Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 05:49 pm GMT

PDB ID	:	4WJL
Title	:	Structure of human dipeptidyl peptidase 10 (DPPY): a modulator of neuronal Kv4 channels
Authors	:	Bezerra, G.A.; Dobrovetsky, E.; Seitova, A.; Fedosyuk, S.; Dhe-Paganon, S.; Gruber, K.
Deposited on	:	2014-09-30
Resolution	:	3.40 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

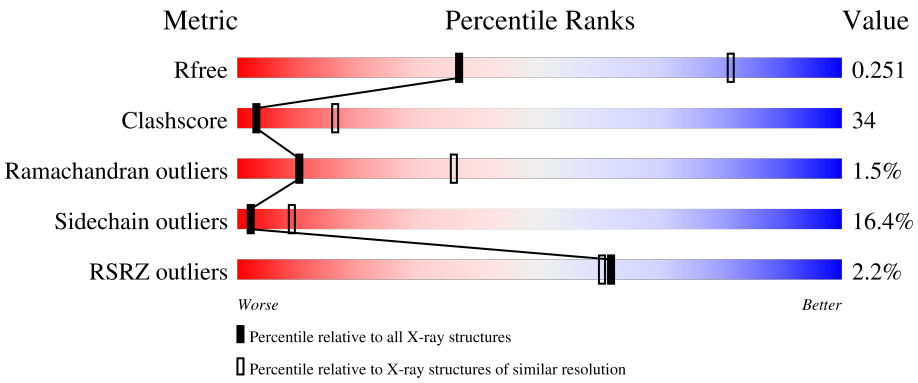
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	719	2%, 45%, 43%, 11%
1	B	719	2%, 44%, 45%, 10%
2	C	4	100%
3	D	2	100%
3	E	2	50%, 50%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
4	F	3	67% 33%

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	B	809	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11829 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 Inactive dipeptidyl peptidase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	717	5794	3730	959	1080	25	0	0	0
1	B	719	5806	3736	960	1085	25	0	0	0

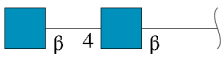
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	MET	VAL	variant	UNP Q8N608
A	401	ILE	VAL	variant	UNP Q8N608
B	288	MET	VAL	variant	UNP Q8N608
B	401	ILE	VAL	variant	UNP Q8N608

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

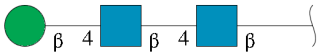
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	4	50	28	2	20	0	0	0

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



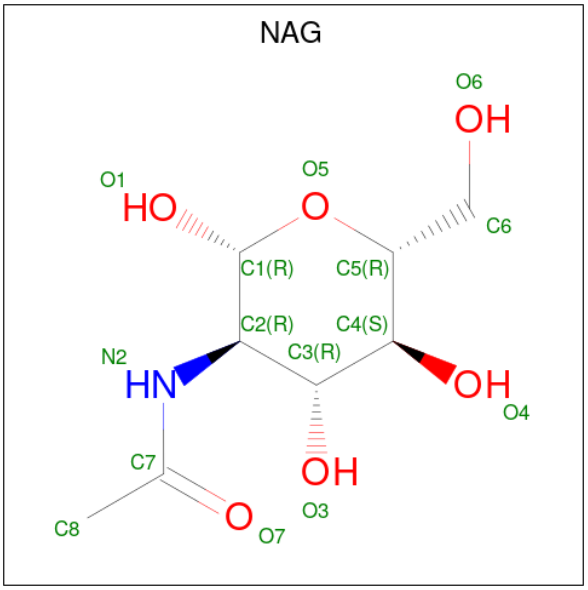
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0
3	E	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0

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



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

- 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
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0

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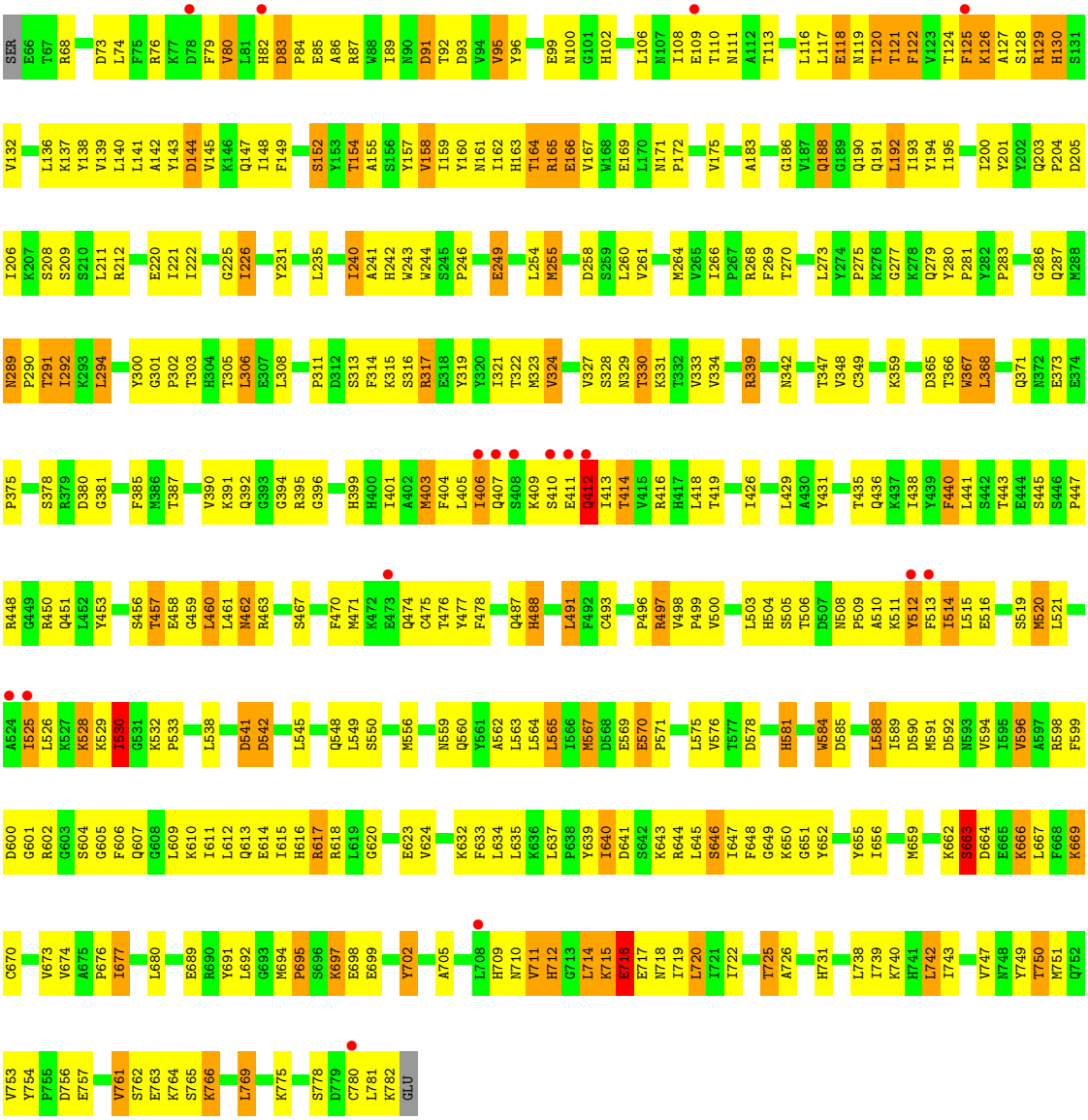
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

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.

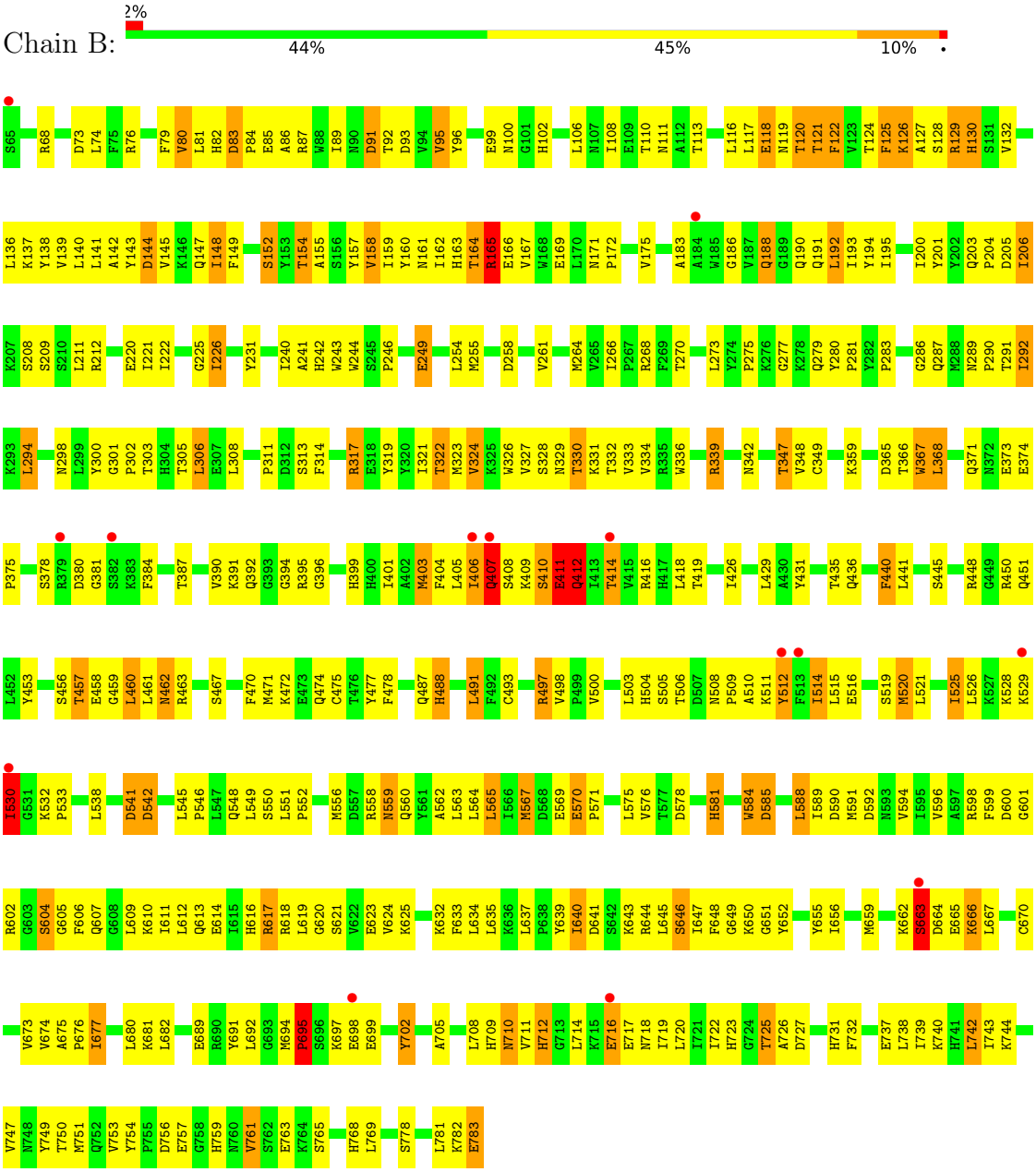
- Molecule 1: Inactive dipeptidyl peptidase 10

Chain A:



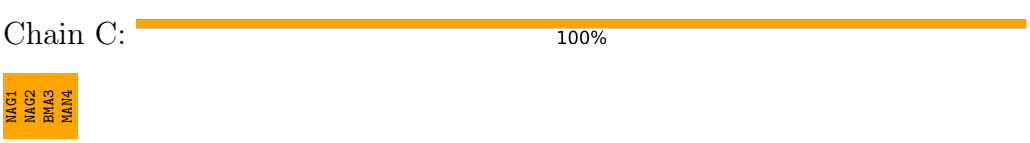
- Molecule 1: Inactive dipeptidyl peptidase 10

Chain B:



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

Chain C:



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

Chain D:

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

Chain E:

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

Chain G:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.91Å 143.73Å 176.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.55 – 3.40 66.55 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.55-3.40) 99.9 (66.55-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.207 , 0.242 0.223 , 0.251	Depositor DCC
R_{free} test set	1476 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11829	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, BMA

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	0.39	0/5940	0.63	1/8052 (0.0%)
1	B	0.41	0/5952	0.64	1/8069 (0.0%)
All	All	0.40	0/11892	0.63	2/16121 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	585	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	714	LEU	N-CA-C	-5.20	96.95	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	GLN	Peptide,Mainchain
1	B	407	GLN	Peptide
1	B	412	GLN	Mainchain
1	B	695	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	B	710	ASN	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5794	0	5719	404	0
1	B	5806	0	5720	392	0
2	C	50	0	43	4	0
3	D	28	0	25	4	0
3	E	28	0	25	3	0
3	G	28	0	25	4	0
4	F	39	0	34	4	0
5	A	28	0	26	1	0
5	B	28	0	26	6	0
All	All	11829	0	11643	794	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 34.

All (794) 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:A:165:ARG:CD	1:A:165:ARG:H	1.60	1.14
1:A:165:ARG:H	1:A:165:ARG:HD2	1.08	1.08
1:A:488:HIS:HB3	1:A:505:SER:HA	1.38	1.05
1:A:644:ARG:HD2	1:A:781:LEU:O	1.57	1.04
1:B:488:HIS:HB3	1:B:505:SER:HA	1.39	1.03
1:B:165:ARG:H	1:B:165:ARG:HD2	1.18	1.03
1:A:165:ARG:HD2	1:A:165:ARG:N	1.72	1.02
1:B:644:ARG:HD2	1:B:781:LEU:O	1.58	1.02
1:B:165:ARG:HD2	1:B:165:ARG:N	1.72	1.01
1:A:118:GLU:HG3	1:A:119:ASN:H	1.28	0.98
1:B:118:GLU:HG3	1:B:119:ASN:N	1.80	0.95
1:A:602:ARG:HD2	1:A:614:GLU:HG2	1.47	0.94
1:B:118:GLU:HG3	1:B:119:ASN:H	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:ARG:HD2	1:B:614:GLU:HG2	1.48	0.94
1:A:775:LYS:NZ	5:B:809:NAG:H62	1.83	0.93
1:A:118:GLU:HG3	1:A:119:ASN:N	1.82	0.92
1:B:710:ASN:O	1:B:712:HIS:N	2.01	0.91
1:A:201:TYR:CE1	1:A:212:ARG:HG3	2.05	0.91
1:A:570:GLU:HG3	1:A:571:PRO:HD2	1.52	0.91
1:B:201:TYR:CE1	1:B:212:ARG:HG3	2.10	0.87
1:A:409:LYS:HG2	1:A:410:SER:H	1.40	0.87
1:A:775:LYS:CE	5:B:809:NAG:H62	2.05	0.86
1:A:710:ASN:C	1:A:712:HIS:H	1.78	0.85
1:B:570:GLU:HG3	1:B:571:PRO:HD2	1.57	0.85
1:B:742:LEU:HD23	1:B:747:VAL:HB	1.58	0.85
1:A:399:HIS:CE1	1:A:609:LEU:HD21	2.12	0.85
1:A:742:LEU:HD23	1:A:747:VAL:HB	1.59	0.84
1:A:695:PRO:HA	1:A:702:TYR:CD2	2.13	0.84
1:A:440:PHE:HE1	1:A:453:TYR:HB3	1.43	0.83
1:B:399:HIS:HE1	1:B:609:LEU:HD21	1.43	0.83
1:B:195:ILE:HD12	1:B:226:ILE:HG23	1.61	0.83
1:B:440:PHE:HE1	1:B:453:TYR:HB3	1.43	0.82
1:B:440:PHE:CE1	1:B:453:TYR:CB	2.63	0.82
1:A:609:LEU:HB3	1:A:613:GLN:HE21	1.45	0.82
1:B:399:HIS:CE1	1:B:609:LEU:HD21	2.14	0.82
1:A:440:PHE:CE1	1:A:453:TYR:CB	2.63	0.82
1:A:195:ILE:HD12	1:A:226:ILE:HG23	1.63	0.81
1:A:399:HIS:HE1	1:A:609:LEU:HD21	1.44	0.81
1:A:753:VAL:HG11	1:B:753:VAL:HG11	1.63	0.81
1:B:411:GLU:O	1:B:412:GLN:HB2	1.80	0.80
1:B:673:VAL:HG11	1:B:676:PRO:HB3	1.64	0.80
1:A:460:LEU:HD13	1:A:460:LEU:H	1.47	0.79
1:B:609:LEU:HB3	1:B:613:GLN:HE21	1.46	0.78
1:B:460:LEU:HD13	1:B:460:LEU:H	1.47	0.78
1:B:644:ARG:HD3	1:B:783:GLU:OE2	1.83	0.78
1:B:448:ARG:HG3	1:B:448:ARG:HH11	1.48	0.78
1:B:287:GLN:HE21	1:B:287:GLN:HA	1.49	0.78
1:B:695:PRO:HA	1:B:702:TYR:CD2	2.18	0.78
1:B:440:PHE:HE1	1:B:453:TYR:CB	1.96	0.78
1:A:673:VAL:HG11	1:A:676:PRO:HB3	1.66	0.78
1:A:607:GLN:HG3	1:A:611:ILE:HD12	1.66	0.78
1:B:145:VAL:HA	1:B:155:ALA:HB2	1.64	0.78
1:A:145:VAL:HA	1:A:155:ALA:HB2	1.64	0.77
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.46	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:VAL:CG1	1:B:676:PRO:HB3	2.14	0.77
1:A:440:PHE:CE1	1:A:453:TYR:HB2	2.20	0.76
1:A:83:ASP:OD2	1:A:85:GLU:HG3	1.84	0.76
1:B:607:GLN:HG3	1:B:611:ILE:HD12	1.67	0.76
1:B:440:PHE:CE1	1:B:453:TYR:HB2	2.19	0.76
1:A:260:LEU:HD11	2:C:1:NAG:H62	1.67	0.76
1:A:287:GLN:HE21	1:A:287:GLN:HA	1.49	0.76
1:A:333:VAL:HG12	1:A:348:VAL:HG22	1.68	0.76
1:A:514:ILE:HD12	1:A:514:ILE:H	1.50	0.75
1:B:460:LEU:HD23	1:B:462:ASN:H	1.52	0.75
1:B:761:VAL:HG21	1:B:769:LEU:HD12	1.67	0.75
1:B:411:GLU:O	1:B:412:GLN:CB	2.28	0.75
1:A:270:THR:HG21	1:B:740:LYS:HD2	1.68	0.75
1:A:270:THR:CG2	1:B:740:LYS:HD2	2.17	0.74
1:B:514:ILE:HD12	1:B:514:ILE:H	1.52	0.74
1:A:440:PHE:HE1	1:A:453:TYR:CB	1.97	0.74
1:B:333:VAL:HG12	1:B:348:VAL:HG22	1.68	0.74
1:A:403:MET:HG3	1:A:418:LEU:HD21	1.70	0.74
1:A:761:VAL:HG21	1:A:769:LEU:HD12	1.68	0.74
1:A:460:LEU:HD23	1:A:462:ASN:H	1.53	0.73
1:B:562:ALA:HB1	1:B:781:LEU:HD13	1.71	0.73
1:B:83:ASP:OD2	1:B:85:GLU:HG3	1.88	0.73
1:B:403:MET:HG3	1:B:418:LEU:HD21	1.71	0.73
1:A:409:LYS:HG2	1:A:410:SER:N	2.02	0.72
1:B:695:PRO:HA	1:B:702:TYR:CE2	2.23	0.72
4:F:1:NAG:H62	4:F:2:NAG:C7	2.19	0.72
1:A:673:VAL:CG1	1:A:676:PRO:HB3	2.17	0.72
1:B:165:ARG:N	1:B:165:ARG:CD	2.49	0.72
1:B:390:VAL:HG23	1:B:392:GLN:HG2	1.71	0.71
1:A:562:ALA:HB1	1:A:781:LEU:HD13	1.72	0.71
1:A:662:LYS:HB3	1:A:712:HIS:HE1	1.56	0.71
1:B:710:ASN:C	1:B:712:HIS:N	2.44	0.71
1:B:477:TYR:O	1:B:493:CYS:O	2.08	0.71
1:A:160:TYR:HE1	1:A:162:ILE:HD12	1.56	0.70
1:A:493:CYS:HB3	1:A:500:VAL:H	1.56	0.70
1:A:440:PHE:CE1	1:A:453:TYR:HB3	2.24	0.70
1:B:478:PHE:CE1	1:B:491:LEU:HD11	2.27	0.70
1:A:201:TYR:HE1	1:A:212:ARG:HG3	1.53	0.70
1:A:292:ILE:HD11	1:A:321:ILE:HG13	1.75	0.69
1:A:695:PRO:HA	1:A:702:TYR:CE2	2.28	0.69
1:A:710:ASN:C	1:A:712:HIS:N	2.46	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:VAL:HG23	1:A:392:GLN:HG2	1.72	0.69
1:B:591:MET:O	1:B:592:ASP:HB2	1.93	0.69
1:A:478:PHE:CE1	1:A:491:LEU:HD11	2.27	0.69
1:B:246:PRO:HD2	1:B:329:ASN:HA	1.73	0.69
1:B:440:PHE:CE1	1:B:453:TYR:HB3	2.23	0.69
1:A:246:PRO:HD2	1:A:329:ASN:HA	1.74	0.69
1:A:695:PRO:HA	1:A:702:TYR:HD2	1.56	0.69
1:B:287:GLN:HA	1:B:287:GLN:NE2	2.08	0.68
1:B:545:LEU:HD13	1:B:601:GLY:HA2	1.75	0.68
1:B:192:LEU:HD23	1:B:203:GLN:HB2	1.76	0.68
1:B:471:MET:HB2	1:B:475:CYS:N	2.09	0.68
1:A:169:GLU:HG2	1:A:171:ASN:HD21	1.57	0.68
1:A:220:GLU:HG3	1:A:281:PRO:HD3	1.76	0.68
1:B:493:CYS:HB3	1:B:500:VAL:H	1.58	0.68
1:B:662:LYS:HB3	1:B:712:HIS:HE1	1.59	0.68
1:A:192:LEU:HD23	1:A:203:GLN:HB2	1.76	0.68
1:A:287:GLN:HA	1:A:287:GLN:NE2	2.07	0.68
1:A:775:LYS:NZ	5:B:809:NAG:C6	2.56	0.68
2:C:2:NAG:O3	2:C:3:BMA:H2	1.94	0.68
1:B:148:ILE:HG13	1:B:154:THR:HG22	1.76	0.68
1:B:201:TYR:HE1	1:B:212:ARG:HG3	1.57	0.67
1:B:655:TYR:OH	1:B:705:ALA:HB1	1.95	0.67
1:B:677:ILE:HG13	1:B:677:ILE:O	1.93	0.67
1:A:139:VAL:HG23	1:A:162:ILE:HD13	1.75	0.67
1:A:148:ILE:HG13	1:A:154:THR:HG22	1.75	0.67
1:A:581:HIS:ND1	1:A:581:HIS:C	2.47	0.67
1:A:324:VAL:HB	1:A:334:VAL:HG22	1.75	0.67
1:B:169:GLU:HG2	1:B:171:ASN:HD21	1.58	0.67
1:A:477:TYR:O	1:A:493:CYS:O	2.11	0.67
1:B:139:VAL:HG23	1:B:162:ILE:HD13	1.77	0.67
1:A:73:ASP:HA	1:A:76:ARG:HG3	1.76	0.66
1:A:270:THR:HG22	1:A:270:THR:O	1.95	0.66
1:B:373:GLU:CD	1:B:387:THR:HG22	2.16	0.66
1:B:581:HIS:ND1	1:B:581:HIS:C	2.47	0.66
1:A:373:GLU:CD	1:A:387:THR:HG22	2.16	0.66
1:A:419:THR:HG21	1:A:440:PHE:HE2	1.61	0.66
1:B:160:TYR:HE1	1:B:162:ILE:HD12	1.59	0.66
1:A:129:ARG:HB3	1:A:142:ALA:HB3	1.77	0.66
1:B:407:GLN:HB3	1:B:408:SER:OG	1.95	0.66
3:D:1:NAG:H4	3:D:2:NAG:C7	2.24	0.66
1:A:591:MET:O	1:A:592:ASP:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PRO:HG3	1:B:516:GLU:CB	2.26	0.66
1:B:467:SER:HB2	1:B:478:PHE:CE2	2.31	0.66
1:B:450:ARG:NH2	1:B:606:PHE:CD2	2.64	0.66
1:A:445:SER:OG	1:A:451:GLN:HG3	1.95	0.66
1:A:132:VAL:HG11	1:A:136:LEU:HD23	1.78	0.65
1:B:475:CYS:HB3	1:B:478:PHE:CZ	2.31	0.65
1:A:195:ILE:HG21	1:A:226:ILE:HG12	1.79	0.65
1:A:84:PRO:HG3	1:A:516:GLU:CB	2.25	0.65
1:A:655:TYR:OH	1:A:705:ALA:HB1	1.97	0.65
1:A:545:LEU:HD13	1:A:601:GLY:HA2	1.77	0.65
1:B:292:ILE:HD11	1:B:321:ILE:HG13	1.79	0.65
1:B:549:LEU:HD21	1:B:634:LEU:HD21	1.77	0.65
1:A:68:ARG:HB2	1:A:590:ASP:OD2	1.96	0.65
1:A:467:SER:HB2	1:A:478:PHE:CE2	2.32	0.65
1:A:677:ILE:HG13	1:A:677:ILE:O	1.94	0.65
1:B:220:GLU:HG3	1:B:281:PRO:HD3	1.78	0.65
1:A:674:VAL:HG22	1:A:722:ILE:HB	1.79	0.65
1:A:538:LEU:HD21	1:A:633:PHE:CD2	2.32	0.65
1:B:132:VAL:HG11	1:B:136:LEU:HD23	1.79	0.65
1:A:143:TYR:O	1:A:155:ALA:HB1	1.97	0.65
1:B:129:ARG:HB3	1:B:142:ALA:HB3	1.78	0.65
1:B:419:THR:HG21	1:B:440:PHE:HE2	1.62	0.64
1:B:270:THR:O	1:B:270:THR:HG22	1.95	0.64
1:B:652:TYR:O	1:B:655:TYR:HB3	1.96	0.64
1:B:324:VAL:HB	1:B:334:VAL:HG22	1.80	0.64
1:A:775:LYS:HE2	5:B:809:NAG:H62	1.80	0.64
3:G:1:NAG:H4	3:G:2:NAG:C7	2.27	0.64
1:B:457:THR:HG23	1:B:458:GLU:H	1.63	0.64
1:A:450:ARG:NH2	1:A:606:PHE:CD2	2.66	0.64
1:B:445:SER:OG	1:B:451:GLN:HG3	1.97	0.63
1:B:102:HIS:HE2	3:E:1:NAG:HO6	1.45	0.63
1:A:457:THR:HG23	1:A:458:GLU:H	1.63	0.63
1:A:775:LYS:HZ3	5:B:809:NAG:C6	2.09	0.63
1:A:775:LYS:HZ3	5:B:809:NAG:H62	1.63	0.63
1:A:471:MET:HB2	1:A:475:CYS:N	2.13	0.63
1:B:609:LEU:HB3	1:B:613:GLN:NE2	2.14	0.63
1:A:475:CYS:HB3	1:A:478:PHE:CZ	2.33	0.63
1:B:73:ASP:HA	1:B:76:ARG:HG3	1.80	0.63
1:A:286:GLY:HA3	1:A:695:PRO:HG3	1.80	0.62
1:B:195:ILE:HG21	1:B:226:ILE:HG12	1.81	0.62
1:B:436:GLN:O	1:B:457:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:TYR:O	1:A:655:TYR:HB3	1.98	0.62
1:B:407:GLN:O	1:B:409:LYS:O	2.16	0.62
1:B:68:ARG:HB2	1:B:590:ASP:OD2	1.98	0.62
1:B:172:PRO:HG2	1:B:175:VAL:HB	1.82	0.62
1:A:530:ILE:HG23	1:A:530:ILE:O	2.00	0.62
1:A:416:ARG:HH11	1:A:461:LEU:HD21	1.65	0.62
1:A:694:MET:HB3	1:A:697:LYS:HB2	1.81	0.62
1:A:436:GLN:O	1:A:457:THR:HG22	2.00	0.62
1:A:609:LEU:HB3	1:A:613:GLN:NE2	2.13	0.62
1:A:401:ILE:HD11	1:A:440:PHE:CD2	2.35	0.62
1:B:530:ILE:HG23	1:B:530:ILE:O	1.98	0.62
1:A:549:LEU:HD21	1:A:634:LEU:HD21	1.81	0.61
1:A:504:HIS:ND1	1:A:511:LYS:HA	2.15	0.61
1:A:710:ASN:O	1:A:712:HIS:N	2.22	0.61
1:B:436:GLN:O	1:B:457:THR:N	2.32	0.61
1:B:530:ILE:O	1:B:530:ILE:CG2	2.48	0.61
1:B:674:VAL:HG22	1:B:722:ILE:HB	1.81	0.61
1:A:378:SER:HB3	1:A:381:GLY:H	1.65	0.61
1:B:538:LEU:HD21	1:B:633:PHE:CD2	2.35	0.61
1:A:220:GLU:HG2	1:A:279:GLN:O	2.01	0.61
1:B:86:ALA:HA	1:B:96:TYR:HA	1.81	0.61
1:A:172:PRO:HG2	1:A:175:VAL:HB	1.82	0.61
1:B:403:MET:HB2	1:B:416:ARG:O	2.00	0.61
1:B:694:MET:HB3	1:B:697:LYS:HB2	1.82	0.61
1:B:416:ARG:HH11	1:B:461:LEU:HD21	1.66	0.61
1:A:121:THR:HG22	1:A:127:ALA:HB3	1.82	0.60
1:B:120:THR:O	1:B:122:PHE:N	2.32	0.60
1:B:714:LEU:HD13	1:B:719:ILE:HD12	1.82	0.60
1:A:86:ALA:HA	1:A:96:TYR:HA	1.82	0.60
1:A:403:MET:HB2	1:A:416:ARG:O	2.00	0.60
1:A:448:ARG:HD3	1:A:576:VAL:HG12	1.83	0.60
1:B:616:HIS:NE2	1:B:617:ARG:HD2	2.16	0.60
1:A:342:ASN:HA	1:A:368:LEU:HD23	1.84	0.60
1:A:294:LEU:HD23	1:A:308:LEU:HB2	1.84	0.60
1:A:585:ASP:OD2	1:A:598:ARG:NH2	2.35	0.60
1:B:143:TYR:O	1:B:155:ALA:HB1	2.02	0.60
1:B:231:TYR:OH	1:B:292:ILE:HG21	2.01	0.60
1:A:436:GLN:O	1:A:457:THR:N	2.33	0.60
1:A:530:ILE:O	1:A:530:ILE:CG2	2.50	0.60
1:A:328:SER:HG	1:A:331:LYS:H	1.50	0.60
1:B:695:PRO:CA	1:B:702:TYR:CE2	2.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:HB3	1:A:578:ASP:OD1	2.02	0.59
1:A:403:MET:HG2	1:A:418:LEU:HD11	1.83	0.59
1:A:194:TYR:CE2	1:A:201:TYR:HD2	2.20	0.59
1:B:448:ARG:HD3	1:B:576:VAL:HG12	1.84	0.59
1:A:79:PHE:O	1:A:80:VAL:HB	2.00	0.59
1:B:192:LEU:CD2	1:B:203:GLN:HB2	2.33	0.59
1:A:317:ARG:O	1:A:319:TYR:HD1	1.85	0.59
3:D:1:NAG:H4	3:D:2:NAG:N2	2.16	0.59
1:A:342:ASN:C	1:A:368:LEU:HD23	2.23	0.59
1:B:125:PHE:O	1:B:126:LYS:C	2.42	0.59
1:B:279:GLN:O	1:B:279:GLN:HG3	2.02	0.59
1:A:331:LYS:HA	1:A:349:CYS:O	2.03	0.59
1:B:317:ARG:O	1:B:319:TYR:HD1	1.85	0.59
1:A:764:LYS:HD3	1:B:744:LYS:HD2	1.85	0.58
1:B:339:ARG:HD2	1:B:689:GLU:OE1	2.03	0.58
1:B:342:ASN:HA	1:B:368:LEU:HD23	1.84	0.58
1:B:592:ASP:OD1	1:B:778:SER:HB2	2.04	0.58
1:B:589:ILE:HG22	1:B:590:ASP:N	2.17	0.58
1:B:698:GLU:C	1:B:699:GLU:HG2	2.22	0.58
1:B:644:ARG:CD	1:B:783:GLU:OE2	2.52	0.58
1:A:563:LEU:HB3	1:A:645:LEU:HD22	1.85	0.58
1:A:641:ASP:OD1	1:A:643:LYS:HB2	2.04	0.58
1:B:450:ARG:HG3	1:B:450:ARG:HH11	1.69	0.58
1:B:563:LEU:HB3	1:B:645:LEU:HD22	1.85	0.58
1:B:448:ARG:HB3	1:B:578:ASP:OD1	2.04	0.57
1:B:270:THR:O	1:B:270:THR:CG2	2.52	0.57
1:A:192:LEU:CD2	1:A:203:GLN:HB2	2.34	0.57
1:B:121:THR:HG22	1:B:127:ALA:HB3	1.84	0.57
1:A:616:HIS:NE2	1:A:617:ARG:HD2	2.20	0.57
1:B:471:MET:HB3	1:B:474:GLN:HB2	1.85	0.57
1:B:401:ILE:HD11	1:B:440:PHE:CD2	2.40	0.57
1:A:698:GLU:C	1:A:699:GLU:HG2	2.23	0.57
1:A:714:LEU:HD13	1:A:719:ILE:HD12	1.86	0.57
4:F:2:NAG:H61	4:F:3:BMA:O2	2.05	0.57
1:A:231:TYR:OH	1:A:292:ILE:HG21	2.05	0.57
1:B:342:ASN:C	1:B:368:LEU:HD23	2.25	0.57
1:B:504:HIS:ND1	1:B:511:LYS:HA	2.20	0.57
1:A:165:ARG:H	1:A:165:ARG:HD3	1.61	0.56
1:A:270:THR:CG2	1:A:270:THR:O	2.52	0.56
1:A:450:ARG:HH11	1:A:450:ARG:HG3	1.70	0.56
1:A:538:LEU:HD12	1:A:599:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:LYS:C	1:A:717:GLU:H	2.08	0.56
1:B:220:GLU:HG2	1:B:279:GLN:O	2.05	0.56
1:A:339:ARG:HD2	1:A:689:GLU:OE1	2.05	0.56
1:A:739:ILE:HD13	1:A:751:MET:HE3	1.87	0.56
1:A:740:LYS:HD2	1:B:270:THR:CG2	2.35	0.56
1:B:694:MET:HE3	1:B:695:PRO:HD2	1.86	0.56
1:B:79:PHE:O	1:B:80:VAL:HB	2.04	0.56
1:B:323:MET:HE2	1:B:373:GLU:O	2.05	0.56
1:A:125:PHE:O	1:A:126:LYS:C	2.43	0.56
1:B:378:SER:HB3	1:B:381:GLY:H	1.70	0.56
1:A:89:ILE:HD11	1:A:95:VAL:HB	1.87	0.56
1:A:279:GLN:O	1:A:279:GLN:HG3	2.06	0.56
1:B:331:LYS:HA	1:B:349:CYS:O	2.06	0.56
1:B:448:ARG:HG3	1:B:448:ARG:NH1	2.20	0.56
1:B:488:HIS:ND1	1:B:488:HIS:N	2.53	0.56
1:A:471:MET:HB3	1:A:474:GLN:HB2	1.87	0.56
1:A:589:ILE:HG22	1:A:590:ASP:N	2.20	0.56
1:B:394:GLY:O	1:B:395:ARG:CB	2.52	0.56
1:B:225:GLY:C	1:B:241:ALA:HB3	2.25	0.56
1:A:394:GLY:O	1:A:395:ARG:CB	2.54	0.55
1:B:186:GLY:HA3	1:B:191:GLN:HG3	1.88	0.55
1:A:575:LEU:HD22	1:A:598:ARG:HD3	1.89	0.55
1:A:589:ILE:HG13	1:A:596:VAL:HG13	1.89	0.55
1:B:510:ALA:C	1:B:512:TYR:H	2.10	0.55
1:A:663:SER:HB3	1:A:712:HIS:CE1	2.41	0.55
1:B:96:TYR:CG	1:B:96:TYR:O	2.59	0.55
1:B:403:MET:HG2	1:B:418:LEU:HD11	1.88	0.55
1:B:695:PRO:CA	1:B:702:TYR:HE2	2.20	0.55
1:A:563:LEU:HB3	1:A:645:LEU:CD2	2.36	0.55
1:B:563:LEU:HB3	1:B:645:LEU:CD2	2.36	0.55
1:A:194:TYR:CE2	1:A:201:TYR:CD2	2.95	0.54
3:D:1:NAG:H2	3:D:2:NAG:O7	2.06	0.54
1:A:110:THR:O	1:A:111:ASN:HB2	2.07	0.54
1:A:565:LEU:HD22	1:A:567:MET:CE	2.37	0.54
1:B:89:ILE:HD11	1:B:95:VAL:HB	1.89	0.54
1:B:102:HIS:CD2	3:E:1:NAG:HO6	2.26	0.54
1:B:471:MET:HG3	1:B:475:CYS:SG	2.46	0.54
1:A:118:GLU:CG	1:A:119:ASN:N	2.64	0.54
1:A:592:ASP:OD1	1:A:778:SER:HB2	2.07	0.54
1:B:84:PRO:HG3	1:B:516:GLU:HB2	1.89	0.54
1:B:194:TYR:CE2	1:B:201:TYR:HD2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:LEU:HD13	1:B:598:ARG:HB3	1.88	0.54
1:A:695:PRO:CA	1:A:702:TYR:CE2	2.91	0.54
1:B:431:TYR:HE1	1:B:457:THR:HG21	1.73	0.54
1:A:120:THR:O	1:A:122:PHE:N	2.41	0.54
1:A:488:HIS:ND1	1:A:488:HIS:N	2.54	0.54
1:A:575:LEU:HD13	1:A:598:ARG:HB3	1.90	0.54
1:A:225:GLY:C	1:A:241:ALA:HB3	2.27	0.53
1:A:431:TYR:HE1	1:A:457:THR:HG21	1.73	0.53
1:A:694:MET:HE3	1:A:695:PRO:HD2	1.90	0.53
1:B:538:LEU:HD12	1:B:599:PHE:CE1	2.43	0.53
1:A:84:PRO:HG3	1:A:516:GLU:HB2	1.90	0.53
1:B:725:THR:HG22	1:B:756:ASP:H	1.74	0.53
1:A:448:ARG:HG3	1:A:448:ARG:NH1	2.18	0.53
1:B:110:THR:O	1:B:111:ASN:HB2	2.08	0.53
1:B:663:SER:HB3	1:B:712:HIS:CE1	2.43	0.53
1:B:739:ILE:HD13	1:B:751:MET:CE	2.38	0.53
1:A:715:LYS:C	1:A:717:GLU:N	2.61	0.53
1:B:460:LEU:HD23	1:B:462:ASN:HB3	1.89	0.53
1:A:411:GLU:C	1:A:412:GLN:O	2.44	0.53
1:B:160:TYR:CE1	1:B:162:ILE:HD12	2.44	0.53
1:B:450:ARG:HG3	1:B:450:ARG:NH1	2.23	0.53
1:A:165:ARG:CD	1:A:165:ARG:N	2.37	0.53
1:A:739:ILE:HD13	1:A:751:MET:CE	2.38	0.53
1:B:670:CYS:CB	1:B:718:ASN:HB3	2.39	0.53
1:B:725:THR:CG2	1:B:756:ASP:H	2.22	0.53
1:A:141:LEU:HB2	1:A:158:VAL:HG12	1.91	0.53
1:A:169:GLU:HG2	1:A:171:ASN:ND2	2.24	0.53
1:A:258:ASP:OD1	1:A:290:PRO:HB3	2.09	0.53
1:A:694:MET:CE	1:A:697:LYS:HG3	2.39	0.53
1:B:193:ILE:HD11	1:B:242:HIS:CD2	2.44	0.53
1:B:589:ILE:HG13	1:B:596:VAL:HG13	1.90	0.53
1:B:294:LEU:HD23	1:B:308:LEU:HB2	1.90	0.52
1:B:322:THR:HG21	1:B:371:GLN:OE1	2.07	0.52
1:B:714:LEU:HD13	1:B:719:ILE:CD1	2.38	0.52
1:A:96:TYR:O	1:A:96:TYR:CG	2.62	0.52
1:B:709:HIS:O	1:B:710:ASN:HB2	2.09	0.52
1:A:73:ASP:OD1	1:A:76:ARG:NH1	2.43	0.52
1:A:584:TRP:HH2	1:A:648:PHE:CE1	2.28	0.52
1:B:584:TRP:HH2	1:B:648:PHE:CZ	2.27	0.52
1:A:725:THR:CG2	1:A:756:ASP:H	2.22	0.52
1:B:339:ARG:NH1	1:B:689:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:TRP:HH2	1:B:648:PHE:CE1	2.27	0.52
1:A:725:THR:HG22	1:A:756:ASP:H	1.74	0.52
1:B:102:HIS:NE2	3:E:1:NAG:O6	2.38	0.52
1:A:510:ALA:C	1:A:512:TYR:H	2.11	0.52
1:B:328:SER:HG	1:B:331:LYS:H	1.58	0.52
1:B:695:PRO:HA	1:B:702:TYR:HD2	1.69	0.52
1:B:264:MET:HE2	1:B:264:MET:HA	1.92	0.52
1:B:623:GLU:HG3	1:B:656:ILE:CD1	2.40	0.52
1:B:739:ILE:HD13	1:B:751:MET:HE3	1.91	0.52
1:A:186:GLY:HA3	1:A:191:GLN:HG3	1.90	0.52
1:A:193:ILE:HD11	1:A:242:HIS:CD2	2.44	0.52
1:B:641:ASP:OD1	1:B:643:LYS:HB2	2.09	0.52
1:B:677:ILE:HD11	1:B:680:LEU:HD22	1.90	0.52
1:A:520:MET:HG2	1:A:521:LEU:N	2.25	0.51
1:A:623:GLU:HG3	1:A:656:ILE:CD1	2.40	0.51
1:B:511:LYS:O	1:B:512:TYR:C	2.49	0.51
1:B:694:MET:CE	1:B:697:LYS:HG3	2.41	0.51
3:G:1:NAG:H2	3:G:2:NAG:O7	2.10	0.51
1:A:118:GLU:C	1:A:120:THR:H	2.14	0.51
1:A:188:GLN:O	1:A:191:GLN:HG2	2.09	0.51
1:B:520:MET:HG2	1:B:521:LEU:N	2.24	0.51
1:B:95:VAL:HG13	1:B:95:VAL:O	2.10	0.51
1:A:322:THR:HG21	1:A:371:GLN:OE1	2.10	0.51
1:A:426:ILE:HD12	1:A:450:ARG:HG2	1.93	0.51
1:A:132:VAL:HG22	1:A:139:VAL:HG22	1.93	0.51
1:A:670:CYS:CB	1:A:718:ASN:HB3	2.41	0.51
1:A:401:ILE:HD11	1:A:440:PHE:HD2	1.75	0.51
1:A:403:MET:O	1:A:405:LEU:HD22	2.11	0.51
1:B:169:GLU:HG2	1:B:171:ASN:ND2	2.26	0.51
1:B:584:TRP:CH2	1:B:648:PHE:CZ	2.99	0.51
1:A:193:ILE:HG23	1:A:244:TRP:CH2	2.45	0.51
1:A:588:LEU:HD22	1:A:594:VAL:HB	1.93	0.51
1:B:588:LEU:HD22	1:B:594:VAL:HB	1.93	0.50
1:A:95:VAL:HG13	1:A:95:VAL:O	2.11	0.50
1:A:440:PHE:N	1:A:440:PHE:CD1	2.78	0.50
1:A:644:ARG:CD	1:A:781:LEU:O	2.46	0.50
1:B:141:LEU:HB2	1:B:158:VAL:HG12	1.93	0.50
1:B:460:LEU:HD22	1:B:460:LEU:N	2.26	0.50
2:C:2:NAG:O3	2:C:4:MAN:H3	2.10	0.50
1:A:159:ILE:HG21	1:A:206:ILE:HD11	1.93	0.50
1:B:508:ASN:OD1	1:B:510:ALA:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:CE1	1:A:162:ILE:HD12	2.41	0.50
1:A:450:ARG:HG3	1:A:450:ARG:NH1	2.25	0.50
1:A:567:MET:SD	1:A:647:ILE:HD11	2.51	0.50
1:B:403:MET:O	1:B:405:LEU:HD22	2.10	0.50
1:B:550:SER:HB2	1:B:596:VAL:HG22	1.92	0.50
1:B:73:ASP:OD2	1:B:528:LYS:NZ	2.45	0.50
1:A:460:LEU:N	1:A:460:LEU:HD22	2.26	0.50
1:A:513:PHE:HB3	5:A:801:NAG:H61	1.93	0.50
1:B:194:TYR:CE2	1:B:201:TYR:CD2	2.99	0.50
1:B:567:MET:SD	1:B:647:ILE:HD11	2.52	0.50
1:A:460:LEU:HD23	1:A:462:ASN:HB3	1.94	0.50
1:A:508:ASN:OD1	1:A:510:ALA:HB2	2.12	0.50
1:B:646:SER:HA	1:B:670:CYS:O	2.12	0.50
1:A:264:MET:HG2	1:A:731:HIS:NE2	2.27	0.49
1:A:403:MET:CG	1:A:418:LEU:HD11	2.42	0.49
1:B:188:GLN:O	1:B:191:GLN:HG2	2.12	0.49
1:B:249:GLU:HG3	1:B:300:TYR:CE2	2.47	0.49
1:B:405:LEU:HB2	1:B:414:THR:HG23	1.94	0.49
1:B:73:ASP:OD1	1:B:76:ARG:NH1	2.44	0.49
1:B:694:MET:HE2	1:B:697:LYS:HG3	1.94	0.49
1:B:193:ILE:HG23	1:B:244:TRP:CH2	2.46	0.49
1:B:264:MET:HG2	1:B:731:HIS:NE2	2.28	0.49
1:B:367:TRP:CD1	1:B:367:TRP:C	2.85	0.49
1:B:410:SER:C	1:B:411:GLU:O	2.51	0.49
1:A:373:GLU:OE2	1:A:387:THR:HG22	2.12	0.49
1:B:142:ALA:HB2	1:B:157:TYR:CE2	2.47	0.49
1:B:488:HIS:HB2	1:B:504:HIS:O	2.11	0.49
1:A:488:HIS:HB2	1:A:504:HIS:O	2.12	0.49
1:A:714:LEU:HD13	1:A:719:ILE:CD1	2.43	0.49
1:B:102:HIS:CE1	1:B:119:ASN:OD1	2.66	0.49
1:B:132:VAL:HG22	1:B:139:VAL:HG22	1.95	0.49
1:B:161:ASN:ND2	1:B:164:THR:HG23	2.28	0.49
1:B:620:GLY:N	1:B:623:GLU:OE1	2.40	0.49
1:A:511:LYS:O	1:A:512:TYR:C	2.50	0.49
1:A:525:ILE:HD13	1:A:526:LEU:N	2.28	0.49
1:A:550:SER:HB2	1:A:596:VAL:HG22	1.95	0.49
1:A:666:LYS:NZ	1:A:666:LYS:HB3	2.27	0.49
1:B:562:ALA:CB	1:B:781:LEU:HD13	2.41	0.49
1:A:677:ILE:HD11	1:A:680:LEU:HD22	1.95	0.49
1:A:121:THR:CG2	1:A:127:ALA:HB3	2.42	0.49
1:B:286:GLY:HA3	1:B:695:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:NH1	1:A:689:GLU:OE2	2.46	0.49
1:A:670:CYS:HB3	1:A:718:ASN:HB3	1.95	0.49
1:B:373:GLU:OE2	1:B:387:THR:HG22	2.13	0.48
1:A:695:PRO:CA	1:A:702:TYR:HE2	2.27	0.48
1:B:450:ARG:H	1:B:477:TYR:HA	1.78	0.48
1:B:663:SER:O	1:B:664:ASP:C	2.50	0.48
1:B:710:ASN:O	1:B:712:HIS:CG	2.67	0.48
4:F:1:NAG:H4	4:F:2:NAG:O7	2.14	0.48
1:A:669:LYS:HD2	1:A:780:CYS:O	2.13	0.48
1:B:159:ILE:HG21	1:B:206:ILE:HD11	1.95	0.48
1:A:268:ARG:NH1	1:A:277:GLY:HA2	2.29	0.48
1:A:409:LYS:CG	1:A:410:SER:H	2.10	0.48
1:A:694:MET:HE2	1:A:697:LYS:HG3	1.95	0.48
1:B:195:ILE:CD1	1:B:226:ILE:HG23	2.38	0.48
1:B:575:LEU:HD22	1:B:598:ARG:HD3	1.95	0.48
1:A:512:TYR:HB3	1:A:513:PHE:H	1.54	0.48
1:A:640:ILE:HD13	1:A:640:ILE:O	2.13	0.48
1:A:751:MET:HG2	1:A:751:MET:O	2.13	0.48
1:B:470:PHE:CE1	1:B:491:LEU:HD12	2.49	0.48
1:A:378:SER:C	1:A:380:ASP:H	2.17	0.48
1:A:584:TRP:HH2	1:A:648:PHE:CZ	2.32	0.48
1:B:143:TYR:O	1:B:144:ASP:HB2	2.14	0.48
1:B:429:LEU:HD11	1:B:441:LEU:CD2	2.44	0.48
1:B:666:LYS:NZ	1:B:666:LYS:HB3	2.29	0.48
1:A:646:SER:HA	1:A:670:CYS:O	2.13	0.48
1:B:159:ILE:HD13	1:B:206:ILE:HD11	1.96	0.48
1:B:666:LYS:HB3	1:B:666:LYS:HZ2	1.79	0.48
1:A:471:MET:HG3	1:A:475:CYS:SG	2.54	0.48
1:B:440:PHE:CD1	1:B:440:PHE:N	2.81	0.48
1:A:243:TRP:HH2	1:A:254:LEU:HG	1.78	0.47
1:B:602:ARG:HA	1:B:611:ILE:HG23	1.96	0.47
1:B:670:CYS:HB3	1:B:718:ASN:HB3	1.96	0.47
1:A:695:PRO:C	1:A:697:LYS:N	2.68	0.47
1:B:637:LEU:HD13	1:B:639:TYR:CZ	2.49	0.47
1:A:166:GLU:H	1:A:166:GLU:HG3	1.47	0.47
1:A:562:ALA:CB	1:A:781:LEU:HD13	2.43	0.47
1:B:525:ILE:HD13	1:B:526:LEU:N	2.29	0.47
1:B:118:GLU:CG	1:B:119:ASN:N	2.64	0.47
3:D:1:NAG:H4	3:D:2:NAG:O7	2.14	0.47
1:A:488:HIS:CB	1:A:504:HIS:O	2.62	0.47
1:B:460:LEU:HD23	1:B:462:ASN:N	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HB2	1:A:414:THR:HG23	1.97	0.47
1:B:121:THR:CG2	1:B:127:ALA:HB3	2.44	0.47
1:B:648:PHE:CD1	1:B:648:PHE:C	2.87	0.47
1:B:738:LEU:HG	1:B:742:LEU:HD12	1.95	0.47
1:A:138:TYR:CD1	1:A:161:ASN:HA	2.50	0.47
1:B:426:ILE:HD12	1:B:450:ARG:HG2	1.96	0.47
1:B:488:HIS:CB	1:B:504:HIS:O	2.63	0.47
1:B:571:PRO:HD3	1:B:652:TYR:CD2	2.50	0.47
1:B:585:ASP:HB2	1:B:596:VAL:HG11	1.97	0.47
1:B:605:GLY:HA2	1:B:612:LEU:HD13	1.97	0.47
1:A:301:GLY:HA3	1:A:302:PRO:HD3	1.80	0.47
1:A:431:TYR:CE1	1:A:457:THR:HG21	2.50	0.47
1:B:158:VAL:HG13	1:B:167:VAL:HG13	1.97	0.47
1:B:268:ARG:NH1	1:B:277:GLY:HA2	2.29	0.47
1:A:163:HIS:ND1	1:A:163:HIS:C	2.68	0.47
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.80	0.47
1:A:584:TRP:CH2	1:A:648:PHE:CZ	3.03	0.47
1:A:591:MET:O	1:A:592:ASP:CB	2.63	0.47
1:B:92:THR:O	1:B:108:ILE:HG12	2.15	0.47
1:B:410:SER:O	1:B:411:GLU:O	2.32	0.47
1:B:751:MET:O	1:B:751:MET:HG2	2.14	0.47
1:A:648:PHE:C	1:A:648:PHE:CD1	2.87	0.47
1:A:666:LYS:HB3	1:A:666:LYS:HZ2	1.79	0.47
1:A:738:LEU:HG	1:A:742:LEU:HD12	1.97	0.47
1:A:753:VAL:HG13	1:B:751:MET:HE2	1.97	0.47
1:B:645:LEU:HD12	1:B:667:LEU:O	2.15	0.47
1:A:126:LYS:HE3	1:A:126:LYS:HA	1.98	0.46
1:B:431:TYR:CE1	1:B:457:THR:HG21	2.50	0.46
1:A:740:LYS:HD2	1:B:270:THR:HG21	1.96	0.46
1:B:80:VAL:HG12	1:B:80:VAL:O	2.15	0.46
1:B:258:ASP:OD1	1:B:290:PRO:HB3	2.14	0.46
1:A:249:GLU:HG3	1:A:300:TYR:CE2	2.51	0.46
1:B:163:HIS:ND1	1:B:163:HIS:C	2.68	0.46
1:B:754:TYR:HB3	1:B:757:GLU:HG3	1.98	0.46
1:A:292:ILE:HD11	1:A:321:ILE:CG1	2.45	0.46
1:A:470:PHE:HE2	1:A:511:LYS:HG3	1.80	0.46
1:A:158:VAL:HG13	1:A:167:VAL:HG13	1.98	0.46
1:A:367:TRP:CD1	1:A:367:TRP:C	2.89	0.46
1:A:450:ARG:H	1:A:477:TYR:HA	1.80	0.46
1:B:328:SER:HG	1:B:331:LYS:N	2.13	0.46
1:B:617:ARG:NH2	1:B:699:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:ILE:HD13	1:B:640:ILE:O	2.15	0.46
1:A:80:VAL:HG12	1:A:80:VAL:O	2.14	0.46
1:A:142:ALA:HB2	1:A:157:TYR:CE2	2.51	0.46
1:A:328:SER:OG	1:A:330:THR:HG23	2.15	0.46
1:A:403:MET:O	1:A:404:PHE:C	2.54	0.46
1:A:541:ASP:HB3	1:A:542:ASP:H	1.38	0.46
1:A:73:ASP:OD2	1:A:528:LYS:NZ	2.49	0.46
1:A:195:ILE:CD1	1:A:226:ILE:HG23	2.40	0.46
1:A:602:ARG:HA	1:A:611:ILE:HG23	1.98	0.46
1:A:409:LYS:CG	1:A:410:SER:N	2.67	0.46
1:A:436:GLN:HG2	1:A:458:GLU:HB2	1.97	0.46
1:A:753:VAL:HG11	1:B:753:VAL:CG1	2.41	0.46
1:B:609:LEU:HD13	1:B:613:GLN:NE2	2.31	0.46
1:B:126:LYS:HE3	1:B:126:LYS:HA	1.98	0.46
1:B:161:ASN:OD1	1:B:161:ASN:C	2.55	0.46
1:B:644:ARG:NH1	1:B:781:LEU:O	2.49	0.46
1:A:273:LEU:HD23	1:B:682:LEU:HD23	1.97	0.46
1:A:719:ILE:O	1:A:750:THR:HG23	2.16	0.46
1:B:436:GLN:HG2	1:B:458:GLU:HB2	1.97	0.46
1:A:268:ARG:HH12	1:A:277:GLY:HA2	1.81	0.45
1:A:301:GLY:O	1:A:303:THR:HG23	2.16	0.45
1:A:460:LEU:HD23	1:A:462:ASN:N	2.26	0.45
1:B:714:LEU:HD12	1:B:747:VAL:HG11	1.97	0.45
3:G:1:NAG:O3	3:G:2:NAG:N2	2.49	0.45
1:A:545:LEU:HB3	1:A:600:ASP:O	2.17	0.45
1:A:644:ARG:NH1	1:A:781:LEU:O	2.49	0.45
1:A:172:PRO:HG2	1:A:175:VAL:CB	2.45	0.45
1:A:497:ARG:HD3	1:A:498:VAL:O	2.16	0.45
1:A:548:GLN:HB2	1:A:576:VAL:HG22	1.99	0.45
1:A:564:LEU:HD22	1:A:588:LEU:HD12	1.99	0.45
1:B:82:HIS:HB3	1:B:516:GLU:OE2	2.16	0.45
1:B:172:PRO:HG2	1:B:175:VAL:CB	2.46	0.45
1:B:591:MET:O	1:B:592:ASP:CB	2.61	0.45
1:A:147:GLN:HA	1:A:147:GLN:OE1	2.17	0.45
1:A:411:GLU:O	1:A:412:GLN:O	2.34	0.45
1:A:82:HIS:HB3	1:A:516:GLU:OE2	2.15	0.45
1:A:569:GLU:O	1:A:652:TYR:HB3	2.17	0.45
1:B:124:THR:O	1:B:125:PHE:C	2.55	0.45
1:B:268:ARG:O	1:B:275:PRO:HB2	2.16	0.45
1:B:545:LEU:HB3	1:B:600:ASP:O	2.17	0.45
1:B:548:GLN:HB2	1:B:576:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:NAG:H4	3:G:2:NAG:N2	2.31	0.45
1:A:92:THR:O	1:A:108:ILE:HG12	2.17	0.45
1:A:221:ILE:HG22	1:A:222:ILE:HG13	1.98	0.45
1:B:403:MET:CG	1:B:418:LEU:HD11	2.46	0.45
1:B:471:MET:O	1:B:472:LYS:HB2	2.17	0.45
1:B:691:TYR:N	1:B:691:TYR:CD1	2.85	0.45
1:A:157:TYR:CE2	1:A:183:ALA:HB3	2.52	0.45
1:A:193:ILE:HG12	1:A:244:TRP:HZ2	1.81	0.45
1:A:327:VAL:HG23	1:A:328:SER:H	1.81	0.45
1:A:645:LEU:HD12	1:A:667:LEU:O	2.17	0.45
1:B:403:MET:O	1:B:404:PHE:C	2.53	0.45
1:B:541:ASP:HB3	1:B:542:ASP:H	1.37	0.45
1:A:143:TYR:O	1:A:144:ASP:HB2	2.17	0.45
1:A:161:ASN:ND2	1:A:164:THR:HG23	2.32	0.45
1:A:268:ARG:O	1:A:275:PRO:HB2	2.17	0.45
1:A:637:LEU:HD13	1:A:639:TYR:CZ	2.52	0.45
1:A:691:TYR:N	1:A:691:TYR:CD1	2.85	0.45
1:A:754:TYR:HB3	1:A:757:GLU:HG3	1.97	0.45
1:A:264:MET:HG2	1:A:731:HIS:CD2	2.52	0.45
1:B:564:LEU:HD22	1:B:588:LEU:HD12	1.99	0.45
1:A:762:SER:O	1:A:766:LYS:HB2	2.16	0.44
1:B:147:GLN:OE1	1:B:147:GLN:HA	2.17	0.44
1:B:401:ILE:HD11	1:B:440:PHE:HD2	1.80	0.44
1:A:102:HIS:HD1	1:A:118:GLU:HA	1.82	0.44
1:A:450:ARG:HD2	1:A:477:TYR:CZ	2.52	0.44
1:A:460:LEU:H	1:A:460:LEU:CD1	2.16	0.44
1:A:498:VAL:CG1	1:A:521:LEU:HD22	2.47	0.44
1:A:666:LYS:HD2	1:A:717:GLU:HG3	2.00	0.44
1:A:126:LYS:O	1:A:126:LYS:HG3	2.17	0.44
1:A:255:MET:SD	1:A:255:MET:C	2.95	0.44
1:A:584:TRP:CD1	1:A:585:ASP:N	2.86	0.44
1:A:617:ARG:NH2	1:A:699:GLU:OE2	2.50	0.44
1:A:709:HIS:O	1:A:710:ASN:HB2	2.17	0.44
1:B:193:ILE:HD11	1:B:242:HIS:NE2	2.32	0.44
1:B:488:HIS:HB3	1:B:505:SER:CA	2.29	0.44
1:B:624:VAL:HG21	1:B:659:MET:HB2	1.99	0.44
1:B:749:TYR:CD1	1:B:749:TYR:C	2.91	0.44
1:A:193:ILE:HD11	1:A:242:HIS:NE2	2.32	0.44
1:A:241:ALA:HB1	1:A:254:LEU:HB2	1.98	0.44
1:A:609:LEU:HD13	1:A:613:GLN:NE2	2.33	0.44
1:A:666:LYS:HE2	1:A:716:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:LEU:HD12	1:A:747:VAL:HG11	1.99	0.44
1:A:739:ILE:O	1:A:743:ILE:HG13	2.17	0.44
1:B:204:PRO:HG2	1:B:208:SER:HB2	2.00	0.44
1:B:301:GLY:O	1:B:303:THR:HG23	2.17	0.44
1:B:498:VAL:CG1	1:B:521:LEU:HD22	2.47	0.44
1:B:565:LEU:HD22	1:B:567:MET:CE	2.48	0.44
1:A:506:THR:O	1:A:509:PRO:HD3	2.18	0.44
1:B:497:ARG:HD3	1:B:498:VAL:O	2.17	0.44
1:B:648:PHE:CD1	1:B:649:GLY:N	2.85	0.44
1:B:662:LYS:HB3	1:B:712:HIS:CE1	2.47	0.44
1:B:666:LYS:HE2	1:B:716:GLU:HG2	1.99	0.44
1:B:695:PRO:CA	1:B:702:TYR:CD2	2.97	0.44
1:A:165:ARG:O	1:A:166:GLU:C	2.55	0.44
1:A:620:GLY:N	1:A:623:GLU:OE1	2.42	0.44
1:B:366:THR:OG1	1:B:367:TRP:N	2.50	0.44
1:B:450:ARG:HD2	1:B:477:TYR:CZ	2.53	0.44
1:B:551:LEU:HA	1:B:552:PRO:HD3	1.89	0.44
1:A:159:ILE:HD13	1:A:206:ILE:HD11	1.98	0.44
1:A:161:ASN:C	1:A:161:ASN:OD1	2.57	0.44
1:A:172:PRO:HA	1:A:194:TYR:OH	2.17	0.44
1:A:315:LYS:O	1:A:316:SER:OG	2.27	0.44
1:A:739:ILE:CD1	1:A:751:MET:HE3	2.48	0.44
1:B:183:ALA:O	1:B:193:ILE:O	2.36	0.44
1:A:87:ARG:HB3	1:A:95:VAL:HG12	2.00	0.44
1:A:648:PHE:CD1	1:A:649:GLY:N	2.86	0.44
1:B:190:GLN:HG3	1:B:205:ASP:HA	2.00	0.44
1:B:243:TRP:HH2	1:B:254:LEU:HG	1.82	0.44
1:B:666:LYS:CE	1:B:716:GLU:HG2	2.48	0.44
1:B:138:TYR:CD1	1:B:161:ASN:HA	2.53	0.43
1:B:292:ILE:O	1:B:292:ILE:HD13	2.17	0.43
1:B:394:GLY:O	1:B:395:ARG:HB2	2.17	0.43
1:B:268:ARG:HH12	1:B:277:GLY:HA2	1.82	0.43
1:B:396:GLY:HA3	1:B:610:LYS:HB2	2.00	0.43
1:B:532:LYS:HA	1:B:533:PRO:HD3	1.55	0.43
1:B:681:LYS:HB2	1:B:681:LYS:HE3	1.70	0.43
1:B:157:TYR:CE2	1:B:183:ALA:HB3	2.53	0.43
1:B:221:ILE:HG22	1:B:222:ILE:HG13	2.00	0.43
1:B:126:LYS:HG3	1:B:126:LYS:O	2.17	0.43
1:B:172:PRO:HA	1:B:194:TYR:OH	2.17	0.43
1:B:193:ILE:HG12	1:B:244:TRP:HZ2	1.83	0.43
1:A:584:TRP:CG	1:A:585:ASP:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:C	1:B:122:PHE:N	2.72	0.43
1:B:366:THR:OG1	1:B:613:GLN:OE1	2.30	0.43
1:A:183:ALA:O	1:A:193:ILE:O	2.36	0.43
1:A:311:PRO:HG2	1:A:314:PHE:HB2	2.00	0.43
1:A:328:SER:HG	1:A:331:LYS:N	2.15	0.43
1:A:148:ILE:HB	1:A:152:SER:HB3	2.00	0.43
1:A:289:ASN:HD22	1:A:289:ASN:HA	1.57	0.43
1:A:532:LYS:HA	1:A:533:PRO:HD3	1.57	0.43
1:B:148:ILE:HG13	1:B:154:THR:CG2	2.47	0.43
1:B:194:TYR:CZ	1:B:201:TYR:HD2	2.37	0.43
1:B:460:LEU:H	1:B:460:LEU:CD1	2.16	0.43
1:B:545:LEU:HA	1:B:546:PRO:HD3	1.74	0.43
1:A:429:LEU:HD11	1:A:441:LEU:CD2	2.48	0.43
1:A:498:VAL:HA	1:A:499:PRO:HD3	1.92	0.43
1:A:624:VAL:HG21	1:A:659:MET:HB2	2.01	0.43
1:A:663:SER:O	1:A:664:ASP:C	2.56	0.43
1:A:124:THR:O	1:A:125:PHE:C	2.57	0.43
1:A:194:TYR:CZ	1:A:201:TYR:HD2	2.36	0.43
1:A:270:THR:HG23	1:B:740:LYS:HD2	1.98	0.43
1:A:764:LYS:CE	1:B:744:LYS:HD2	2.49	0.43
1:B:121:THR:HG23	1:B:141:LEU:HD12	2.00	0.43
1:B:292:ILE:HD11	1:B:321:ILE:CG1	2.48	0.43
1:B:328:SER:OG	1:B:330:THR:HG23	2.18	0.43
1:B:515:LEU:HA	1:B:515:LEU:HD12	1.70	0.43
1:B:650:LYS:HG2	1:B:651:GLY:N	2.34	0.43
1:A:605:GLY:HA2	1:A:612:LEU:HD13	2.00	0.43
1:A:662:LYS:HB3	1:A:712:HIS:CE1	2.45	0.43
1:B:692:LEU:HD12	1:B:702:TYR:CE1	2.54	0.43
1:A:342:ASN:CA	1:A:368:LEU:HD23	2.49	0.42
1:A:740:LYS:HD2	1:B:270:THR:HG23	2.00	0.42
1:B:374:GLU:HA	1:B:375:PRO:HD2	1.90	0.42
1:B:670:CYS:HB2	1:B:718:ASN:HB3	2.01	0.42
1:A:83:ASP:HA	1:A:84:PRO:HD3	1.81	0.42
1:A:116:LEU:C	1:A:162:ILE:HD11	2.40	0.42
1:A:436:GLN:C	1:A:457:THR:HG22	2.40	0.42
1:A:440:PHE:N	1:A:440:PHE:HD1	2.15	0.42
1:A:585:ASP:HB2	1:A:596:VAL:HG11	2.01	0.42
1:A:749:TYR:CD1	1:A:749:TYR:C	2.92	0.42
1:A:775:LYS:HB2	1:A:775:LYS:HE3	1.71	0.42
1:B:520:MET:HG2	1:B:521:LEU:H	1.84	0.42
1:B:569:GLU:O	1:B:652:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:HD11	2:C:1:NAG:HN2	1.84	0.42
1:B:264:MET:HG2	1:B:731:HIS:CD2	2.54	0.42
1:A:266:ILE:HG23	1:A:726:ALA:HA	2.02	0.42
1:A:396:GLY:HA3	1:A:610:LYS:HB2	2.01	0.42
1:A:419:THR:HG22	1:A:463:ARG:HD3	2.01	0.42
1:A:666:LYS:CE	1:A:716:GLU:HG2	2.49	0.42
1:B:616:HIS:CD2	1:B:617:ARG:HD2	2.55	0.42
1:A:385:PHE:CG	1:A:438:ILE:HD12	2.53	0.42
1:A:584:TRP:CD1	1:A:584:TRP:C	2.92	0.42
1:B:79:PHE:CD1	1:B:79:PHE:N	2.87	0.42
1:B:87:ARG:HB3	1:B:95:VAL:HG12	2.01	0.42
1:A:511:LYS:O	1:A:511:LYS:HG2	2.20	0.42
1:B:74:LEU:HD12	1:B:74:LEU:N	2.34	0.42
1:A:323:MET:HE2	1:A:375:PRO:HD2	2.01	0.42
1:A:650:LYS:HG2	1:A:651:GLY:N	2.34	0.42
1:A:782:LYS:HB2	1:A:782:LYS:HE3	1.22	0.42
1:B:116:LEU:C	1:B:162:ILE:HD11	2.40	0.42
1:B:436:GLN:C	1:B:457:THR:HG22	2.39	0.42
1:B:727:ASP:OD1	1:B:759:HIS:HB2	2.19	0.42
1:A:116:LEU:HB3	1:A:162:ILE:HD11	2.02	0.42
1:A:148:ILE:HG22	1:A:149:PHE:N	2.35	0.42
1:A:650:LYS:CG	1:A:651:GLY:N	2.83	0.42
1:B:378:SER:C	1:B:380:ASP:H	2.23	0.42
1:A:669:LYS:HG3	1:A:670:CYS:N	2.34	0.42
1:A:720:LEU:HA	1:A:750:THR:O	2.19	0.42
1:B:130:HIS:ND1	1:B:130:HIS:C	2.73	0.42
1:B:419:THR:HG22	1:B:463:ARG:HD3	2.02	0.42
1:B:584:TRP:CD1	1:B:584:TRP:C	2.92	0.42
1:B:584:TRP:CD1	1:B:585:ASP:N	2.88	0.42
1:A:95:VAL:O	1:A:96:TYR:C	2.58	0.42
1:A:366:THR:OG1	1:A:367:TRP:N	2.49	0.42
1:A:443:THR:HB	1:A:447:PRO:HA	2.02	0.42
1:A:620:GLY:H	1:A:623:GLU:CD	2.22	0.42
1:B:116:LEU:HB3	1:B:162:ILE:HD11	2.02	0.42
1:B:222:ILE:HD11	4:F:1:NAG:HN2	1.85	0.42
1:B:666:LYS:HD2	1:B:717:GLU:HG3	2.02	0.42
1:A:91:ASP:O	1:A:108:ILE:HD11	2.19	0.41
1:B:298:ASN:OD1	1:B:303:THR:HA	2.20	0.41
1:B:301:GLY:HA3	1:B:302:PRO:HD3	1.78	0.41
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.78	0.41
1:A:87:ARG:HH22	1:A:132:VAL:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:VAL:HG13	1:A:521:LEU:HD22	2.03	0.41
1:A:575:LEU:HA	1:A:575:LEU:HD23	1.82	0.41
1:B:241:ALA:HB1	1:B:254:LEU:HB2	2.02	0.41
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.79	0.41
1:B:306:LEU:N	1:B:306:LEU:HD12	2.35	0.41
1:B:619:LEU:HB2	1:B:692:LEU:HD21	2.02	0.41
1:B:712:HIS:N	1:B:712:HIS:ND1	2.68	0.41
1:A:448:ARG:NH1	1:A:448:ARG:CG	2.82	0.41
1:A:692:LEU:HD12	1:A:702:TYR:CE1	2.55	0.41
1:A:765:SER:HA	1:B:743:ILE:HG21	2.01	0.41
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.93	0.41
1:B:327:VAL:HG23	1:B:328:SER:H	1.84	0.41
1:A:269:PHE:CD1	1:B:732:PHE:HD2	2.39	0.41
1:A:515:LEU:HA	1:A:515:LEU:HD12	1.72	0.41
1:B:93:ASP:HA	1:B:106:LEU:O	2.20	0.41
1:B:287:GLN:HE21	1:B:287:GLN:CA	2.28	0.41
1:B:559:ASN:OD1	1:B:559:ASN:N	2.52	0.41
1:B:601:GLY:O	1:B:604:SER:HB3	2.19	0.41
1:B:644:ARG:HB3	1:B:781:LEU:HD22	2.03	0.41
1:B:675:ALA:HA	1:B:723:HIS:CE1	2.55	0.41
1:A:460:LEU:O	1:A:461:LEU:HB2	2.21	0.41
1:A:476:THR:H	1:A:496:PRO:HD3	1.85	0.41
1:A:726:ALA:HB3	1:A:757:GLU:O	2.21	0.41
1:B:81:LEU:HA	1:B:521:LEU:HD13	2.01	0.41
1:B:148:ILE:HG22	1:B:149:PHE:N	2.35	0.41
1:A:74:LEU:N	1:A:74:LEU:HD12	2.34	0.41
1:A:204:PRO:HG2	1:A:208:SER:HB2	2.03	0.41
1:B:137:LYS:HB2	1:B:137:LYS:HE3	1.92	0.41
1:B:584:TRP:CG	1:B:585:ASP:N	2.88	0.41
1:B:620:GLY:H	1:B:623:GLU:CD	2.22	0.41
1:B:761:VAL:CG1	1:B:765:SER:HB2	2.50	0.41
1:A:240:ILE:H	1:A:240:ILE:HG12	1.60	0.41
1:A:416:ARG:HH11	1:A:461:LEU:CD2	2.31	0.41
1:A:436:GLN:O	1:A:456:SER:HA	2.20	0.41
1:A:620:GLY:O	1:A:624:VAL:HB	2.19	0.41
1:B:782:LYS:HE3	1:B:782:LYS:HB2	1.08	0.41
1:A:190:GLN:HG3	1:A:205:ASP:HA	2.02	0.41
1:A:459:GLY:O	1:A:461:LEU:HD12	2.21	0.41
1:B:148:ILE:HB	1:B:152:SER:HB3	2.03	0.41
1:B:336:TRP:HE1	1:B:347:THR:HB	1.85	0.41
1:B:409:LYS:O	1:B:410:SER:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ARG:HH11	1:B:461:LEU:CD2	2.31	0.41
1:B:621:SER:O	1:B:625:LYS:HG3	2.21	0.41
1:A:137:LYS:HB2	1:A:137:LYS:HE3	1.92	0.41
1:A:261:VAL:HG11	1:A:283:PRO:HD3	2.03	0.41
1:A:294:LEU:CD2	1:A:308:LEU:HB2	2.50	0.41
1:A:306:LEU:HD12	1:A:306:LEU:N	2.36	0.41
1:A:644:ARG:HB3	1:A:781:LEU:HD22	2.03	0.41
1:B:73:ASP:O	1:B:76:ARG:HB2	2.21	0.41
1:B:91:ASP:O	1:B:108:ILE:HD11	2.21	0.41
1:B:231:TYR:CZ	1:B:292:ILE:HG21	2.55	0.41
1:B:411:GLU:O	1:B:412:GLN:CG	2.68	0.41
1:B:708:LEU:HD23	1:B:708:LEU:HA	1.87	0.41
1:A:92:THR:HG22	1:A:109:GLU:HG3	2.03	0.41
1:A:148:ILE:HG13	1:A:154:THR:CG2	2.46	0.41
1:A:200:ILE:C	1:A:201:TYR:HD1	2.25	0.41
1:A:615:ILE:O	1:A:615:ILE:CG2	2.70	0.41
1:B:83:ASP:HA	1:B:84:PRO:HD3	1.80	0.41
1:B:200:ILE:O	1:B:201:TYR:HD1	2.04	0.41
1:B:326:TRP:HA	1:B:332:THR:HG22	2.03	0.41
1:B:384:PHE:HD2	1:B:406:ILE:HG13	1.86	0.41
1:B:506:THR:O	1:B:509:PRO:HD3	2.21	0.41
1:B:650:LYS:CG	1:B:651:GLY:N	2.84	0.41
1:B:765:SER:O	1:B:768:HIS:N	2.54	0.41
1:A:394:GLY:O	1:A:395:ARG:HB2	2.20	0.40
1:A:652:TYR:HA	1:A:677:ILE:HG23	2.03	0.40
1:B:261:VAL:HG11	1:B:283:PRO:HD3	2.03	0.40
1:A:93:ASP:HA	1:A:106:LEU:O	2.21	0.40
1:A:130:HIS:ND1	1:A:130:HIS:C	2.74	0.40
1:A:542:ASP:OD1	1:A:542:ASP:N	2.48	0.40
1:A:571:PRO:HD3	1:A:652:TYR:CD2	2.57	0.40
1:B:459:GLY:O	1:B:461:LEU:HD12	2.20	0.40
1:A:270:THR:HG23	1:B:737:GLU:OE2	2.21	0.40
1:B:266:ILE:HG23	1:B:726:ALA:HA	2.03	0.40
1:A:79:PHE:CD1	1:A:79:PHE:N	2.88	0.40
1:B:311:PRO:HG2	1:B:314:PHE:HB2	2.03	0.40
1:B:342:ASN:CA	1:B:368:LEU:HD23	2.50	0.40
1:B:436:GLN:O	1:B:456:SER:HA	2.21	0.40
1:A:73:ASP:O	1:A:76:ARG:HB2	2.21	0.40
1:A:231:TYR:HA	1:A:235:LEU:HB2	2.04	0.40
1:A:264:MET:HA	1:A:264:MET:CE	2.51	0.40
1:A:291:THR:C	1:A:292:ILE:HG22	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HG3	1:A:406:ILE:CD1	2.52	0.40
1:B:359:LYS:HG3	1:B:406:ILE:CD1	2.52	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	715/719 (99%)	632 (88%)	71 (10%)	12 (2%)	9 34
1	B	717/719 (100%)	635 (89%)	72 (10%)	10 (1%)	11 37
All	All	1432/1438 (100%)	1267 (88%)	143 (10%)	22 (2%)	10 36

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	A	413	ILE
1	A	663	SER
1	A	711	VAL
1	B	165	ARG
1	B	711	VAL
1	A	695	PRO
1	A	766	LYS
1	B	411	GLU
1	B	663	SER
1	B	695	PRO
1	A	715	LYS
1	A	716	GLU
1	A	529	LYS
1	A	697	LYS
1	B	410	SER

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Mol	Chain	Res	Type
1	B	412	GLN
1	B	529	LYS
1	A	80	VAL
1	B	80	VAL
1	A	530	ILE
1	B	530	ILE

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	645/650 (99%)	540 (84%)	105 (16%)	2 9
1	B	646/650 (99%)	539 (83%)	107 (17%)	2 8
All	All	1291/1300 (99%)	1079 (84%)	212 (16%)	2 9

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	91	ASP
1	A	95	VAL
1	A	99	GLU
1	A	100	ASN
1	A	113	THR
1	A	117	LEU
1	A	118	GLU
1	A	120	THR
1	A	121	THR
1	A	122	PHE
1	A	125	PHE
1	A	126	LYS
1	A	128	SER
1	A	129	ARG
1	A	130	HIS
1	A	140	LEU

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Mol	Chain	Res	Type
1	A	144	ASP
1	A	152	SER
1	A	154	THR
1	A	158	VAL
1	A	164	THR
1	A	165	ARG
1	A	166	GLU
1	A	188	GLN
1	A	192	LEU
1	A	209	SER
1	A	211	LEU
1	A	226	ILE
1	A	240	ILE
1	A	249	GLU
1	A	255	MET
1	A	280	TYR
1	A	289	ASN
1	A	291	THR
1	A	292	ILE
1	A	294	LEU
1	A	305	THR
1	A	306	LEU
1	A	313	SER
1	A	317	ARG
1	A	324	VAL
1	A	330	THR
1	A	339	ARG
1	A	347	THR
1	A	365	ASP
1	A	367	TRP
1	A	368	LEU
1	A	391	LYS
1	A	403	MET
1	A	406	ILE
1	A	407	GLN
1	A	412	GLN
1	A	414	THR
1	A	435	THR
1	A	440	PHE
1	A	457	THR
1	A	460	LEU
1	A	462	ASN

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Mol	Chain	Res	Type
1	A	487	GLN
1	A	488	HIS
1	A	491	LEU
1	A	497	ARG
1	A	503	LEU
1	A	512	TYR
1	A	514	ILE
1	A	519	SER
1	A	520	MET
1	A	525	ILE
1	A	528	LYS
1	A	530	ILE
1	A	541	ASP
1	A	542	ASP
1	A	556	MET
1	A	559	ASN
1	A	560	GLN
1	A	565	LEU
1	A	567	MET
1	A	570	GLU
1	A	581	HIS
1	A	584	TRP
1	A	588	LEU
1	A	596	VAL
1	A	604	SER
1	A	617	ARG
1	A	618	ARG
1	A	632	LYS
1	A	635	LEU
1	A	640	ILE
1	A	646	SER
1	A	663	SER
1	A	666	LYS
1	A	669	LYS
1	A	677	ILE
1	A	702	TYR
1	A	711	VAL
1	A	712	HIS
1	A	716	GLU
1	A	720	LEU
1	A	725	THR
1	A	742	LEU

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Mol	Chain	Res	Type
1	A	750	THR
1	A	761	VAL
1	A	763	GLU
1	A	769	LEU
1	B	83	ASP
1	B	91	ASP
1	B	95	VAL
1	B	99	GLU
1	B	100	ASN
1	B	113	THR
1	B	117	LEU
1	B	118	GLU
1	B	120	THR
1	B	121	THR
1	B	122	PHE
1	B	125	PHE
1	B	126	LYS
1	B	128	SER
1	B	129	ARG
1	B	130	HIS
1	B	140	LEU
1	B	144	ASP
1	B	148	ILE
1	B	152	SER
1	B	154	THR
1	B	158	VAL
1	B	164	THR
1	B	165	ARG
1	B	166	GLU
1	B	188	GLN
1	B	192	LEU
1	B	206	ILE
1	B	209	SER
1	B	211	LEU
1	B	226	ILE
1	B	240	ILE
1	B	249	GLU
1	B	255	MET
1	B	280	TYR
1	B	289	ASN
1	B	291	THR
1	B	292	ILE

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Mol	Chain	Res	Type
1	B	294	LEU
1	B	305	THR
1	B	306	LEU
1	B	313	SER
1	B	317	ARG
1	B	322	THR
1	B	324	VAL
1	B	330	THR
1	B	339	ARG
1	B	347	THR
1	B	365	ASP
1	B	367	TRP
1	B	368	LEU
1	B	391	LYS
1	B	403	MET
1	B	406	ILE
1	B	407	GLN
1	B	411	GLU
1	B	412	GLN
1	B	414	THR
1	B	435	THR
1	B	440	PHE
1	B	457	THR
1	B	460	LEU
1	B	462	ASN
1	B	487	GLN
1	B	488	HIS
1	B	491	LEU
1	B	497	ARG
1	B	503	LEU
1	B	512	TYR
1	B	514	ILE
1	B	519	SER
1	B	520	MET
1	B	525	ILE
1	B	530	ILE
1	B	541	ASP
1	B	542	ASP
1	B	556	MET
1	B	558	ARG
1	B	559	ASN
1	B	560	GLN

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Mol	Chain	Res	Type
1	B	565	LEU
1	B	567	MET
1	B	570	GLU
1	B	581	HIS
1	B	584	TRP
1	B	588	LEU
1	B	604	SER
1	B	617	ARG
1	B	618	ARG
1	B	632	LYS
1	B	635	LEU
1	B	640	ILE
1	B	646	SER
1	B	663	SER
1	B	665	GLU
1	B	666	LYS
1	B	677	ILE
1	B	702	TYR
1	B	712	HIS
1	B	716	GLU
1	B	720	LEU
1	B	725	THR
1	B	742	LEU
1	B	750	THR
1	B	761	VAL
1	B	763	GLU
1	B	783	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	B	287	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.50	0	17,19,21	1.57	3 (17%)
2	NAG	C	2	2	14,14,15	0.64	0	17,19,21	1.50	3 (17%)
2	BMA	C	3	2	11,11,12	0.69	0	15,15,17	2.74	5 (33%)
2	MAN	C	4	2	11,11,12	0.47	0	15,15,17	1.68	3 (20%)
3	NAG	D	1	3,1	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	NAG	D	2	3	14,14,15	0.55	0	17,19,21	1.36	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	1.68	3 (17%)
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	0.76	0
4	NAG	F	1	4,1	14,14,15	0.75	0	17,19,21	1.00	0
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	0.72	0
4	BMA	F	3	4	11,11,12	0.55	0	15,15,17	1.35	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.63	0	17,19,21	1.62	6 (35%)
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	1.51	1 (5%)

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

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	2.00	1.55	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	BMA	C1-C2-C3	-8.25	99.52	109.67
3	G	2	NAG	C1-O5-C5	5.32	119.40	112.19
2	C	1	NAG	C2-N2-C7	-5.22	115.47	122.90
3	E	1	NAG	O5-C1-C2	-5.14	103.17	111.29
3	D	2	NAG	C1-O5-C5	4.61	118.44	112.19
2	C	4	MAN	C1-O5-C5	4.10	117.74	112.19
4	F	3	BMA	C1-O5-C5	4.06	117.69	112.19
2	C	3	BMA	C3-C4-C5	3.70	116.84	110.24
3	D	1	NAG	O5-C1-C2	-3.58	105.64	111.29
2	C	2	NAG	C1-O5-C5	3.43	116.83	112.19
2	C	4	MAN	O5-C5-C6	3.10	112.06	107.20
2	C	3	BMA	C1-O5-C5	3.05	116.32	112.19
3	G	1	NAG	O4-C4-C3	2.73	116.65	110.35
3	D	1	NAG	C1-O5-C5	2.56	115.66	112.19
3	G	1	NAG	C4-C3-C2	-2.51	107.34	111.02
2	C	3	BMA	O5-C5-C4	2.49	116.88	110.83
3	G	1	NAG	O5-C5-C6	2.42	111.00	107.20
2	C	3	BMA	O2-C2-C1	2.29	113.84	109.15
2	C	2	NAG	C3-C4-C5	2.26	114.27	110.24
3	E	1	NAG	C3-C4-C5	2.17	114.11	110.24
3	G	1	NAG	O5-C1-C2	-2.17	107.87	111.29
3	E	1	NAG	C4-C3-C2	2.16	114.19	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	O4-C4-C5	-2.14	103.99	109.30
2	C	1	NAG	C1-O5-C5	2.14	115.09	112.19
2	C	4	MAN	C2-C3-C4	-2.08	107.29	110.89
3	G	1	NAG	C3-C4-C5	-2.02	106.63	110.24
3	G	1	NAG	O3-C3-C4	2.02	115.01	110.35
2	C	1	NAG	O5-C5-C6	2.01	110.36	107.20

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C8-C7-N2-C2
2	C	4	MAN	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	E	2	NAG	C3-C2-N2-C7
3	G	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

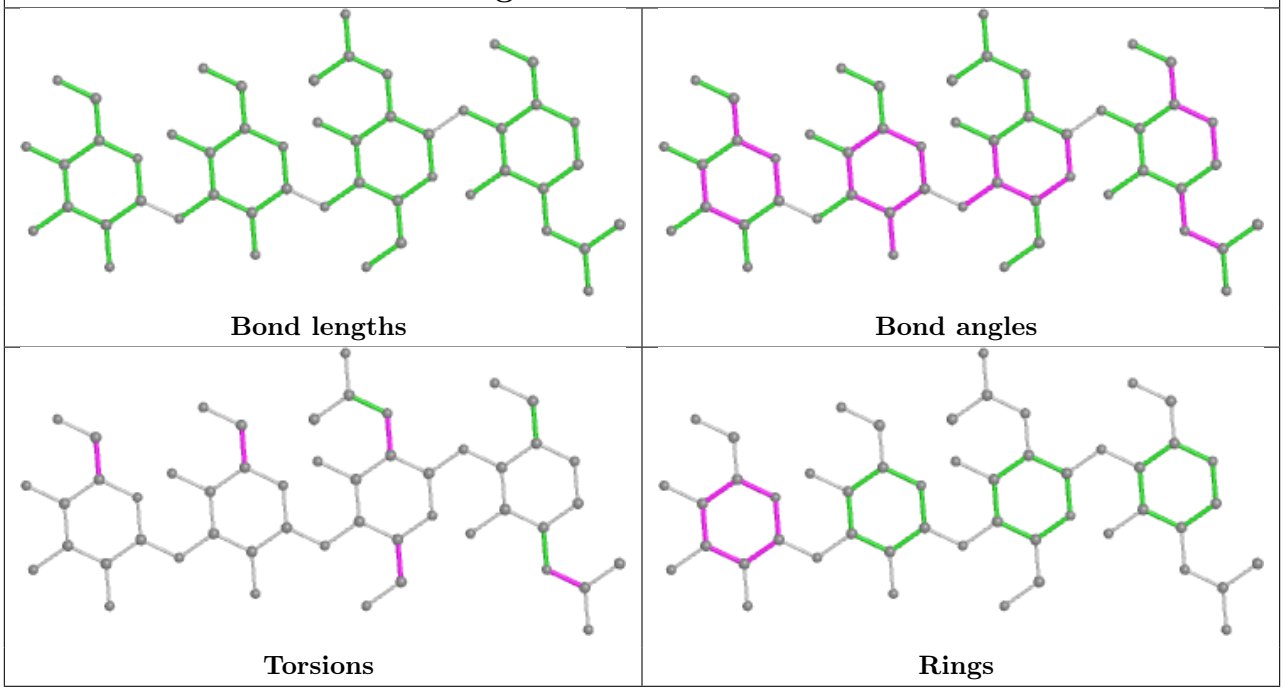
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 19 short contacts:

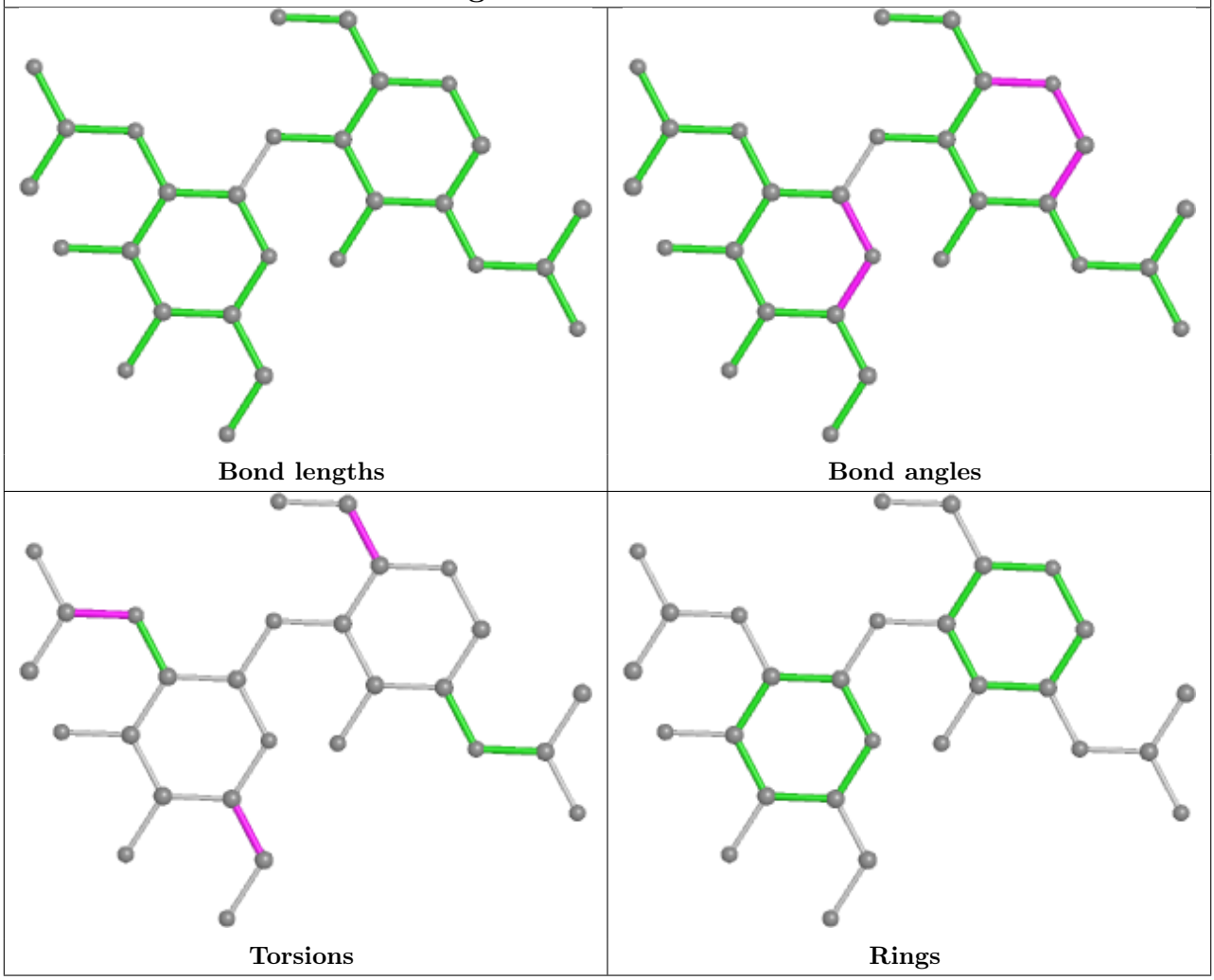
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	3	0
4	F	1	NAG	3	0
4	F	3	BMA	1	0
2	C	4	MAN	1	0
2	C	2	NAG	2	0
2	C	3	BMA	1	0
3	E	1	NAG	3	0
3	G	2	NAG	4	0
3	G	1	NAG	4	0
3	D	2	NAG	4	0
2	C	1	NAG	2	0
3	D	1	NAG	4	0

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

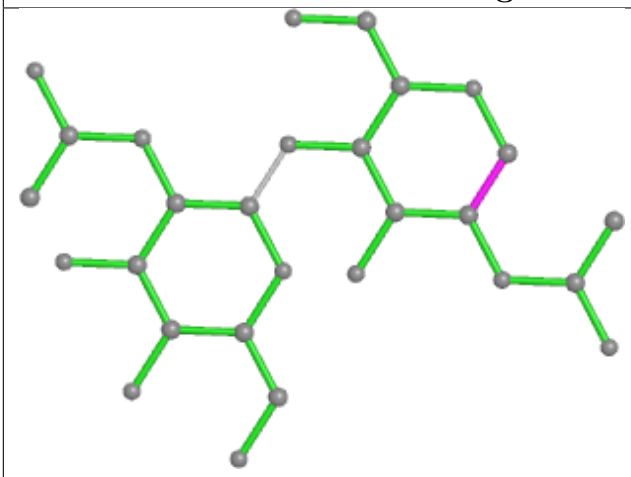
Oligosaccharide Chain C



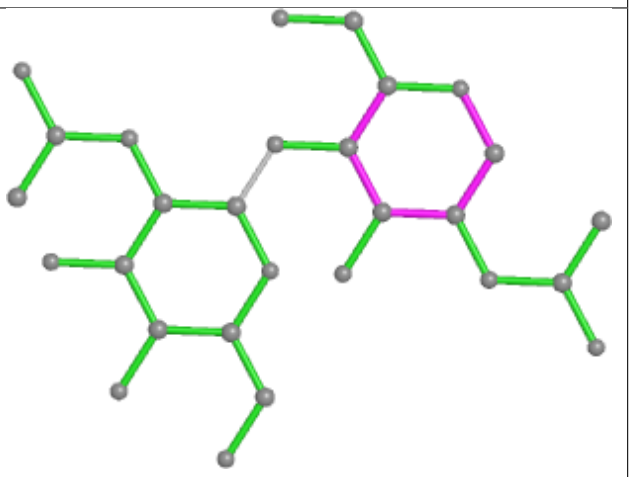
Oligosaccharide Chain D



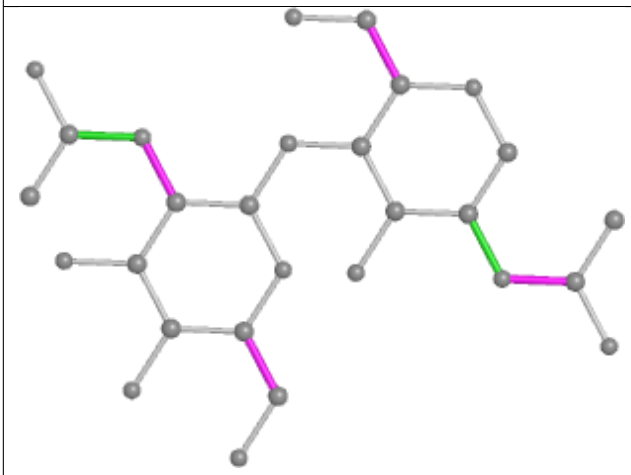
Oligosaccharide Chain E



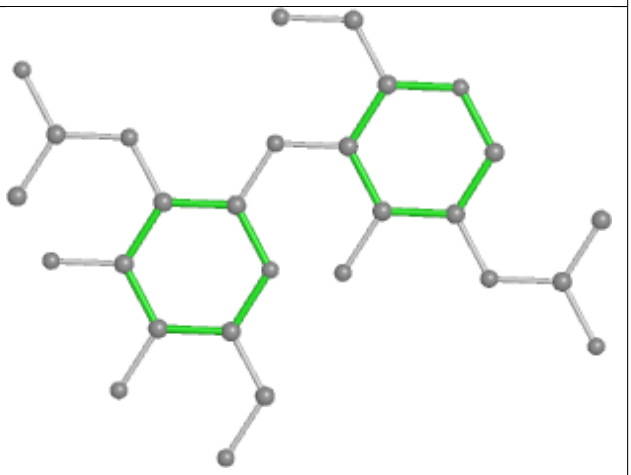
Bond lengths



Bond angles

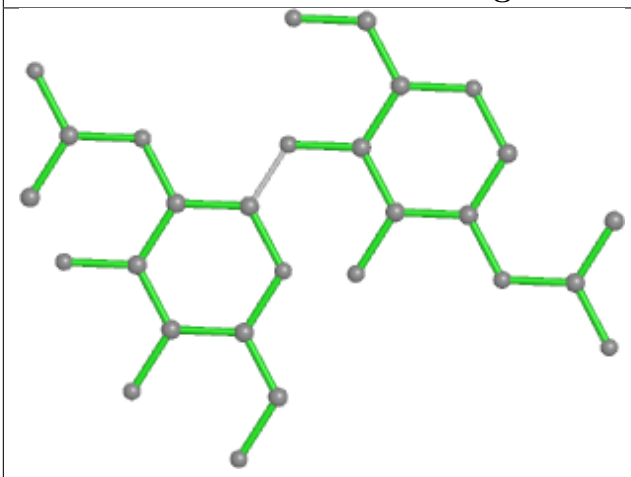


Torsions

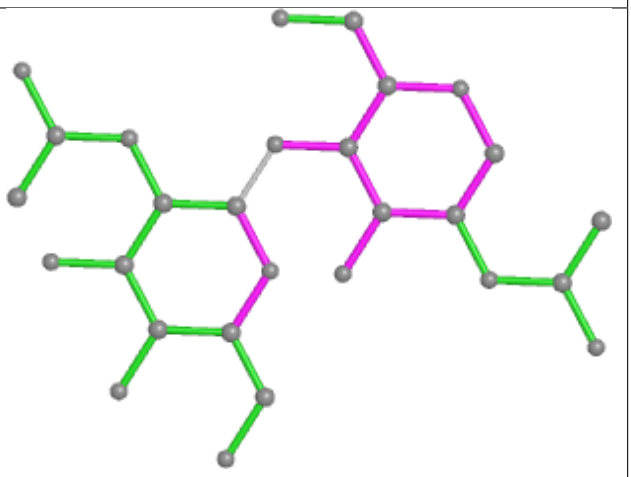


Rings

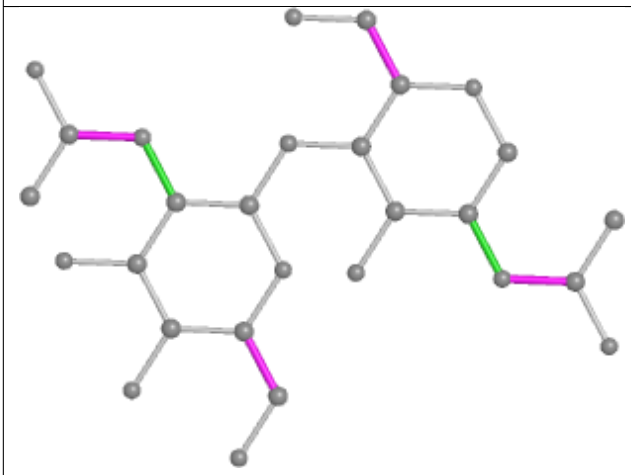
Oligosaccharide Chain G



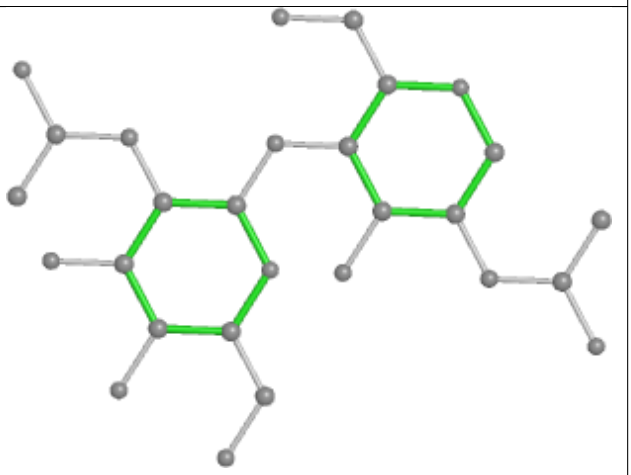
Bond lengths



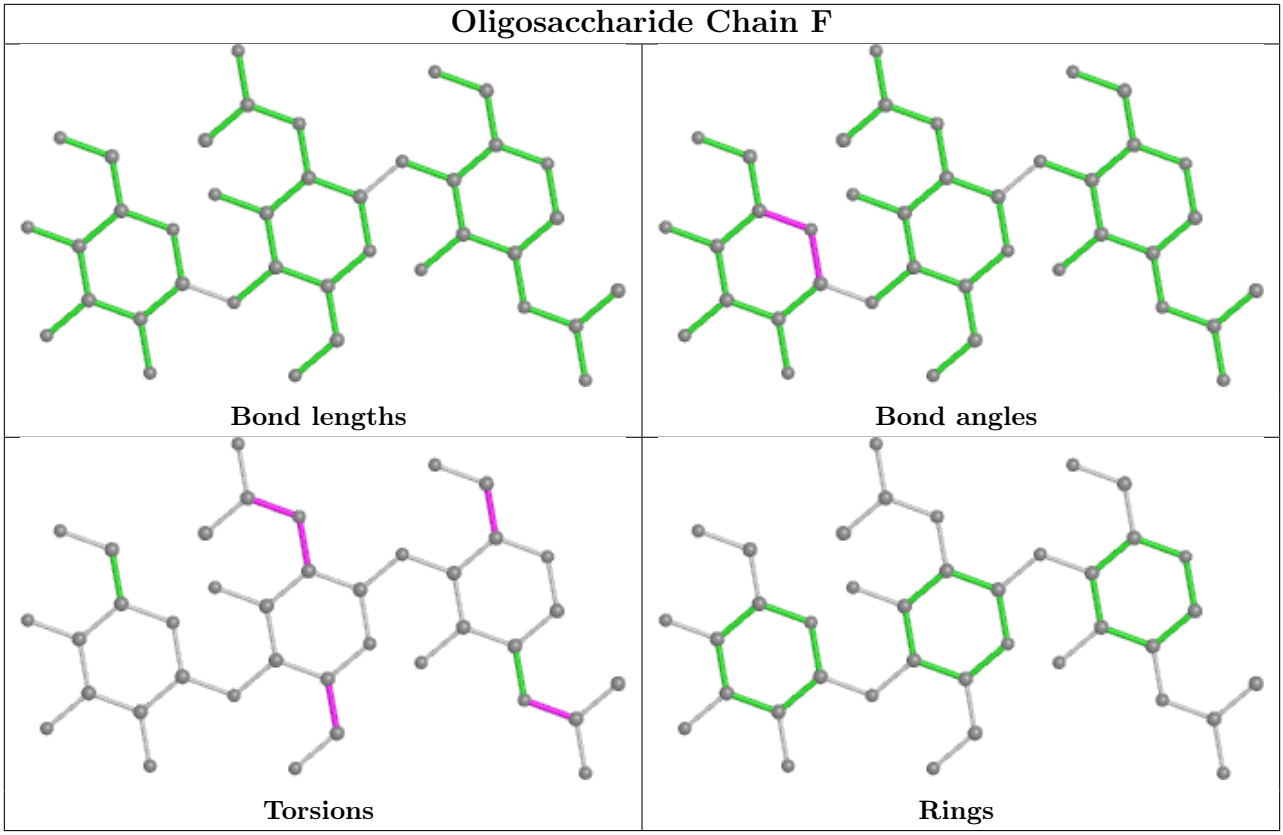
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	809	1	14,14,15	0.61	0	17,19,21	1.44	3 (17%)
5	NAG	B	801	1	14,14,15	0.43	0	17,19,21	1.81	2 (11%)
5	NAG	A	802	1	14,14,15	0.56	0	17,19,21	1.99	3 (17%)
5	NAG	A	801	1	14,14,15	0.65	0	17,19,21	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	809	1	-	4/6/23/26	0/1/1/1
5	NAG	B	801	1	-	5/6/23/26	0/1/1/1
5	NAG	A	802	1	-	5/6/23/26	0/1/1/1
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	801	NAG	C1-O5-C5	6.20	120.59	112.19
5	A	802	NAG	O5-C1-C2	-5.77	102.17	111.29
5	B	809	NAG	C6-C5-C4	-3.53	104.74	113.00
5	A	802	NAG	O5-C5-C6	3.27	112.33	107.20
5	A	802	NAG	C2-N2-C7	3.25	127.53	122.90
5	B	809	NAG	C1-O5-C5	2.86	116.07	112.19
5	B	809	NAG	C3-C4-C5	2.37	114.47	110.24
5	B	801	NAG	C2-N2-C7	2.14	125.95	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	802	NAG	C3-C2-N2-C7
5	B	801	NAG	C3-C2-N2-C7
5	B	801	NAG	C8-C7-N2-C2
5	B	801	NAG	O7-C7-N2-C2
5	B	809	NAG	O5-C5-C6-O6
5	A	802	NAG	O5-C5-C6-O6
5	A	802	NAG	C8-C7-N2-C2
5	B	801	NAG	O5-C5-C6-O6
5	B	809	NAG	C4-C5-C6-O6
5	A	802	NAG	O7-C7-N2-C2
5	B	809	NAG	C8-C7-N2-C2
5	A	802	NAG	C4-C5-C6-O6
5	B	809	NAG	O7-C7-N2-C2
5	A	801	NAG	C8-C7-N2-C2
5	B	801	NAG	C4-C5-C6-O6
5	A	801	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	809	NAG	6	0
5	A	801	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	717/719 (99%)	0.21	17 (2%)	59	57	33, 69, 138, 251	19 (2%)
1	B	719/719 (100%)	0.24	14 (1%)	66	65	32, 67, 129, 227	11 (1%)
All	All	1436/1438 (99%)	0.23	31 (2%)	62	60	32, 68, 131, 251	30 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	GLN	6.2
1	A	411	GLU	4.8
1	B	716	GLU	4.7
1	B	65	SER	4.6
1	A	408	SER	4.4
1	B	512	TYR	3.7
1	A	410	SER	3.5
1	B	513	PHE	3.5
1	B	406	ILE	3.4
1	A	406	ILE	3.3
1	B	382	SER	3.2
1	A	512	TYR	3.0
1	A	78	ASP	3.0
1	A	780	CYS	2.8
1	B	184	ALA	2.7
1	A	412	GLN	2.5
1	A	513	PHE	2.4
1	A	109	GLU	2.4
1	A	708	LEU	2.3
1	B	698	GLU	2.3
1	B	530	ILE	2.2
1	A	125	PHE	2.2
1	A	82	HIS	2.2
1	B	407	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	529	LYS	2.1
1	B	379	ARG	2.1
1	B	663	SER	2.1
1	A	473	GLU	2.0
1	A	524	ALA	2.0
1	A	525	ILE	2.0
1	B	414	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)

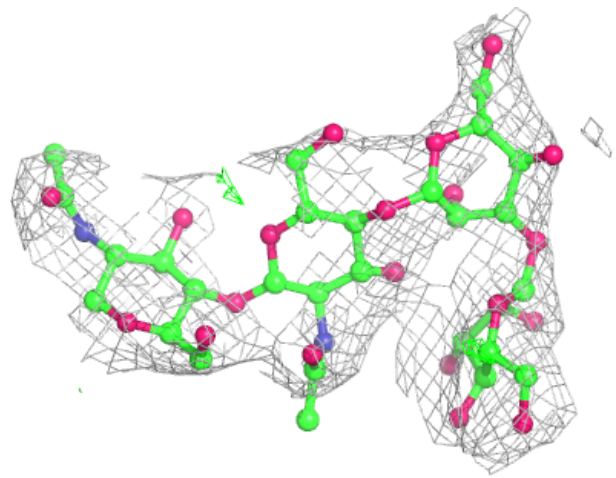
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

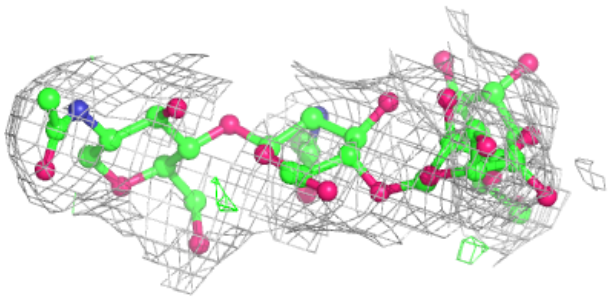
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	C	4	11/12	0.72	0.28	113,113,113,113	0
3	NAG	D	2	14/15	0.73	0.28	131,131,131,131	0
3	NAG	E	2	14/15	0.80	0.34	128,128,128,128	0
4	BMA	F	3	11/12	0.81	0.23	127,127,127,127	0
2	BMA	C	3	11/12	0.83	0.23	135,135,135,135	0
3	NAG	G	2	14/15	0.84	0.26	128,128,128,128	0
4	NAG	F	2	14/15	0.87	0.30	113,113,113,113	0
4	NAG	F	1	14/15	0.87	0.25	83,83,83,83	0
2	NAG	C	2	14/15	0.88	0.20	88,88,88,88	0
2	NAG	C	1	14/15	0.92	0.15	74,74,74,74	0
3	NAG	D	1	14/15	0.92	0.21	77,77,77,77	0
3	NAG	E	1	14/15	0.93	0.19	69,69,69,69	0
3	NAG	G	1	14/15	0.93	0.22	71,71,71,71	0

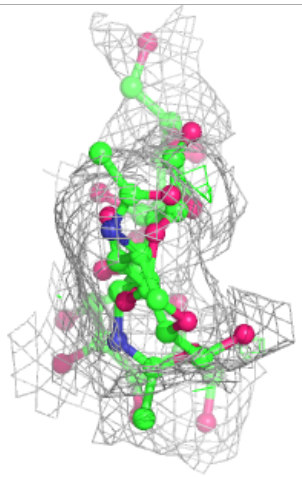
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

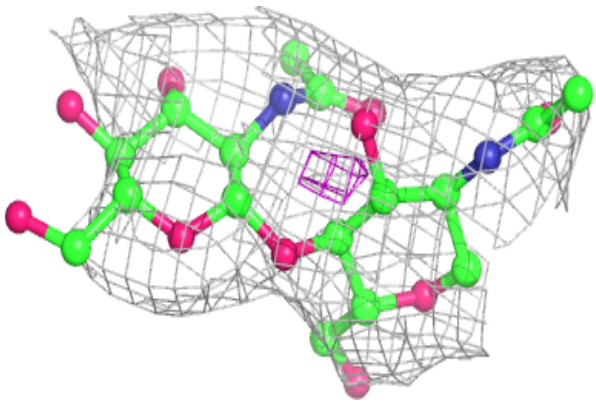


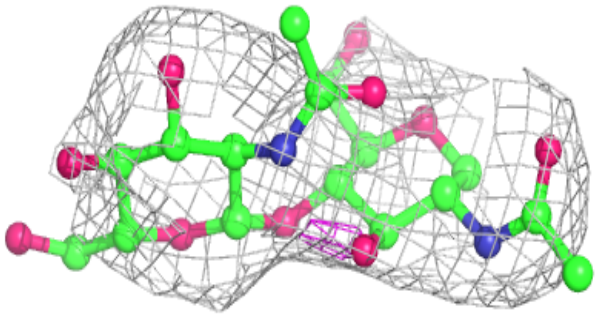


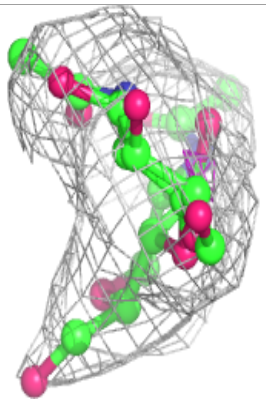


Electron density around Chain D:

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

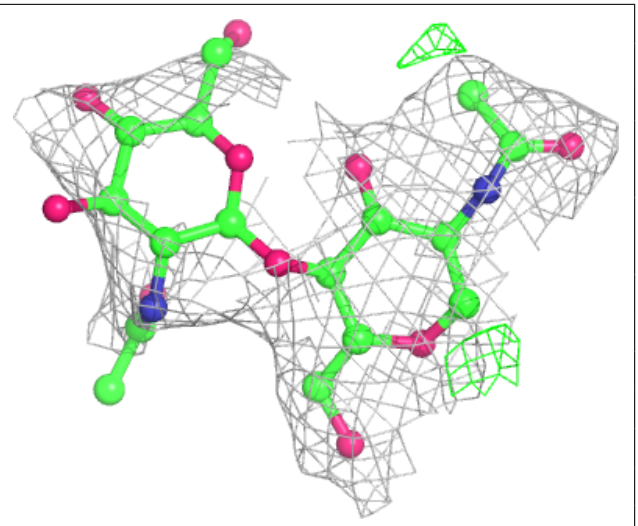


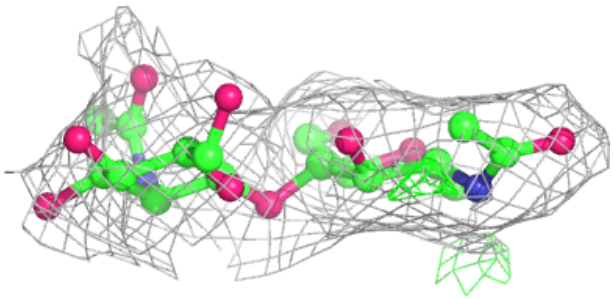


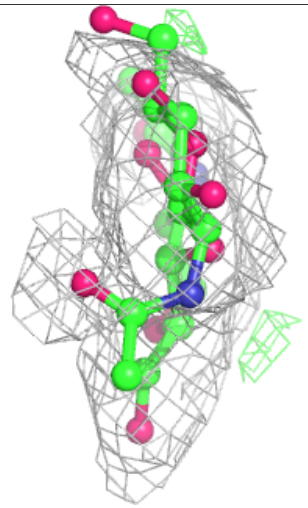


Electron density around Chain E:

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

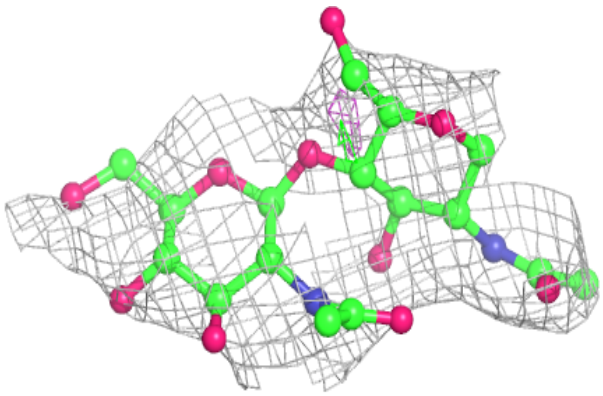


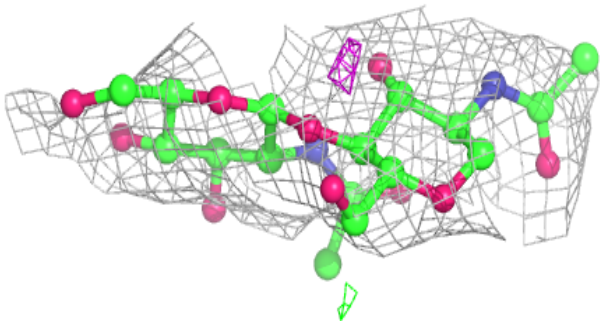


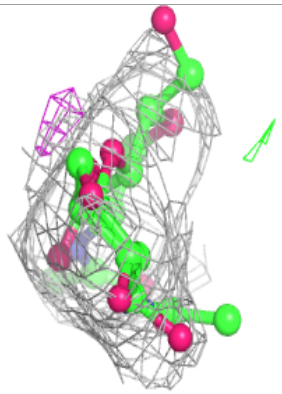


Electron density around Chain G:

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

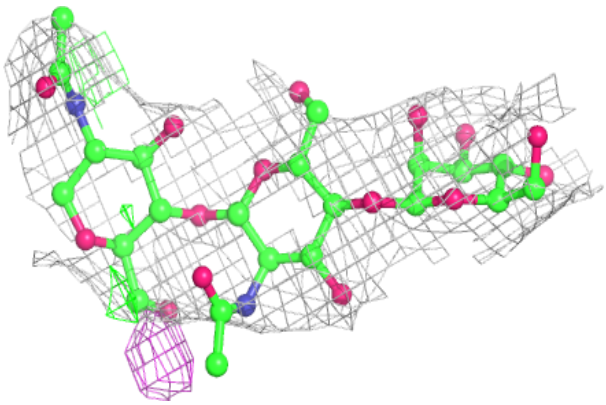


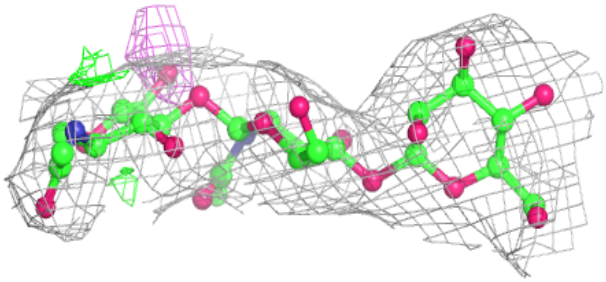


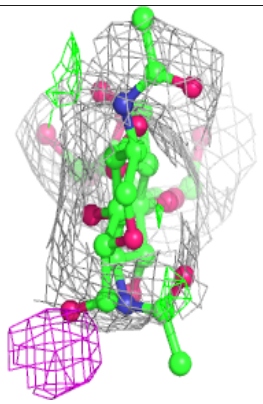


Electron density around Chain F:

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







6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	809	14/15	0.73	0.48	189,189,189,189	0
5	NAG	A	801	14/15	0.82	0.27	109,109,109,109	0
5	NAG	B	801	14/15	0.84	0.25	106,106,106,106	0
5	NAG	A	802	14/15	0.89	0.25	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.