%)	0.32	21 (4%)	32	30	61, 111, 178, 259	0
All	All	2526/2550 (99%)	0.25	78 (3%)	49	48	47, 95, 170, 284	3 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	HIS	13.3
1	A	308	SER	7.1
1	C	299	PRO	5.1
1	E	292	HIS	4.7
2	F	983	TYR	4.5
2	F	1320	TYR	4.4
1	A	297	THR	4.4
2	F	1004	TYR	4.1
2	F	1058	THR	3.9
1	A	298	LEU	3.8
2	B	1320	TYR	3.8
2	B	1270	PHE	3.6
2	D	1350	TYR	3.6
1	C	292	HIS	3.5
2	D	1023	VAL	3.3
2	D	1022	LEU	3.3
2	B	1085	LEU	3.2
1	C	221	GLY	3.2
2	D	1001	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	1387	PHE	3.1
2	F	1308	TRP	3.1
2	D	1210	PHE	3.0
1	E	319	ASN	3.0
1	E	290	PRO	3.0
2	B	991	GLU	2.9
2	D	1159	ASP	2.8
2	D	1354	ASP	2.8
2	B	1323	LEU	2.7
1	E	286	VAL	2.7
2	D	1340	LEU	2.7
2	D	1211	HIS	2.7
2	F	1023	VAL	2.6
1	C	297	THR	2.6
2	B	1058	THR	2.6
2	B	1009	ILE	2.6
2	B	1004	TYR	2.6
2	F	1208	LYS	2.6
2	B	1073	GLU	2.6
2	B	992	VAL	2.5
2	F	1366	LEU	2.5
2	B	1367	GLN	2.5
2	B	1271	LYS	2.5
1	A	280	TYR	2.5
2	D	1338	LEU	2.4
2	D	1226	TYR	2.4
2	F	975	GLU	2.4
2	B	1132	ILE	2.4
2	F	1005	CYS	2.4
2	B	1357	PRO	2.4
2	B	1086	ILE	2.4
2	D	1036	LEU	2.4
2	B	1356	PRO	2.3
2	D	1353	VAL	2.3
2	F	1144	LYS	2.3
1	E	322	LEU	2.3
2	F	1223	LEU	2.3
2	D	1272	ALA	2.2
1	A	389	LEU	2.2
2	D	1186	TYR	2.2
2	B	1272	ALA	2.2
2	F	1283	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	291	ASP	2.1
2	F	1034	GLY	2.1
2	F	981	PHE	2.1
2	F	1325	PHE	2.1
2	F	1205	LEU	2.1
2	D	1007	LYS	2.1
2	B	1366	LEU	2.1
2	B	1387	PHE	2.1
1	A	321	GLN	2.1
2	D	1290	ILE	2.1
2	B	1052	TYR	2.0
2	F	943	ILE	2.0
1	E	285	GLN	2.0
2	B	976	THR	2.0
2	F	991	GLU	2.0
2	F	977	PHE	2.0
2	F	1361	THR	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	BMA	N	3	11/12	0.52	0.17	173,182,191,193	0
3	BMA	G	3	11/12	0.57	0.21	128,134,138,144	0
3	MAN	G	4	11/12	0.59	0.24	162,165,175,180	0
3	MAN	N	5	11/12	0.63	0.21	192,201,209,213	0
3	MAN	J	4	11/12	0.64	0.26	160,166,178,180	0
3	MAN	J	5	11/12	0.67	0.22	196,201,205,206	0
3	NAG	N	1	14/15	0.68	0.24	119,123,127,130	0
3	MAN	H	4	11/12	0.68	0.24	181,194,208,211	0
3	MAN	N	4	11/12	0.69	0.24	188,194,206,206	0
3	MAN	K	5	11/12	0.69	0.20	190,201,222,227	0
3	MAN	M	5	11/12	0.70	0.21	181,190,197,200	0

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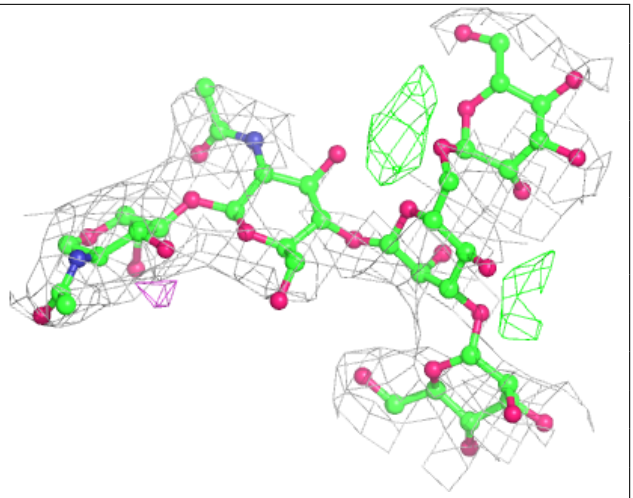
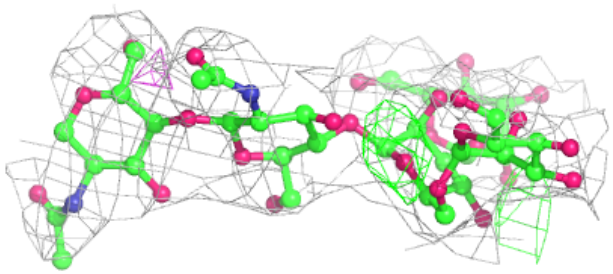
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	G	5	11/12	0.72	0.23	190,195,201,202	0
3	NAG	H	1	14/15	0.73	0.21	113,122,130,135	0
3	MAN	H	5	11/12	0.75	0.22	184,197,219,223	0
3	BMA	M	3	11/12	0.76	0.19	129,131,147,153	0
4	NAG	O	2	14/15	0.77	0.25	160,167,171,175	0
4	NAG	L	2	14/15	0.78	0.25	163,170,176,178	0
3	NAG	K	1	14/15	0.79	0.20	107,122,135,136	0
3	NAG	H	2	14/15	0.79	0.20	159,171,180,183	0
4	NAG	I	2	14/15	0.81	0.19	150,155,171,178	0
3	NAG	K	2	14/15	0.82	0.18	151,172,184,186	0
3	BMA	K	3	11/12	0.82	0.12	167,179,190,190	0
3	MAN	K	4	11/12	0.83	0.15	172,185,203,208	0
3	BMA	J	3	11/12	0.83	0.15	138,144,154,155	0
3	BMA	H	3	11/12	0.83	0.10	167,178,184,188	0
3	NAG	N	2	14/15	0.83	0.20	163,175,188,193	0
4	NAG	I	1	14/15	0.86	0.23	121,132,136,139	0
4	NAG	O	1	14/15	0.88	0.23	119,136,140,142	0
4	NAG	L	1	14/15	0.89	0.19	125,138,141,143	0
3	MAN	M	4	11/12	0.89	0.17	169,175,195,202	0
3	NAG	M	2	14/15	0.91	0.21	89,97,107,109	0
3	NAG	G	2	14/15	0.92	0.24	90,95,103,104	0
3	NAG	J	2	14/15	0.94	0.20	89,98,103,104	0
3	NAG	M	1	14/15	0.95	0.22	53,78,96,106	0
3	NAG	J	1	14/15	0.95	0.23	59,75,86,91	0
3	NAG	G	1	14/15	0.96	0.26	58,73,97,103	0

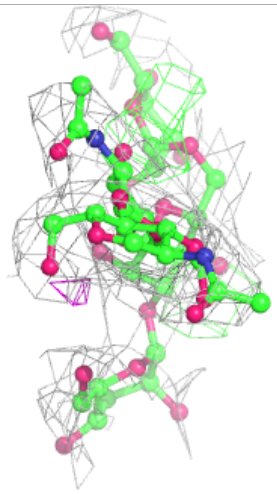
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

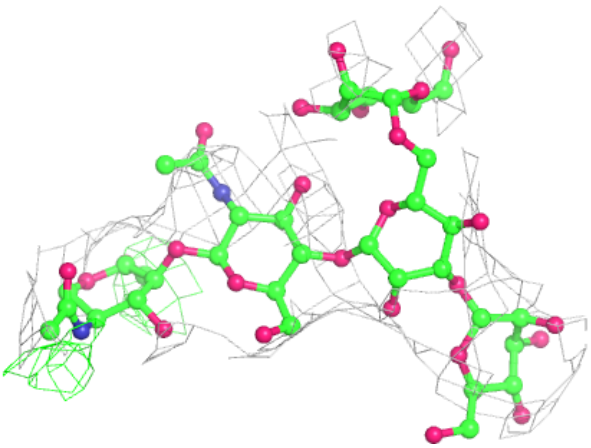


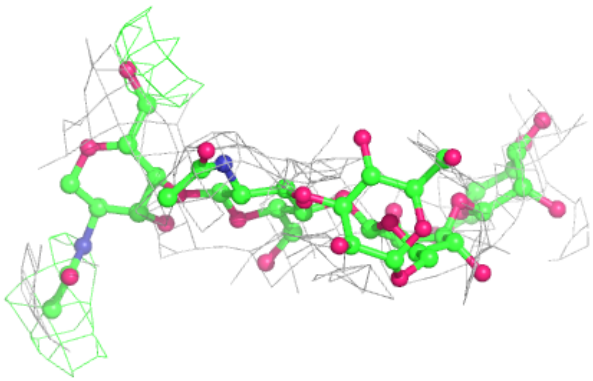


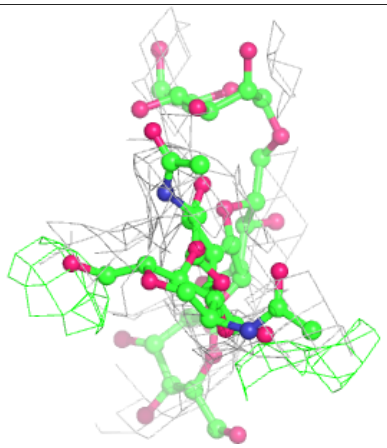


Electron density around Chain H:

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

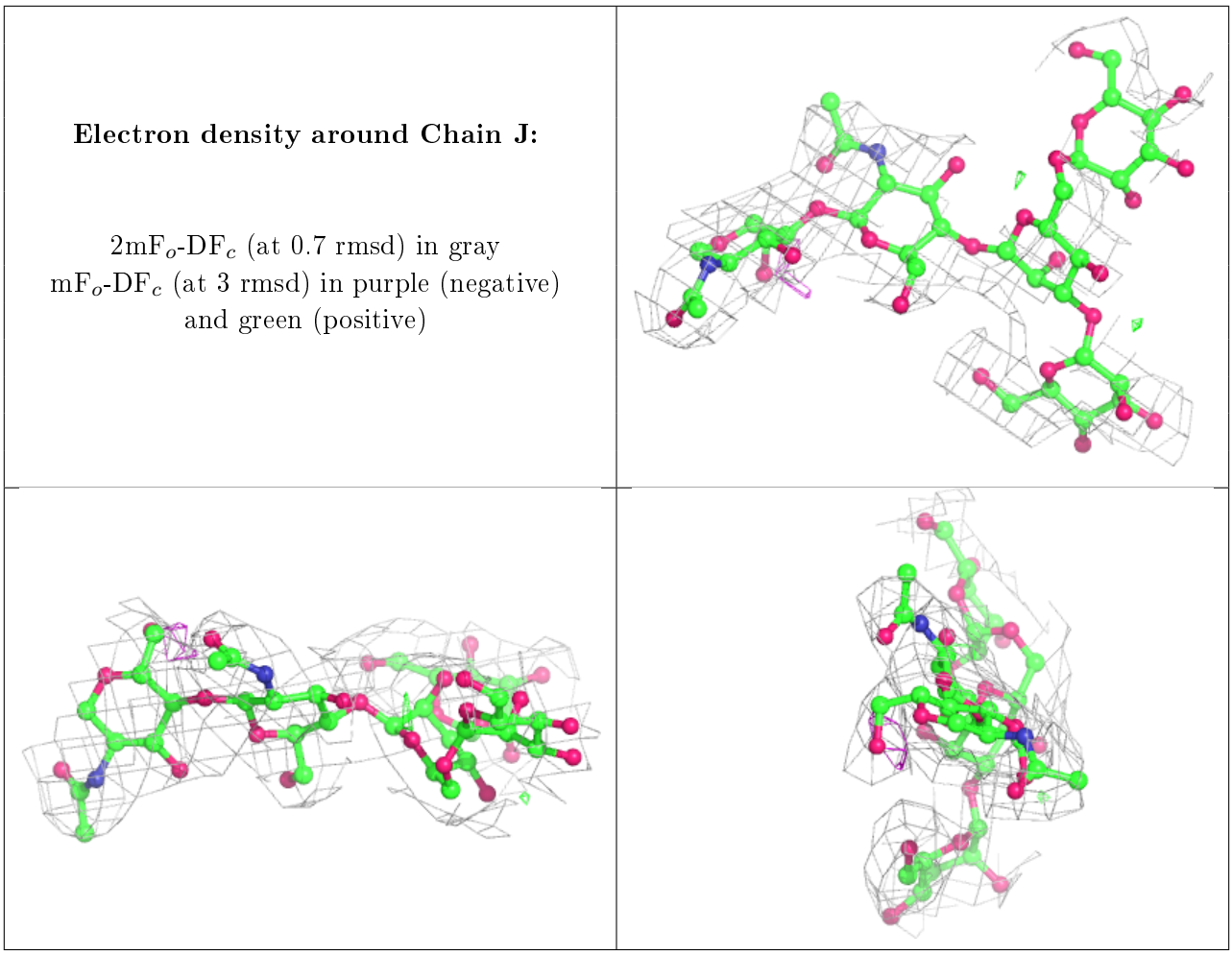






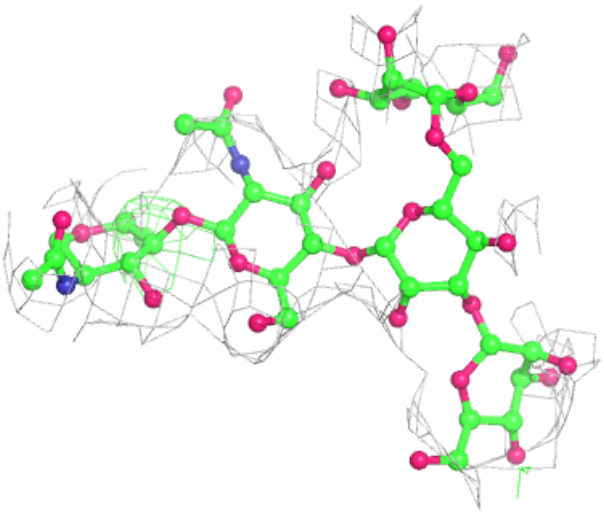
Electron density around Chain J:

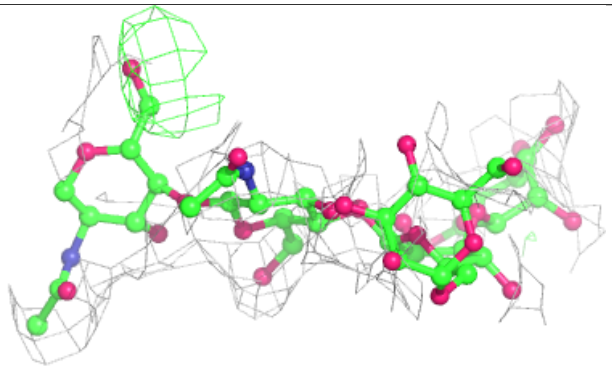
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

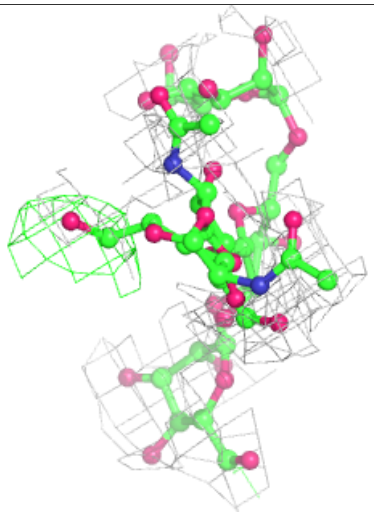


Electron density around Chain K:

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

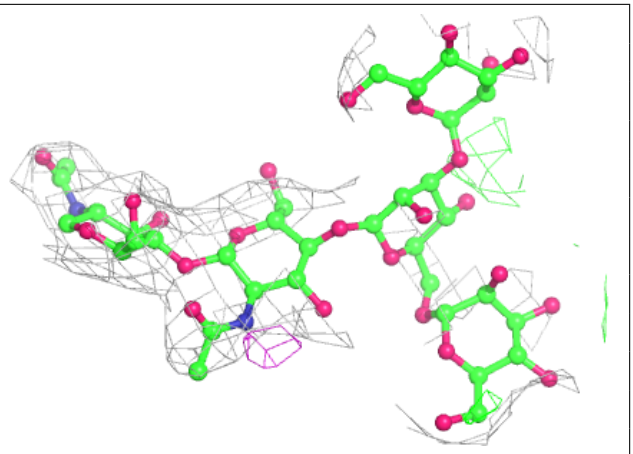


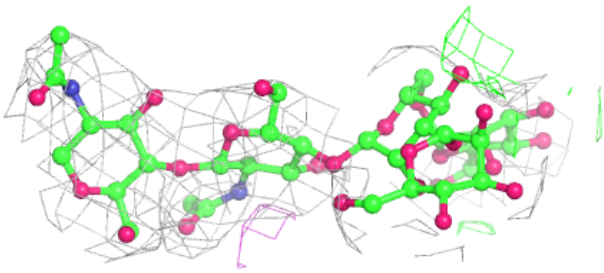


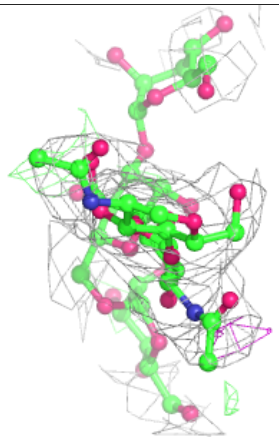


Electron density around Chain M:

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

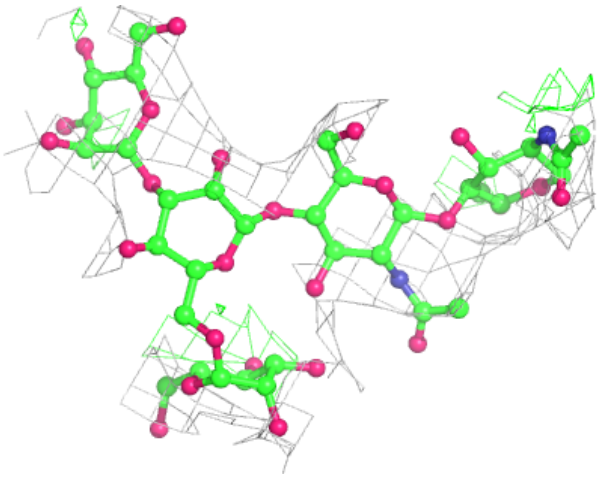


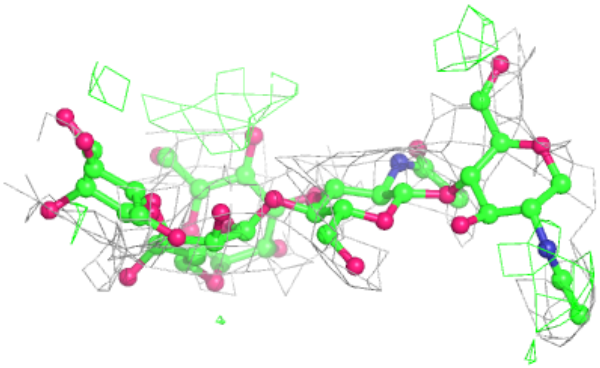


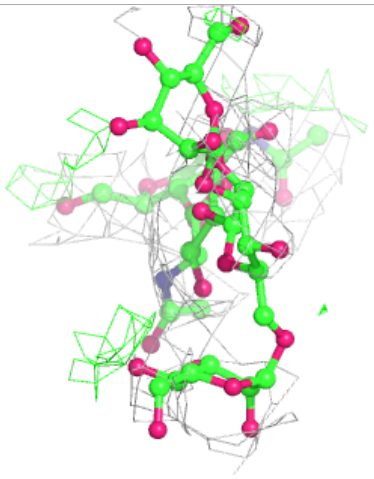


Electron density around Chain N:

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

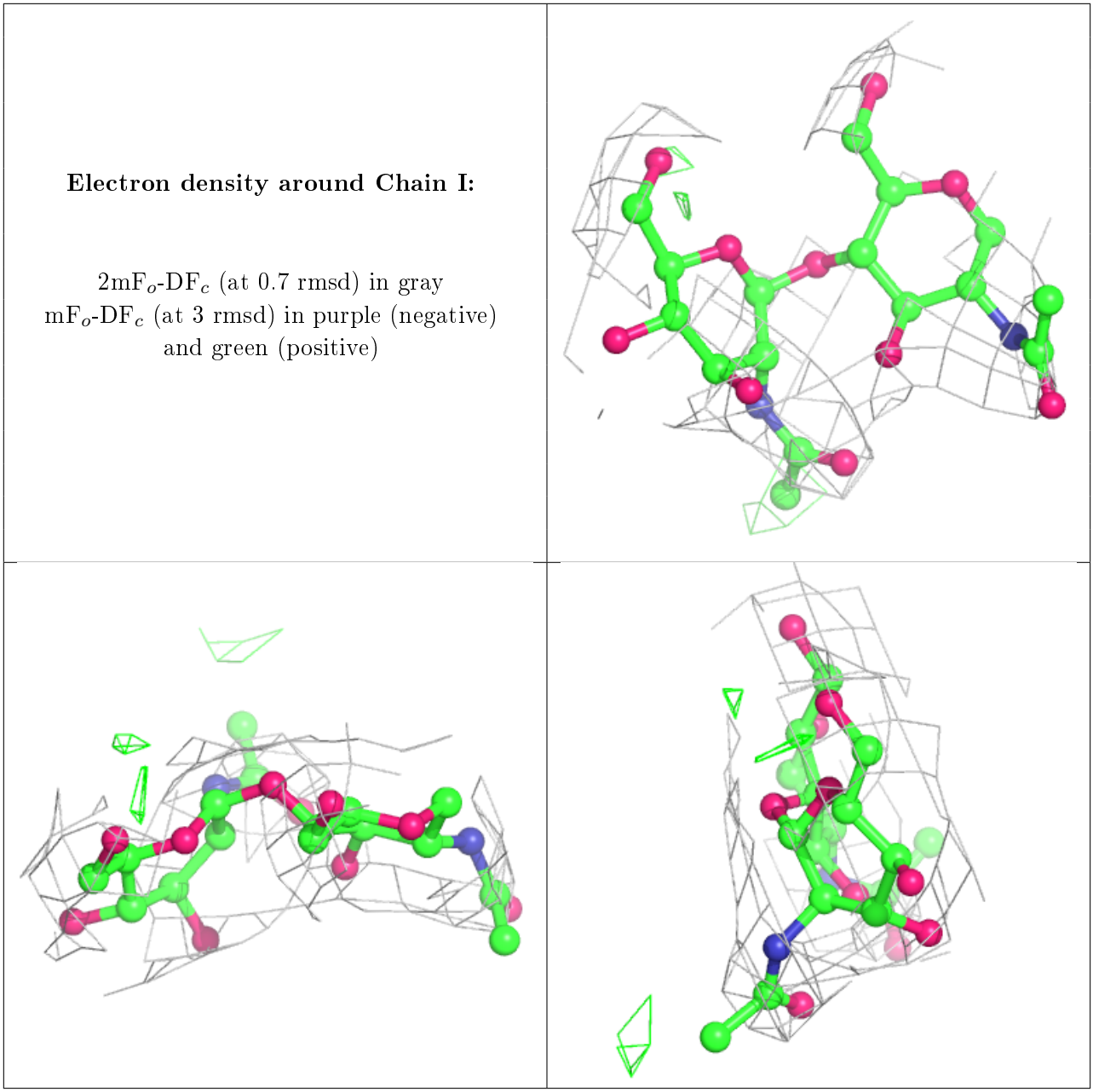






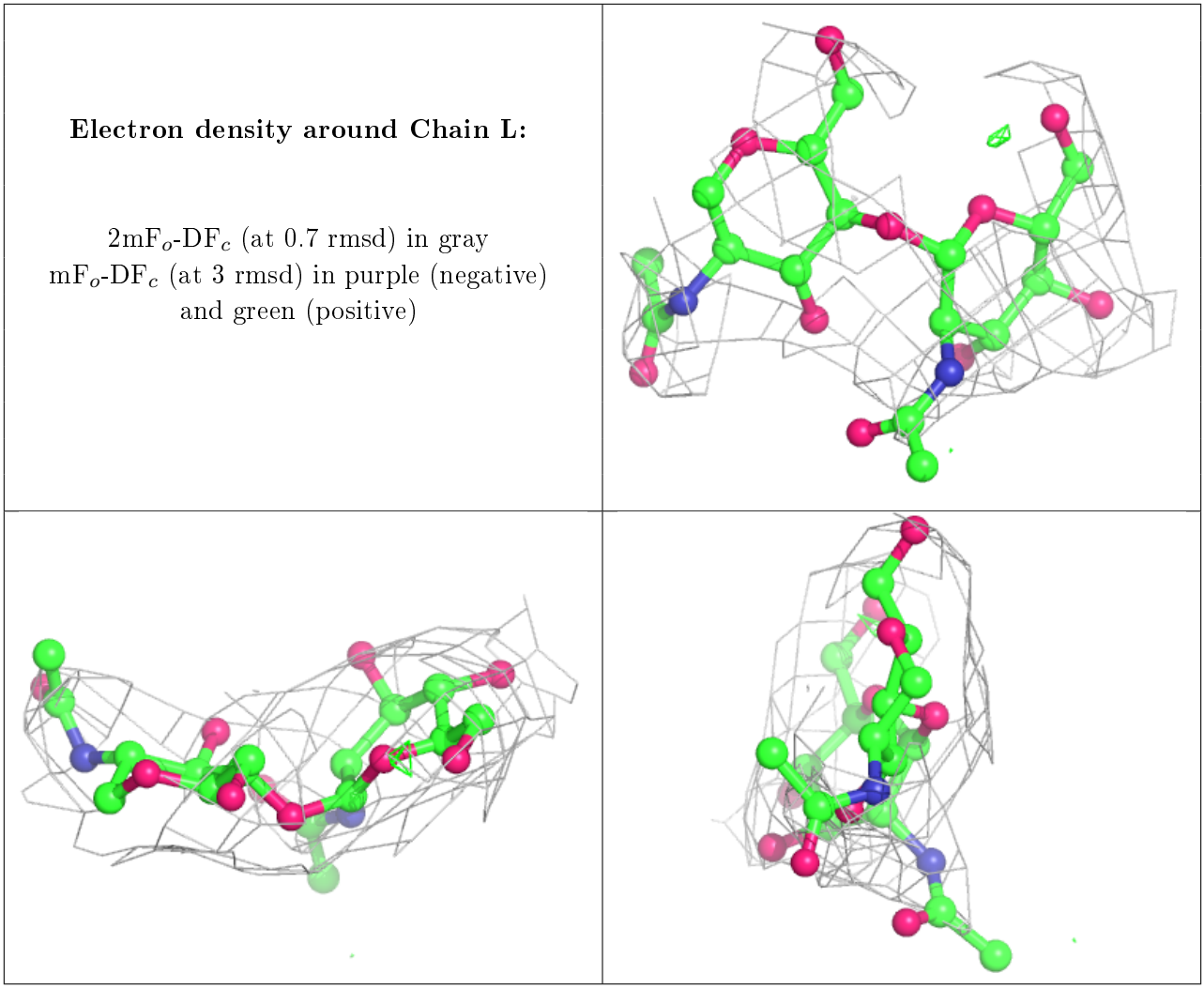
Electron density around Chain I:

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



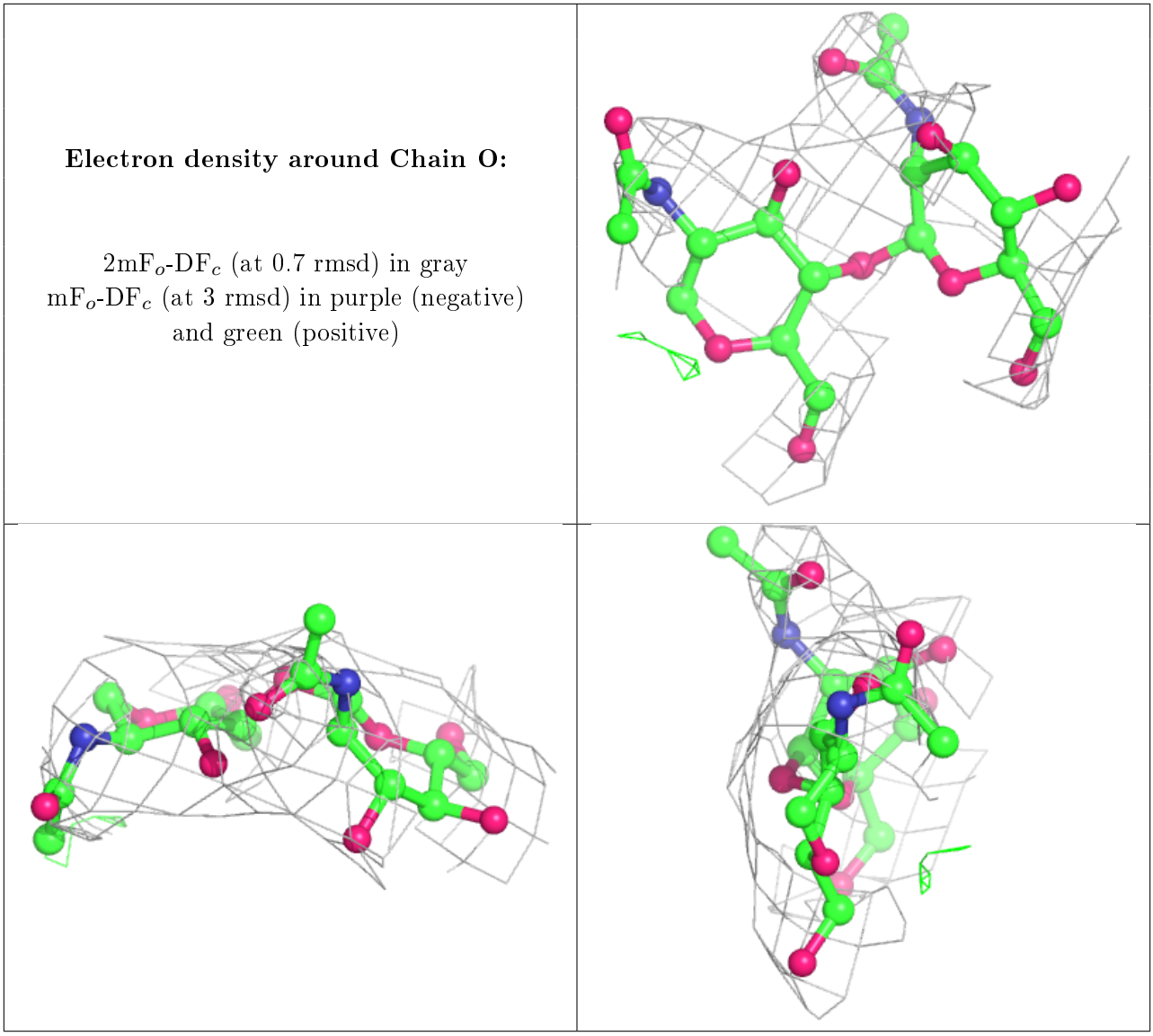
Electron density around Chain L:

$2mF_o$-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 O:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	NAG	F	2001	14/15	0.37	0.29	192,198,201,203	0
5	NAG	F	2008	14/15	0.47	0.28	190,198,203,205	0
5	NAG	B	2008	14/15	0.48	0.33	196,198,198,199	0
5	NAG	F	2013	14/15	0.59	0.29	162,176,180,183	0
5	NAG	F	2012	14/15	0.69	0.22	139,157,192,194	0
5	NAG	D	2001	14/15	0.69	0.19	187,191,196,197	0

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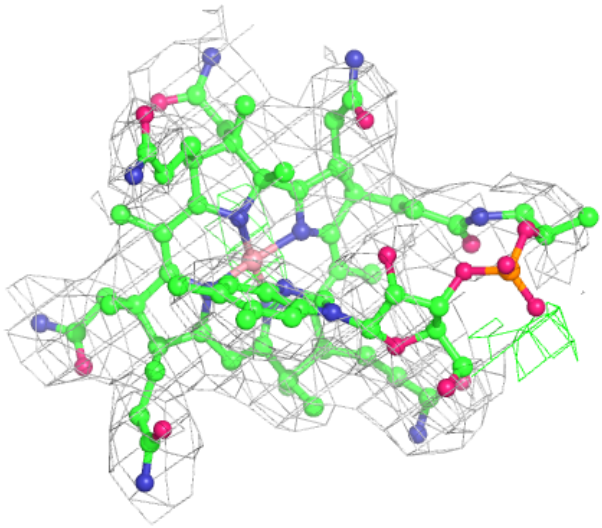
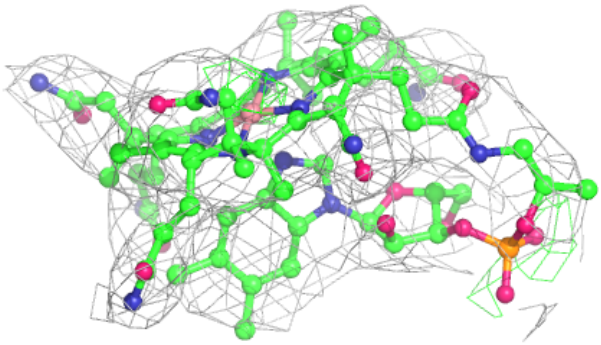
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	D	2008	14/15	0.69	0.20	196,203,209,210	0
5	NAG	B	2012	14/15	0.71	0.21	146,163,198,200	0
5	NAG	F	2007	14/15	0.72	0.31	151,172,188,195	0
5	NAG	F	2009	14/15	0.73	0.35	185,189,191,192	0
5	NAG	D	2009	14/15	0.73	0.41	188,192,195,195	0
5	NAG	D	2013	14/15	0.76	0.20	168,182,187,189	0
7	CA	F	2014	1/1	0.77	0.06	151,151,151,151	0
5	NAG	B	2009	14/15	0.78	0.45	185,193,199,199	0
5	NAG	B	2007	14/15	0.78	0.26	149,179,202,211	0
5	NAG	D	2012	14/15	0.80	0.25	145,163,197,200	0
7	CA	B	2014	1/1	0.81	0.14	140,140,140,140	0
5	NAG	B	2013	14/15	0.83	0.17	157,169,174,176	0
5	NAG	B	2001	14/15	0.84	0.20	195,202,205,206	0
5	NAG	C	2001	14/15	0.86	0.28	45,49,52,54	14
5	NAG	E	2001	14/15	0.88	0.29	50,55,60,61	14
5	NAG	A	2001	14/15	0.89	0.32	50,54,57,60	14
5	NAG	D	2007	14/15	0.90	0.13	166,193,216,223	0
7	CA	F	2016	1/1	0.93	0.10	144,144,144,144	0
7	CA	D	2014	1/1	0.93	0.10	163,163,163,163	0
7	CA	F	2017	1/1	0.94	0.22	80,80,80,80	0
6	B12	A	2007	91/91	0.95	0.29	45,64,92,100	0
7	CA	B	2016	1/1	0.96	0.12	147,147,147,147	0
7	CA	B	2017	1/1	0.96	0.14	82,82,82,82	0
6	B12	E	2007	91/91	0.96	0.29	40,66,91,95	0
7	CA	D	2015	1/1	0.97	0.23	60,60,60,60	0
6	B12	C	2007	91/91	0.97	0.28	46,65,81,88	0
7	CA	D	2017	1/1	0.97	0.22	79,79,79,79	0
7	CA	D	2016	1/1	0.98	0.10	139,139,139,139	0
7	CA	F	2015	1/1	0.98	0.15	58,58,58,58	0
7	CA	B	2015	1/1	0.99	0.19	54,54,54,54	0

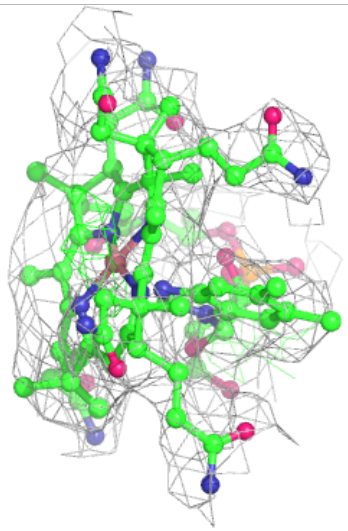
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B12 A 2007:

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

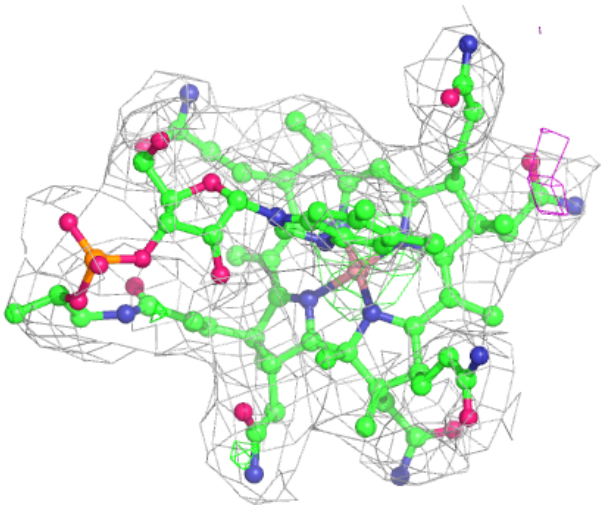


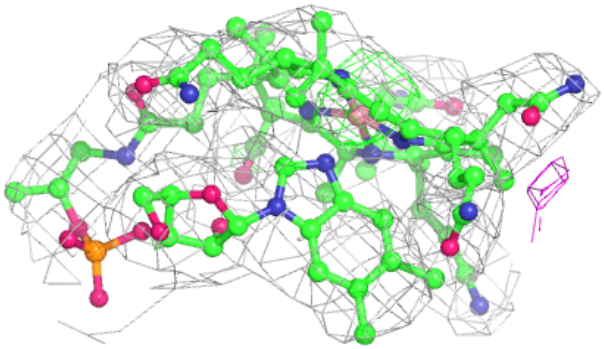


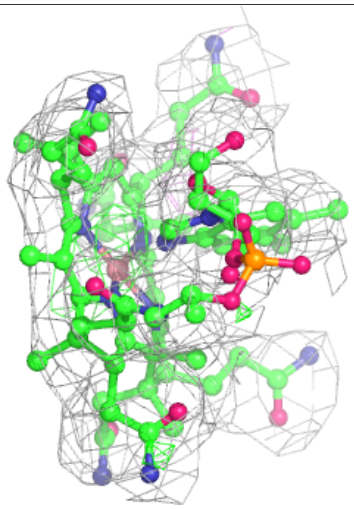


Electron density around B12 E 2007:

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

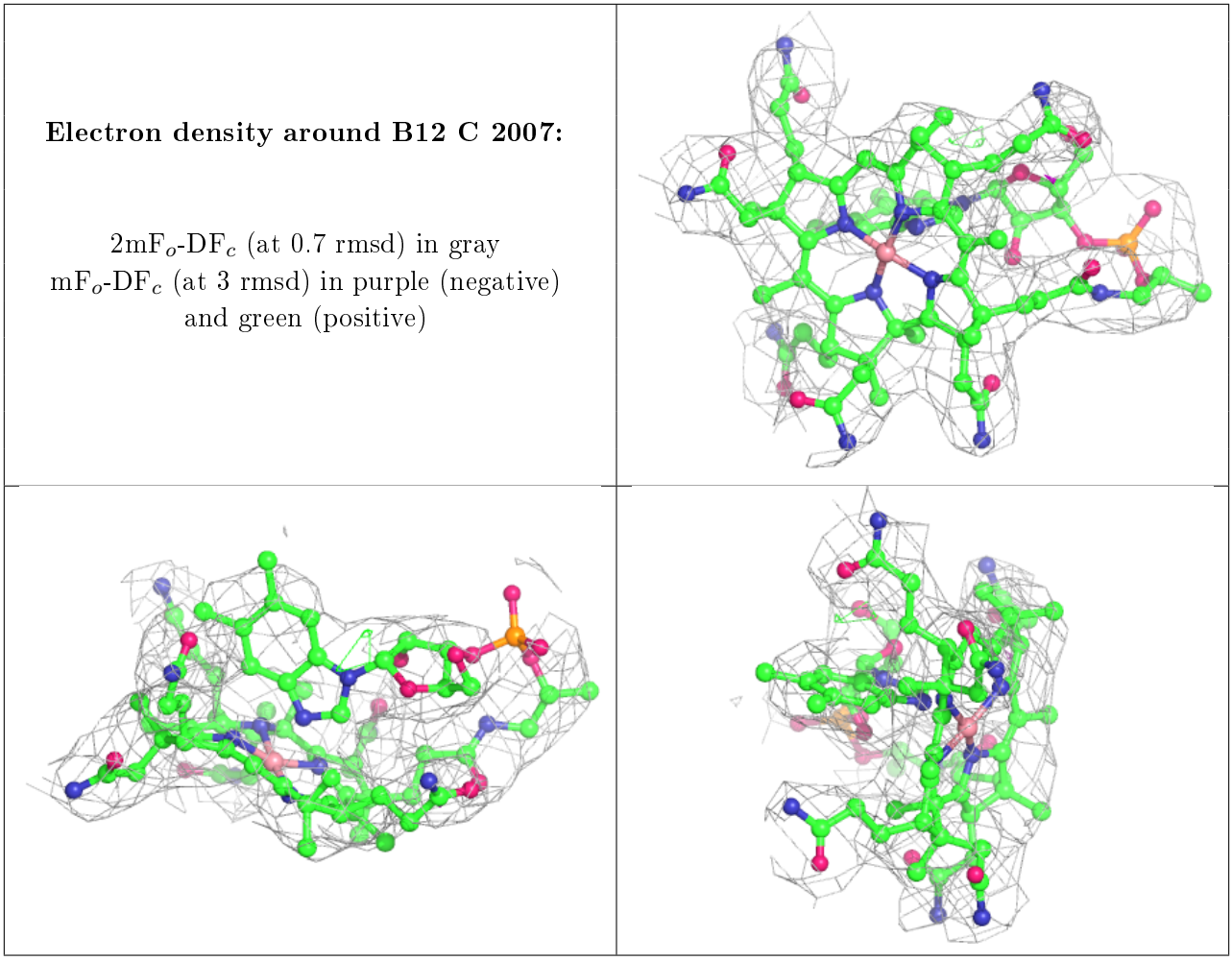






Electron density around B12 C 2007:

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



6.5 Other polymers

There are no such residues in this entry.