



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 01:30 AM EST

PDB ID : 2GD4
Title : Crystal Structure of the Antithrombin-S195A Factor Xa-Pentasaccharide Complex
Authors : Johnson, D.J.; Li, W.; Adams, T.E.; Huntington, J.A.
Deposited on : 2006-03-15
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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
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

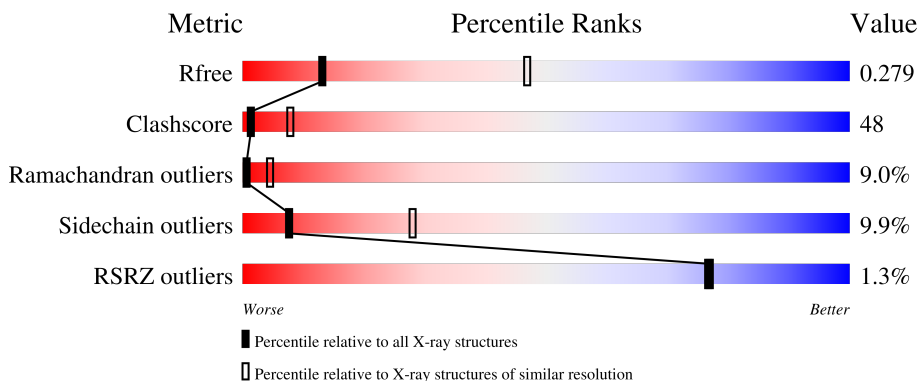
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



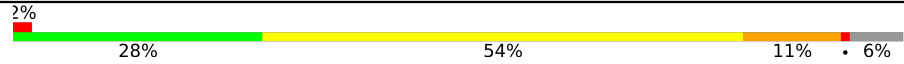
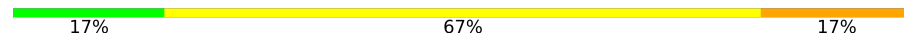
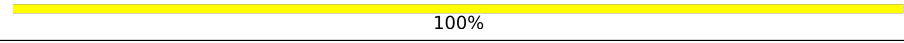

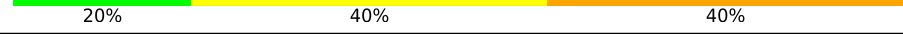
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	58	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 48% 34% 7% 10%</p>
1	L	58	<div style="display: flex; align-items: center;"> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">52% 31% 10% 7%</p>
2	B	241	<div style="display: flex; align-items: center;"> <div style="width: 32%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">32% 55% 10% ..</p>
2	H	241	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">33% 55% 8% ..</p>
3	C	443	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 30% 51% 11% 6%</p>

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Mol	Chain	Length	Quality of chain
3	I	443	
4	D	6	
5	E	2	
6	F	5	
6	G	5	

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
4	MAN	D	4	-	-	-	X
8	NAG	C	701	-	-	-	X
8	NAG	I	701	-	-	-	X

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 11165 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 Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	54	Total	C	N	O	S	0	0	0
			366	219	67	73	7			
1	A	52	Total	C	N	O	S	6	0	0
			349	209	62	71	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	85	MET	-	cloning artifact	UNP P00742
A	85	MET	-	cloning artifact	UNP P00742

- Molecule 2 is a protein called Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	234	Total	C	N	O	S	0	0	0
			1811	1143	312	342	14			
2	B	239	Total	C	N	O	S	3	0	0
			1840	1162	319	345	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	ALA	SER	engineered mutation	UNP P00742
B	104	ALA	SER	engineered mutation	UNP P00742

- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	417	Total	C	N	O	S	14	0	0
			3197	2045	537	599	16			

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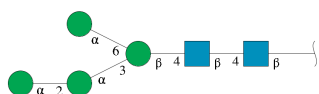
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	418	3200	2048	538	597	17	20	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	engineered mutation	UNP P01008
I	347	ALA	GLU	engineered mutation	UNP P01008
I	348	ALA	LYS	engineered mutation	UNP P01008
I	350	ALA	LYS	engineered mutation	UNP P01008
C	137	ALA	SER	engineered mutation	UNP P01008
C	347	ALA	GLU	engineered mutation	UNP P01008
C	348	ALA	LYS	engineered mutation	UNP P01008
C	350	ALA	LYS	engineered mutation	UNP P01008

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
			Total	C	N	O			
4	D	6	71	40	2	29	0	0	0

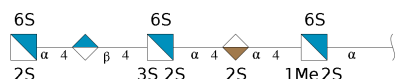
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulf

o-2-(sulfoamino)-alpha-D-glucopyranoside.

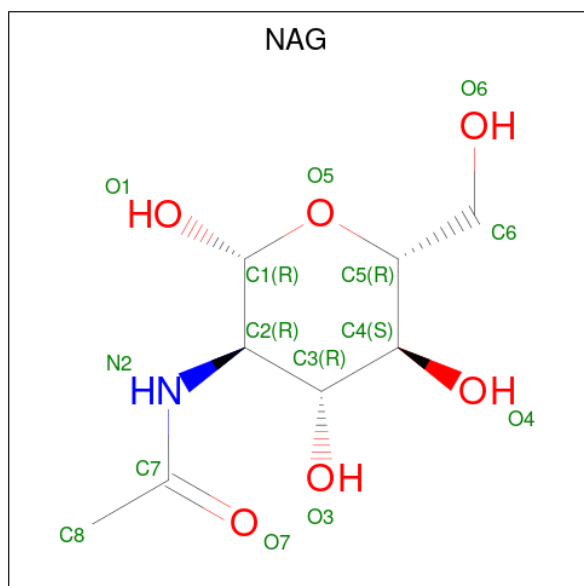


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	5	Total	C	N	O	S	0	0	0
			91	31	3	49	8			
6	G	5	Total	C	N	O	S	0	0	0
			91	31	3	49	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	H	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	3	Total	O	0	0
			3	3		
9	H	10	Total	O	0	0
			10	10		
9	I	22	Total	O	0	0
			22	22		
9	A	2	Total	O	0	0
			2	2		
9	B	9	Total	O	0	0
			9	9		
9	C	17	Total	O	0	0
			17	17		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain L: 



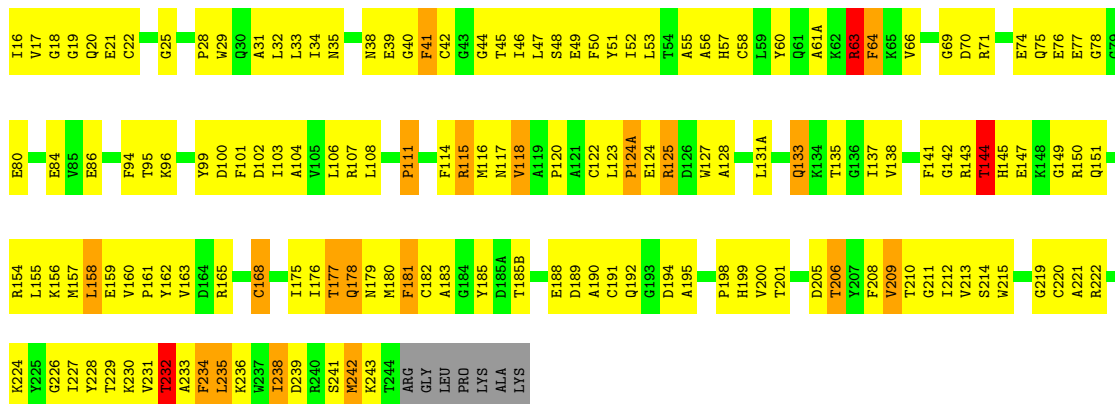
- Molecule 1: Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain A: 



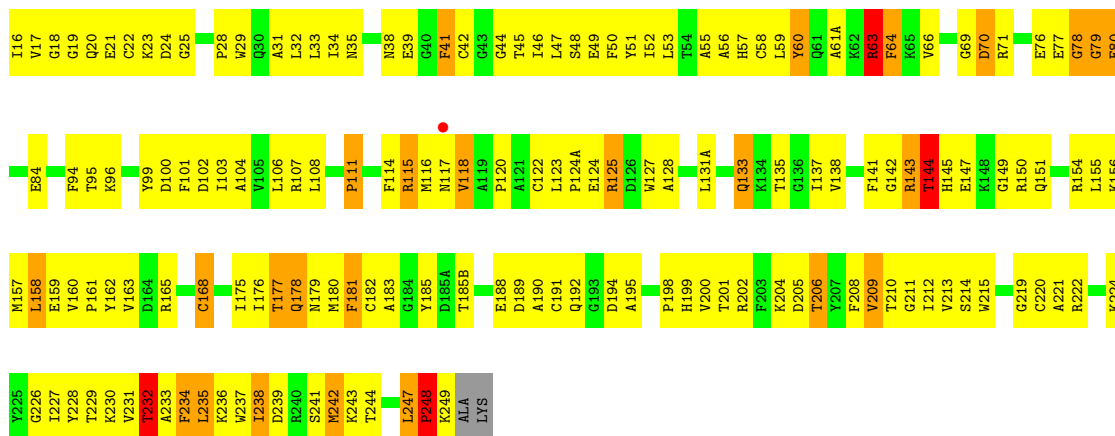
- Molecule 2: Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain H: 

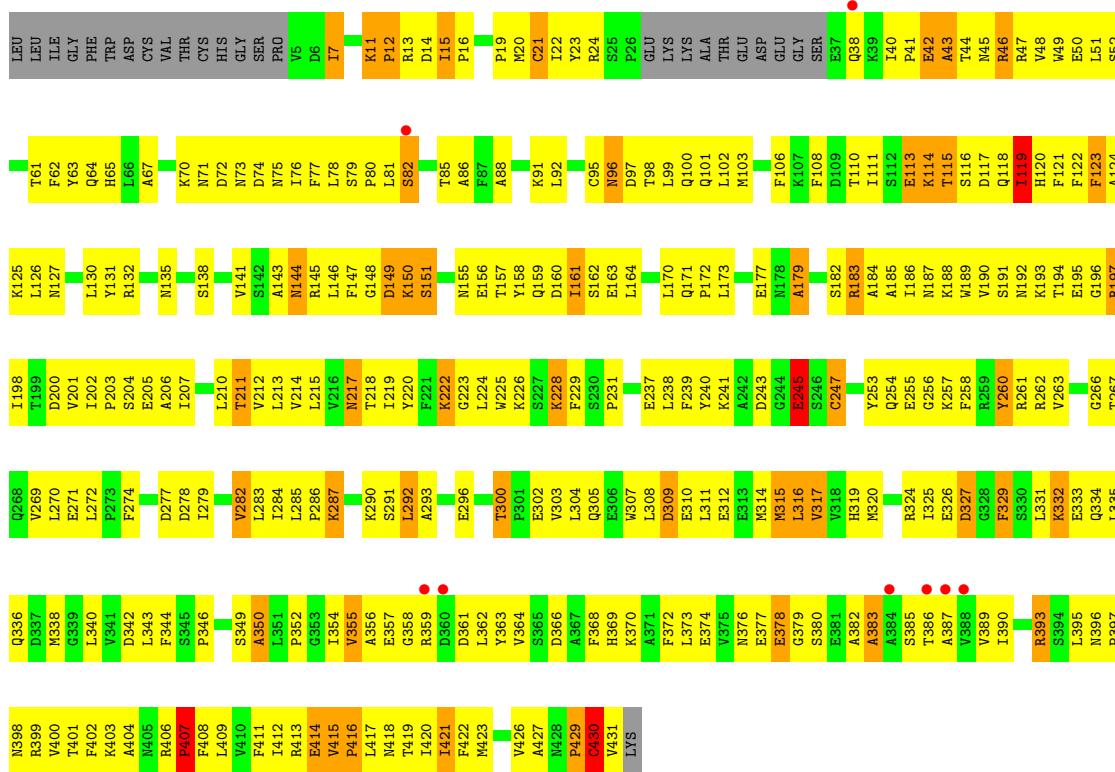


- Molecule 2: Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

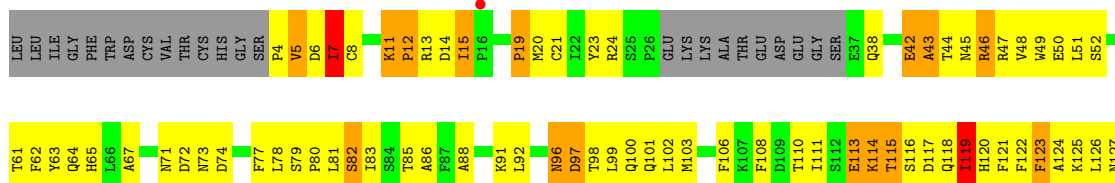
Chain B: 

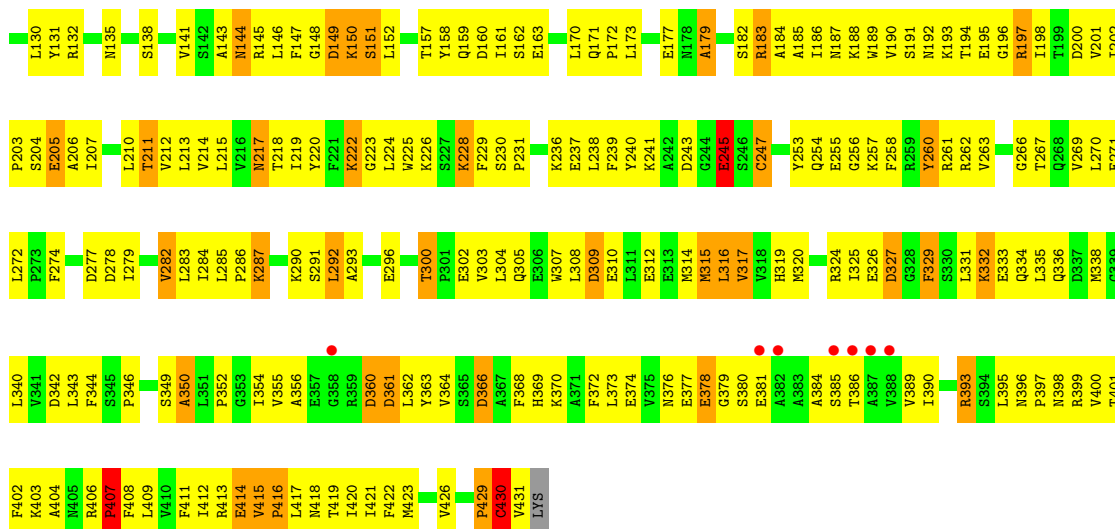


• Molecule 3: Antithrombin-III



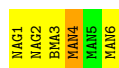
• Molecule 3: Antithrombin-III





- Molecule 4: alpha-D-mannopyranose-(1-2)-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 D: 17% 67% 17%



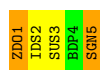
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



- Molecule 6: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain F: 20% 40% 40%



- Molecule 6: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain G: 20% 40% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.26Å 60.59Å 156.17Å 90.00° 113.14° 90.00°	Depositor
Resolution (Å)	36.90 – 3.30 36.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (36.90-3.30) 93.7 (36.92-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.18Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.247 , 0.298 0.235 , 0.279	Depositor DCC
R_{free} test set	1202 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11165	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: IDS, SUS, ZDO, BMA, CA, SGN, NAG, BDP, 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	0.31	0/355	0.61	0/484
1	L	0.31	0/372	0.65	0/506
2	B	0.50	0/1879	0.78	1/2541 (0.0%)
2	H	0.50	0/1849	0.76	1/2500 (0.0%)
3	C	0.43	0/3267	0.72	0/4440
3	I	0.44	0/3263	0.71	0/4435
All	All	0.45	0/10985	0.73	2/14906 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	168	CYS	CA-CB-SG	5.41	123.75	114.00
2	B	168	CYS	CA-CB-SG	5.26	123.47	114.00

There are no chirality outliers.

There are no planarity outliers.

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	349	0	279	30	0
1	L	366	0	296	31	0
2	B	1840	0	1752	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1811	0	1727	176	0
3	C	3200	0	3073	317	0
3	I	3197	0	3072	323	0
4	D	71	0	59	9	0
5	E	28	0	25	8	0
6	F	91	0	27	2	0
6	G	91	0	27	2	0
7	B	1	0	0	0	0
7	H	1	0	0	0	0
8	C	28	0	26	1	0
8	I	28	0	26	1	0
9	A	2	0	0	1	0
9	B	9	0	0	0	0
9	C	17	0	0	2	0
9	H	10	0	0	1	0
9	I	22	0	0	0	0
9	L	3	0	0	0	0
All	All	11165	0	10389	1033	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 48.

All (1033) 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)
4:D:1:NAG:H61	4:D:2:NAG:N2	1.59	1.17
2:B:235:LEU:HD22	2:B:235:LEU:H	1.03	1.14
5:E:1:NAG:H61	5:E:2:NAG:N2	1.59	1.13
2:H:235:LEU:H	2:H:235:LEU:HD22	1.02	1.12
2:B:237:TRP:HD1	2:B:248:PRO:HG2	1.19	1.05
5:E:1:NAG:C6	5:E:2:NAG:HN2	1.71	1.03
4:D:1:NAG:C6	4:D:2:NAG:HN2	1.70	1.03
4:D:3:BMA:H2	4:D:4:MAN:H5	1.42	1.01
3:I:144:ASN:HB3	3:I:217:ASN:HA	1.45	0.98
3:C:144:ASN:HB3	3:C:217:ASN:HA	1.46	0.96
3:C:340:LEU:HD21	3:C:343:LEU:HD23	1.49	0.95
3:I:340:LEU:HD21	3:I:343:LEU:HD23	1.48	0.95
1:A:130:TYR:HE1	2:B:115:ARG:HA	1.32	0.94
2:B:237:TRP:CD1	2:B:248:PRO:HG2	2.06	0.91
3:I:308:LEU:HD13	3:I:413:ARG:NH1	1.85	0.90
3:C:308:LEU:HD13	3:C:413:ARG:NH1	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:389:VAL:HG12	3:I:390:ILE:H	1.37	0.90
3:I:326:GLU:HB3	3:I:372:PHE:HD2	1.37	0.89
3:C:326:GLU:HB3	3:C:372:PHE:HD2	1.36	0.89
2:H:235:LEU:H	2:H:235:LEU:CD2	1.85	0.89
3:C:326:GLU:HB3	3:C:372:PHE:CD2	2.08	0.89
3:I:326:GLU:HB3	3:I:372:PHE:CD2	2.08	0.89
3:C:389:VAL:HG12	3:C:390:ILE:H	1.37	0.88
2:B:235:LEU:HD22	2:B:235:LEU:N	1.88	0.88
2:H:235:LEU:HD22	2:H:235:LEU:N	1.87	0.88
2:B:235:LEU:H	2:B:235:LEU:CD2	1.86	0.88
3:I:144:ASN:HD22	3:I:144:ASN:N	1.73	0.86
3:I:98:THR:HB	3:I:350:ALA:HB3	1.58	0.86
3:I:355:VAL:HG23	3:I:356:ALA:H	1.38	0.86
3:I:144:ASN:HD22	3:I:144:ASN:H	1.22	0.85
3:C:98:THR:HB	3:C:350:ALA:HB3	1.57	0.85
1:L:130:TYR:HE1	2:H:115:ARG:HA	1.39	0.85
3:I:224:LEU:CD1	3:I:379:GLY:HA2	2.07	0.84
2:B:70:ASP:HB2	2:B:80:GLU:HB3	1.59	0.84
3:C:144:ASN:N	3:C:144:ASN:HD22	1.74	0.84
3:C:224:LEU:CD1	3:C:379:GLY:HA2	2.08	0.84
3:C:144:ASN:HD22	3:C:144:ASN:H	1.23	0.83
1:L:134:LYS:HE2	2:H:206:THR:HG23	1.59	0.83
3:I:183:ARG:HH21	3:I:204:SER:HA	1.44	0.82
3:I:23:TYR:HE2	3:I:100:GLN:HG3	1.44	0.82
2:B:219:GLY:HA3	2:B:222:ARG:HE	1.46	0.81
4:D:3:BMA:H2	4:D:4:MAN:C5	2.12	0.80
2:H:219:GLY:HA3	2:H:222:ARG:HE	1.46	0.80
3:C:183:ARG:HH21	3:C:204:SER:HA	1.44	0.80
3:I:267:THR:HG23	3:I:286:PRO:HA	1.64	0.79
3:I:224:LEU:HD12	3:I:379:GLY:HA2	1.65	0.79
3:C:267:THR:HG23	3:C:286:PRO:HA	1.65	0.79
3:C:319:HIS:HB2	3:C:403:LYS:HA	1.65	0.79
3:I:183:ARG:NH2	3:I:204:SER:HA	1.98	0.78
3:C:183:ARG:NH2	3:C:204:SER:HA	1.98	0.78
2:B:38:ASN:O	2:B:39:GLU:HG2	1.83	0.78
3:C:20:MET:HB3	5:E:2:NAG:H5	1.66	0.77
2:H:38:ASN:O	2:H:39:GLU:HG2	1.83	0.77
3:I:319:HIS:HB2	3:I:403:LYS:HA	1.65	0.77
3:C:218:THR:HG22	3:C:370:LYS:HB3	1.66	0.77
3:C:50:GLU:HG2	3:C:111:ILE:HG22	1.66	0.77
3:C:332:LYS:HG2	3:C:366:ASP:OD1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:50:GLU:HG2	3:I:111:ILE:HG22	1.66	0.77
1:A:130:TYR:CE1	2:B:115:ARG:HA	2.19	0.77
2:B:183:ALA:HB3	2:B:228:TYR:CE1	2.20	0.76
3:I:141:VAL:HG11	3:I:194:THR:HA	1.67	0.76
2:H:183:ALA:HB3	2:H:228:TYR:CE1	2.21	0.76
3:I:218:THR:HG22	3:I:370:LYS:HB3	1.67	0.76
3:C:224:LEU:HD12	3:C:379:GLY:HA2	1.65	0.76
3:C:141:VAL:HG11	3:C:194:THR:HA	1.68	0.75
2:H:232:THR:C	2:H:235:LEU:HD21	2.07	0.75
3:I:63:TYR:HE1	3:I:296:GLU:HG2	1.52	0.75
2:H:195:ALA:HA	2:H:213:VAL:HG12	1.68	0.75
1:A:115:TYR:CE1	1:A:131:PRO:HB2	2.22	0.74
1:A:130:TYR:HE1	2:B:115:ARG:CA	1.99	0.74
3:C:407:PRO:HB2	9:C:907:HOH:O	1.86	0.74
3:C:63:TYR:HE1	3:C:296:GLU:HG2	1.52	0.74
2:B:239:ASP:HA	2:B:242:MET:HB2	1.70	0.74
3:I:326:GLU:CB	3:I:372:PHE:HD2	2.01	0.74
2:B:232:THR:C	2:B:235:LEU:HD21	2.07	0.74
1:L:115:TYR:CE1	1:L:131:PRO:HB2	2.22	0.74
3:C:396:ASN:O	3:C:399:ARG:HG3	1.88	0.74
3:C:229:PHE:CE2	3:C:254:GLN:HG2	2.23	0.73
3:I:23:TYR:CE2	3:I:100:GLN:HG3	2.23	0.73
3:I:229:PHE:CE2	3:I:254:GLN:HG2	2.24	0.73
3:C:412:ILE:HB	3:C:422:PHE:HB2	1.70	0.73
2:B:195:ALA:HA	2:B:213:VAL:HG12	1.68	0.73
3:C:326:GLU:CB	3:C:372:PHE:HD2	2.00	0.73
2:H:19:GLY:HA3	2:H:158:LEU:HB2	1.71	0.73
3:I:12:PRO:HG3	3:I:121:PHE:CD2	2.24	0.73
2:B:124(A):PRO:HB2	2:B:128:ALA:HB2	1.70	0.73
3:C:285:LEU:HD22	3:C:404:ALA:HA	1.71	0.72
1:A:134:LYS:HE2	2:B:206:THR:HG23	1.69	0.72
2:B:78:GLY:O	2:B:80:GLU:N	2.22	0.72
2:H:239:ASP:HA	2:H:242:MET:HB2	1.70	0.72
3:I:49:TRP:HA	3:I:417:LEU:HD11	1.71	0.72
3:I:396:ASN:O	3:I:399:ARG:HG3	1.88	0.72
2:B:19:GLY:HA3	2:B:158:LEU:HB2	1.71	0.72
3:I:170:LEU:HD23	3:I:171:GLN:N	2.05	0.72
1:L:129:PRO:O	1:L:131:PRO:HD3	1.90	0.72
3:I:412:ILE:HB	3:I:422:PHE:HB2	1.71	0.72
2:H:124(A):PRO:HB2	2:H:128:ALA:HB2	1.71	0.72
3:C:49:TRP:HA	3:C:417:LEU:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:THR:HB	2:B:53:LEU:HB3	1.72	0.71
1:A:129:PRO:O	1:A:131:PRO:HD3	1.90	0.71
2:H:189:ASP:CG	2:H:190:ALA:H	1.94	0.71
2:H:45:THR:HB	2:H:53:LEU:HB3	1.72	0.71
3:I:285:LEU:HD22	3:I:404:ALA:HA	1.72	0.71
3:I:344:PHE:HD1	3:I:364:VAL:HB	1.55	0.71
3:I:308:LEU:HD13	3:I:413:ARG:HH11	1.55	0.71
2:B:189:ASP:CG	2:B:190:ALA:H	1.93	0.71
3:C:236:LYS:HD2	3:C:236:LYS:N	2.06	0.71
2:H:56:ALA:HB2	2:H:103:ILE:H	1.54	0.70
3:C:170:LEU:HD23	3:C:171:GLN:N	2.05	0.70
2:B:56:ALA:HB2	2:B:103:ILE:H	1.55	0.70
3:C:344:PHE:HD1	3:C:364:VAL:HB	1.55	0.70
3:I:271:GLU:OE2	3:I:413:ARG:NH2	2.24	0.70
2:B:209:VAL:HG22	2:B:231:VAL:HG21	1.73	0.70
3:I:207:ILE:HG23	3:I:211:THR:HG21	1.73	0.70
3:C:308:LEU:HD13	3:C:413:ARG:HH11	1.55	0.70
2:B:128:ALA:HA	2:B:131(A):LEU:HD23	1.73	0.69
2:H:161:PRO:HD3	2:H:185:TYR:CZ	2.27	0.69
2:B:150:ARG:HG2	3:C:253:TYR:CD1	2.28	0.69
3:I:144:ASN:CB	3:I:217:ASN:HA	2.21	0.69
3:C:207:ILE:HG23	3:C:211:THR:HG21	1.73	0.69
3:C:271:GLU:OE2	3:C:413:ARG:NH2	2.26	0.69
3:C:144:ASN:CB	3:C:217:ASN:HA	2.22	0.69
3:C:257:LYS:HA	3:C:314:MET:O	1.93	0.69
2:B:161:PRO:HD3	2:B:185:TYR:CZ	2.27	0.69
3:C:135:ASN:HA	3:C:138:SER:O	1.92	0.69
3:C:47:ARG:HD3	3:C:115:THR:HG23	1.75	0.69
2:H:209:VAL:HG22	2:H:231:VAL:HG21	1.73	0.68
2:H:150:ARG:HG2	3:I:253:TYR:CD1	2.28	0.68
3:C:415:VAL:HG12	3:C:416:PRO:CD	2.23	0.68
2:H:128:ALA:HA	2:H:131(A):LEU:HD23	1.74	0.68
2:B:28:PRO:HG2	2:B:29:TRP:CE3	2.28	0.68
4:D:3:BMA:C2	4:D:4:MAN:H5	2.21	0.68
3:I:135:ASN:HA	3:I:138:SER:O	1.93	0.68
3:I:415:VAL:HG12	3:I:416:PRO:CD	2.23	0.68
2:H:33:LEU:HD23	2:H:66:VAL:HG22	1.74	0.67
2:H:33:LEU:HD12	2:H:42:CYS:CB	2.25	0.67
3:C:148:GLY:O	3:C:172:PRO:HA	1.94	0.67
2:B:32:LEU:HD22	2:B:141:PHE:CE2	2.30	0.67
3:C:218:THR:CG2	3:C:370:LYS:HB3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:429:PRO:HG2	3:C:430:CYS:H	1.60	0.67
3:I:47:ARG:HD3	3:I:115:THR:HG23	1.76	0.67
2:H:28:PRO:HG2	2:H:29:TRP:CE3	2.29	0.67
2:B:33:LEU:HD23	2:B:66:VAL:HG22	1.76	0.67
1:L:130:TYR:HE1	2:H:115:ARG:CA	2.07	0.67
3:I:257:LYS:HA	3:I:314:MET:O	1.94	0.67
2:H:234:PHE:H	2:H:235:LEU:HD22	1.59	0.67
3:I:148:GLY:O	3:I:172:PRO:HA	1.94	0.67
3:I:389:VAL:HG12	3:I:390:ILE:N	2.09	0.67
2:B:33:LEU:HD12	2:B:42:CYS:CB	2.24	0.67
3:I:102:LEU:HD21	3:I:343:LEU:HD22	1.77	0.67
3:C:327:ASP:O	3:C:370:LYS:HD2	1.95	0.67
3:I:144:ASN:N	3:I:144:ASN:ND2	2.41	0.67
3:I:340:LEU:HD21	3:I:343:LEU:CD2	2.23	0.67
2:H:32:LEU:HD22	2:H:141:PHE:CE2	2.30	0.67
2:B:50:PHE:HE1	2:B:111:PRO:HD3	1.60	0.66
3:C:81:LEU:HD21	3:C:127:ASN:OD1	1.95	0.66
3:I:81:LEU:HD21	3:I:127:ASN:OD1	1.95	0.66
3:I:218:THR:CG2	3:I:370:LYS:HB3	2.25	0.66
3:I:327:ASP:O	3:I:370:LYS:HD2	1.95	0.66
2:B:103:ILE:HG12	2:B:104:ALA:N	2.10	0.66
3:C:159:GLN:HE22	3:C:170:LEU:H	1.42	0.66
3:C:145:ARG:CZ	3:C:171:GLN:HB2	2.25	0.66
3:I:85:THR:O	3:I:88:ALA:HB3	1.96	0.66
3:I:145:ARG:CZ	3:I:171:GLN:HB2	2.26	0.66
2:B:47:LEU:HD22	2:B:123:LEU:HD11	1.75	0.66
3:I:159:GLN:HE22	3:I:170:LEU:H	1.42	0.66
2:B:94:PHE:HB2	2:B:101:PHE:O	1.94	0.66
2:H:47:LEU:HD22	2:H:123:LEU:HD11	1.76	0.66
2:H:94:PHE:HB2	2:H:101:PHE:O	1.96	0.66
3:I:429:PRO:HG2	3:I:430:CYS:H	1.60	0.65
3:I:304:LEU:HD21	3:I:420:ILE:HD11	1.78	0.65
2:B:234:PHE:H	2:B:235:LEU:HD22	1.60	0.65
3:I:159:GLN:NE2	3:I:170:LEU:H	1.95	0.65
3:I:266:GLY:HA3	3:I:287:LYS:HE2	1.78	0.65
3:I:379:GLY:O	3:I:380:SER:HB2	1.97	0.65
3:C:85:THR:O	3:C:88:ALA:HB3	1.96	0.65
3:I:414:GLU:OE1	3:I:417:LEU:N	2.30	0.65
3:C:102:LEU:HD21	3:C:343:LEU:HD22	1.78	0.65
2:H:214:SER:HG	2:H:215:TRP:HD1	1.44	0.65
3:C:266:GLY:HA3	3:C:287:LYS:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:222:LYS:NZ	3:I:374:GLU:HG2	2.12	0.65
3:C:12:PRO:HG3	3:C:121:PHE:CD2	2.32	0.65
3:C:159:GLN:NE2	3:C:170:LEU:H	1.95	0.65
3:C:340:LEU:HD21	3:C:343:LEU:CD2	2.24	0.65
2:B:56:ALA:N	2:B:102:ASP:OD1	2.29	0.64
3:C:415:VAL:HG12	3:C:416:PRO:N	2.11	0.64
2:H:103:ILE:HG12	2:H:104:ALA:N	2.11	0.64
3:I:344:PHE:CD1	3:I:364:VAL:HB	2.33	0.64
3:I:415:VAL:HG12	3:I:416:PRO:N	2.11	0.64
2:B:50:PHE:CE1	2:B:111:PRO:HD3	2.32	0.64
2:H:232:THR:O	2:H:235:LEU:HD21	1.98	0.64
3:C:304:LEU:HD21	3:C:420:ILE:HD11	1.79	0.64
3:C:23:TYR:HE2	3:C:100:GLN:HG3	1.63	0.64
3:C:77:PHE:O	3:C:78:LEU:HB3	1.98	0.64
3:I:77:PHE:O	3:I:78:LEU:HB3	1.98	0.63
2:B:122:CYS:HB2	2:B:208:PHE:CD1	2.33	0.63
2:B:232:THR:O	2:B:235:LEU:HD21	1.98	0.63
3:C:204:SER:O	3:C:205:GLU:HB3	1.99	0.63
3:C:332:LYS:HG3	3:C:333:GLU:N	2.13	0.63
3:C:344:PHE:CD1	3:C:364:VAL:HB	2.33	0.63
2:H:50:PHE:HE1	2:H:111:PRO:HD3	1.62	0.63
3:C:414:GLU:OE1	3:C:417:LEU:N	2.30	0.63
3:C:226:LYS:HD2	3:C:277:ASP:OD1	1.98	0.63
1:L:130:TYR:CE1	2:H:115:ARG:HA	2.28	0.63
3:I:47:ARG:HD2	3:I:122:PHE:CZ	2.34	0.63
2:H:56:ALA:N	2:H:102:ASP:OD1	2.30	0.63
2:B:33:LEU:HD12	2:B:42:CYS:HB3	1.81	0.63
3:I:204:SER:O	3:I:205:GLU:HB3	1.99	0.63
3:C:47:ARG:HD2	3:C:122:PHE:CZ	2.34	0.63
3:I:226:LYS:HD2	3:I:277:ASP:OD1	1.99	0.63
3:I:305:GLN:HE21	3:I:309:ASP:CG	2.02	0.63
2:B:158:LEU:HD21	2:B:160:VAL:HG13	1.81	0.63
3:C:379:GLY:O	3:C:380:SER:HB2	1.99	0.63
2:H:158:LEU:HD21	2:H:160:VAL:HG13	1.79	0.62
2:H:158:LEU:HD21	2:H:160:VAL:CG1	2.29	0.62
1:A:131:PRO:HG2	1:A:134:LYS:HG3	1.81	0.62
1:L:129:PRO:HG2	1:L:130:TYR:H	1.65	0.62
2:H:56:ALA:HB3	2:H:102:ASP:HA	1.81	0.62
2:H:122:CYS:HB2	2:H:208:PHE:CD1	2.34	0.62
2:H:231:VAL:O	2:H:233:ALA:N	2.32	0.62
2:B:77:GLU:O	2:B:77:GLU:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:ARG:O	2:H:144:THR:HG23	1.99	0.62
2:B:56:ALA:HB3	2:B:102:ASP:HA	1.81	0.62
3:C:222:LYS:NZ	3:C:374:GLU:HG2	2.13	0.62
3:I:115:THR:C	3:I:117:ASP:H	2.03	0.62
2:B:158:LEU:HD21	2:B:160:VAL:CG1	2.30	0.62
2:H:50:PHE:CE1	2:H:111:PRO:HD3	2.33	0.62
3:I:141:VAL:CG1	3:I:194:THR:HA	2.30	0.62
3:C:115:THR:C	3:C:117:ASP:H	2.03	0.62
2:B:143:ARG:O	2:B:144:THR:HG23	2.00	0.62
2:H:33:LEU:HD12	2:H:42:CYS:HB3	1.81	0.62
2:B:231:VAL:O	2:B:233:ALA:N	2.33	0.61
3:C:305:GLN:HE21	3:C:309:ASP:CG	2.02	0.61
2:H:201:THR:OG1	2:H:210:THR:HG21	2.00	0.61
3:I:406:ARG:HB2	3:I:407:PRO:HD2	1.83	0.61
3:I:414:GLU:OE1	3:I:416:PRO:HD2	2.01	0.61
3:I:163:GLU:HB3	3:I:164:LEU:HD12	1.82	0.61
3:C:144:ASN:N	3:C:144:ASN:ND2	2.42	0.61
3:C:300:THR:H	3:C:303:VAL:HG12	1.66	0.61
3:I:240:TYR:N	3:I:240:TYR:CD2	2.67	0.61
3:I:349:SER:O	3:I:350:ALA:HB2	2.00	0.61
2:B:201:THR:OG1	2:B:210:THR:HG21	2.00	0.61
3:C:243:ASP:OD1	3:C:245:GLU:HB2	2.01	0.61
1:A:129:PRO:HG2	1:A:130:TYR:H	1.64	0.61
1:L:97:ASP:HB2	1:L:123:ALA:HA	1.83	0.61
3:C:240:TYR:N	3:C:240:TYR:CD2	2.67	0.61
3:C:141:VAL:CG1	3:C:194:THR:HA	2.31	0.61
3:C:349:SER:O	3:C:350:ALA:HB2	1.99	0.61
3:C:414:GLU:OE1	3:C:416:PRO:HD2	2.00	0.61
1:A:97:ASP:HB2	1:A:123:ALA:HA	1.82	0.61
3:I:225:TRP:HB2	3:I:379:GLY:HA3	1.82	0.60
3:C:225:TRP:HB2	3:C:379:GLY:HA3	1.83	0.60
3:C:406:ARG:HB2	3:C:407:PRO:HD2	1.83	0.60
2:B:143:ARG:HD3	2:B:149:GLY:O	2.01	0.60
3:I:115:THR:O	3:I:117:ASP:N	2.35	0.60
1:L:131:PRO:HG2	1:L:134:LYS:HG3	1.81	0.60
3:I:270:LEU:HD21	3:I:272:LEU:HD21	1.84	0.60
2:H:143:ARG:HD3	2:H:149:GLY:O	2.01	0.60
3:I:243:ASP:OD1	3:I:245:GLU:HB2	2.01	0.60
3:I:282:VAL:HG13	3:I:411:PHE:HB2	1.84	0.60
3:I:287:LYS:HG3	3:I:290:LYS:HB2	1.83	0.60
3:C:269:VAL:HG11	3:C:307:TRP:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:ILE:HB	2:H:229:THR:HB	1.84	0.60
3:I:210:LEU:O	3:I:212:VAL:HG13	2.02	0.60
3:C:157:THR:O	3:C:160:ASP:N	2.35	0.60
1:L:134:LYS:CE	2:H:206:THR:HG23	2.31	0.60
3:I:222:LYS:HD3	3:I:374:GLU:CG	2.32	0.60
3:C:115:THR:O	3:C:117:ASP:N	2.35	0.60
3:C:287:LYS:HG3	3:C:290:LYS:HB2	1.83	0.60
2:H:35:ASN:OD1	2:H:38:ASN:N	2.35	0.59
2:H:78:GLY:C	2:H:80:GLU:H	2.05	0.59
2:B:138:VAL:HG11	2:B:228:TYR:CE2	2.36	0.59
2:B:212:ILE:HB	2:B:229:THR:HB	1.84	0.59
3:C:270:LEU:HD21	3:C:272:LEU:HD21	1.84	0.59
3:C:270:LEU:O	3:C:282:VAL:HA	2.02	0.59
3:C:389:VAL:HG12	3:C:390:ILE:N	2.14	0.59
3:I:77:PHE:CE2	3:I:373:LEU:HB2	2.37	0.59
3:C:258:PHE:HB2	3:C:316:LEU:HD11	1.84	0.59
3:C:282:VAL:HG13	3:C:411:PHE:HB2	1.83	0.59
2:H:138:VAL:HG11	2:H:228:TYR:CE2	2.37	0.59
3:I:239:PHE:CD2	3:I:429:PRO:HG3	2.38	0.59
3:C:80:PRO:HD2	3:C:421:ILE:O	2.03	0.59
3:C:182:SER:O	3:C:185:ALA:HB3	2.03	0.59
4:D:1:NAG:O7	4:D:1:NAG:O3	2.18	0.59
3:I:300:THR:H	3:I:303:VAL:HG12	1.67	0.59
3:C:239:PHE:CE1	3:C:406:ARG:HA	2.38	0.59
3:I:355:VAL:HG23	3:I:356:ALA:N	2.13	0.59
2:B:211:GLY:HA2	2:B:229:THR:O	2.03	0.59
2:H:31:ALA:HB3	2:H:44:GLY:HA3	1.85	0.59
3:I:270:LEU:O	3:I:282:VAL:HA	2.03	0.59
3:C:77:PHE:CE2	3:C:373:LEU:HB2	2.38	0.59
3:C:210:LEU:O	3:C:212:VAL:HG13	2.02	0.59
2:H:158:LEU:CD2	2:H:160:VAL:HG13	2.33	0.59
2:B:69:GLY:HA3	2:B:118:VAL:HG22	1.83	0.59
2:H:69:GLY:HA3	2:H:118:VAL:HG22	1.84	0.58
3:C:222:LYS:CE	3:C:374:GLU:HG2	2.33	0.58
3:C:222:LYS:HD3	3:C:374:GLU:CG	2.32	0.58
3:C:239:PHE:CD2	3:C:429:PRO:HG3	2.37	0.58
3:I:157:THR:O	3:I:160:ASP:N	2.35	0.58
3:I:269:VAL:HG11	3:I:307:TRP:O	2.02	0.58
2:H:18:GLY:HA3	2:H:188:GLU:OE2	2.03	0.58
3:I:98:THR:CB	3:I:350:ALA:HB3	2.31	0.58
2:B:35:ASN:OD1	2:B:38:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ASP:CG	2:B:190:ALA:N	2.56	0.58
5:E:1:NAG:H61	5:E:2:NAG:HN2	0.74	0.58
3:I:12:PRO:HG3	3:I:121:PHE:CE2	2.37	0.58
3:I:80:PRO:HD2	3:I:421:ILE:O	2.04	0.58
3:I:96:ASN:O	3:I:98:THR:N	2.37	0.58
3:I:182:SER:O	3:I:185:ALA:HB3	2.03	0.58
3:I:164:LEU:HD12	3:I:164:LEU:H	1.67	0.58
3:I:222:LYS:CE	3:I:374:GLU:HG2	2.32	0.58
2:H:189:ASP:CG	2:H:190:ALA:N	2.57	0.58
2:B:19:GLY:CA	2:B:158:LEU:HB2	2.34	0.58
3:C:12:PRO:HG3	3:C:121:PHE:CE2	2.38	0.58
2:B:100:ASP:OD1	2:B:177:THR:HG21	2.05	0.57
2:B:128:ALA:HA	2:B:131(A):LEU:CD2	2.33	0.57
3:C:202:ILE:HD13	3:C:207:ILE:HD11	1.86	0.57
2:H:19:GLY:CA	2:H:158:LEU:HB2	2.34	0.57
2:H:128:ALA:HA	2:H:131(A):LEU:CD2	2.34	0.57
2:H:211:GLY:HA2	2:H:229:THR:O	2.04	0.57
3:I:239:PHE:CE1	3:I:406:ARG:HA	2.39	0.57
3:I:258:PHE:HB2	3:I:316:LEU:HD11	1.85	0.57
2:B:64:PHE:CD1	2:B:64:PHE:N	2.72	0.57
3:C:23:TYR:CE2	3:C:100:GLN:HG3	2.39	0.57
3:C:98:THR:CB	3:C:350:ALA:HB3	2.31	0.57
2:H:100:ASP:OD1	2:H:177:THR:HG21	2.04	0.57
3:C:19:PRO:HA	5:E:2:NAG:O7	2.04	0.57
3:I:179:ALA:O	3:I:182:SER:N	2.37	0.57
3:I:267:THR:HG23	3:I:286:PRO:CA	2.32	0.57
2:B:34:ILE:HA	2:B:39:GLU:O	2.05	0.57
2:B:195:ALA:HA	2:B:213:VAL:CG1	2.35	0.57
3:C:15:ILE:HD13	3:C:15:ILE:H	1.69	0.57
2:H:151:GLN:CD	3:I:399:ARG:HH12	2.07	0.57
3:I:22:ILE:HD12	3:I:22:ILE:O	2.04	0.57
2:H:44:GLY:O	2:H:198:PRO:HD3	2.05	0.57
2:H:33:LEU:HD12	2:H:42:CYS:HB2	1.87	0.57
2:B:44:GLY:O	2:B:198:PRO:HD3	2.05	0.57
2:B:76:GLU:HA	2:B:80:GLU:OE1	2.05	0.57
3:C:147:PHE:HB2	3:C:214:VAL:HG23	1.87	0.57
3:C:71:ASN:HB3	3:C:74:ASP:OD2	2.05	0.56
4:D:1:NAG:H61	4:D:2:NAG:HN2	0.74	0.56
2:H:77:GLU:OE1	2:H:77:GLU:N	2.39	0.56
2:H:125:ARG:O	2:H:128:ALA:HB3	2.05	0.56
3:I:24:ARG:CZ	3:I:113:GLU:OE1	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:164:LEU:HD12	3:I:164:LEU:N	2.20	0.56
3:I:202:ILE:HD13	3:I:207:ILE:HD11	1.86	0.56
3:I:220:TYR:CD1	3:I:372:PHE:HD1	2.23	0.56
2:B:18:GLY:HA3	2:B:188:GLU:OE2	2.04	0.56
2:B:31:ALA:HB3	2:B:44:GLY:HA3	1.86	0.56
2:B:158:LEU:CD2	2:B:160:VAL:HG13	2.34	0.56
3:I:382:ALA:O	3:I:383:ALA:C	2.43	0.56
2:B:133:GLN:O	2:B:162:TYR:HD2	1.89	0.56
3:I:7:ILE:N	3:I:7:ILE:HD13	2.20	0.56
3:I:219:ILE:HG22	3:I:220:TYR:N	2.21	0.56
3:C:332:LYS:HG3	3:C:333:GLU:H	1.70	0.56
2:H:103:ILE:HG13	2:H:212:ILE:CD1	2.35	0.56
2:B:125:ARG:O	2:B:128:ALA:HB3	2.05	0.56
3:C:267:THR:HG23	3:C:286:PRO:CA	2.33	0.56
2:H:195:ALA:HA	2:H:213:VAL:CG1	2.34	0.56
3:I:71:ASN:HB3	3:I:74:ASP:OD2	2.04	0.56
3:C:228:LYS:O	3:C:254:GLN:NE2	2.39	0.56
2:H:34:ILE:HA	2:H:39:GLU:O	2.05	0.56
2:H:64:PHE:N	2:H:64:PHE:CD1	2.73	0.56
2:B:22:CYS:SG	2:B:157:MET:HB3	2.46	0.56
3:C:91:LYS:HG2	3:C:99:LEU:HD11	1.88	0.56
2:H:77:GLU:O	2:H:77:GLU:HG2	2.05	0.56
2:H:158:LEU:CD1	2:H:188:GLU:HB3	2.36	0.56
3:I:207:ILE:HG23	3:I:211:THR:CG2	2.36	0.56
2:B:33:LEU:HD12	2:B:42:CYS:HB2	1.87	0.56
3:I:91:LYS:HG2	3:I:99:LEU:HD11	1.88	0.56
2:H:211:GLY:HA2	2:H:231:VAL:HG23	1.88	0.55
1:A:116:THR:HG23	1:A:127:THR:OG1	2.07	0.55
3:I:222:LYS:HD3	3:I:374:GLU:HG2	1.88	0.55
3:I:331:LEU:HD11	3:I:369:HIS:HB2	1.88	0.55
3:C:421:ILE:HG22	3:C:422:PHE:CD2	2.41	0.55
3:I:147:PHE:HB2	3:I:214:VAL:HG23	1.88	0.55
2:B:47:LEU:HD13	2:B:123:LEU:HD21	1.88	0.55
3:I:213:LEU:HB3	3:I:363:TYR:O	2.07	0.55
2:B:16:ILE:HG22	2:B:17:VAL:N	2.22	0.55
2:B:158:LEU:CD1	2:B:188:GLU:HB3	2.36	0.55
3:C:224:LEU:O	3:C:274:PHE:HA	2.07	0.55
3:I:421:ILE:HG22	3:I:422:PHE:CD2	2.41	0.55
2:B:103:ILE:HG13	2:B:212:ILE:CD1	2.36	0.55
3:C:222:LYS:HD3	3:C:374:GLU:HG2	1.89	0.55
3:C:213:LEU:HB3	3:C:363:TYR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:THR:HG23	1:L:127:THR:OG1	2.07	0.55
2:B:84:GLU:O	2:B:108:LEU:HD23	2.07	0.55
2:H:133:GLN:O	2:H:162:TYR:HD2	1.89	0.55
3:C:77:PHE:CZ	3:C:373:LEU:HB2	2.42	0.55
3:C:331:LEU:HD11	3:C:369:HIS:HB2	1.89	0.55
2:H:181:PHE:CE2	2:H:228:TYR:HB2	2.42	0.55
3:I:327:ASP:O	3:I:370:LYS:HA	2.07	0.55
2:B:123:LEU:N	2:B:123:LEU:HD12	2.22	0.55
2:H:123:LEU:HD12	2:H:123:LEU:N	2.22	0.54
3:I:159:GLN:HE22	3:I:170:LEU:N	2.05	0.54
3:C:236:LYS:HD2	3:C:236:LYS:H	1.70	0.54
3:I:15:ILE:HD13	3:I:15:ILE:H	1.71	0.54
3:I:63:TYR:HB2	3:I:423:MET:SD	2.47	0.54
3:I:228:LYS:O	3:I:254:GLN:NE2	2.41	0.54
3:I:261:ARG:HD2	3:I:262:ARG:N	2.22	0.54
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.88	0.54
3:C:47:ARG:O	3:C:50:GLU:HB3	2.08	0.54
2:H:47:LEU:HD13	2:H:123:LEU:HD21	1.89	0.54
2:H:51:TYR:CE1	2:H:107:ARG:HG3	2.43	0.54
3:C:11:LYS:H	3:C:11:LYS:CE	2.19	0.54
3:C:220:TYR:CD1	3:C:372:PHE:HD1	2.24	0.54
2:H:16:ILE:HG22	2:H:17:VAL:N	2.22	0.54
3:I:340:LEU:CD2	3:I:343:LEU:HD23	2.32	0.54
3:C:327:ASP:O	3:C:370:LYS:HA	2.07	0.54
3:I:96:ASN:OD1	8:I:501:NAG:H61	2.08	0.54
3:I:352:PRO:O	3:I:356:ALA:HB2	2.07	0.54
3:C:179:ALA:O	3:C:182:SER:N	2.37	0.54
3:I:77:PHE:CZ	3:I:373:LEU:HB2	2.42	0.54
3:C:63:TYR:HB2	3:C:423:MET:SD	2.47	0.54
3:C:147:PHE:CZ	3:C:186:ILE:HG23	2.43	0.54
3:C:219:ILE:HG22	3:C:220:TYR:N	2.21	0.54
3:C:285:LEU:CD2	3:C:404:ALA:HA	2.36	0.54
2:B:51:TYR:HA	2:B:106:LEU:O	2.08	0.54
3:C:207:ILE:HG23	3:C:211:THR:CG2	2.37	0.54
3:C:261:ARG:HD2	3:C:262:ARG:N	2.22	0.54
2:H:56:ALA:HB2	2:H:103:ILE:N	2.23	0.54
2:B:46:ILE:HA	2:B:52:ILE:HD13	1.90	0.54
2:B:181:PHE:CE2	2:B:228:TYR:HB2	2.42	0.54
2:H:200:VAL:HG12	2:H:209:VAL:HA	1.89	0.54
3:I:147:PHE:CZ	3:I:186:ILE:HG23	2.43	0.54
3:C:4:PRO:O	3:C:5:VAL:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:CYS:SG	2:H:157:MET:HB3	2.47	0.54
3:I:70:LYS:HD2	3:I:76:ILE:CD1	2.38	0.54
3:I:171:GLN:HG3	3:I:173:LEU:CD2	2.37	0.54
3:I:186:ILE:O	3:I:189:TRP:HB3	2.08	0.54
2:H:51:TYR:HA	2:H:106:LEU:O	2.08	0.53
2:H:84:GLU:O	2:H:108:LEU:HD23	2.08	0.53
3:I:224:LEU:O	3:I:274:PHE:HA	2.07	0.53
3:C:205:GLU:O	3:C:205:GLU:HG2	2.07	0.53
3:C:231:PRO:HA	3:C:377:GLU:OE2	2.08	0.53
3:I:64:GLN:O	3:I:67:ALA:HB3	2.08	0.53
3:C:260:TYR:CE2	3:C:400:VAL:HG11	2.44	0.53
3:I:11:LYS:CE	3:I:11:LYS:H	2.21	0.53
3:C:96:ASN:OD1	8:C:501:NAG:H61	2.09	0.53
3:I:77:PHE:HB2	3:I:325:ILE:HG21	1.91	0.53
3:I:285:LEU:CD2	3:I:404:ALA:HA	2.37	0.53
1:A:135:GLN:HB3	2:B:25:GLY:O	2.08	0.53
3:C:159:GLN:HE22	3:C:170:LEU:N	2.05	0.53
3:C:186:ILE:O	3:C:189:TRP:HB3	2.08	0.53
2:H:55:ALA:HB3	2:H:58:CYS:SG	2.49	0.53
3:I:304:LEU:CD2	3:I:420:ILE:HD11	2.39	0.53
2:B:151:GLN:OE1	3:C:399:ARG:NH1	2.32	0.53
3:C:96:ASN:O	3:C:98:THR:N	2.42	0.53
3:I:47:ARG:O	3:I:50:GLU:HB3	2.08	0.53
2:B:200:VAL:HG12	2:B:209:VAL:HA	1.90	0.53
2:B:209:VAL:CG2	2:B:231:VAL:HG21	2.38	0.53
2:H:143:ARG:NH1	2:H:192:GLN:HB2	2.24	0.53
3:I:255:GLU:HG2	3:I:315:MET:CE	2.39	0.53
3:I:260:TYR:CE2	3:I:400:VAL:HG11	2.44	0.53
3:C:414:GLU:O	3:C:418:ASN:HA	2.09	0.53
2:B:55:ALA:HB3	2:B:58:CYS:SG	2.48	0.53
3:I:229:PHE:CZ	3:I:254:GLN:HG2	2.44	0.52
1:A:131:PRO:HG2	1:A:134:LYS:CG	2.39	0.52
3:C:304:LEU:CD2	3:C:420:ILE:HD11	2.39	0.52
3:I:376:ASN:ND2	3:I:378:GLU:HG3	2.23	0.52
3:C:64:GLN:O	3:C:67:ALA:HB3	2.08	0.52
2:B:103:ILE:HG12	2:B:104:ALA:H	1.73	0.52
2:H:215:TRP:CE2	2:H:227:ILE:HG21	2.45	0.52
3:I:231:PRO:HA	3:I:377:GLU:OE2	2.09	0.52
2:B:47:LEU:O	2:B:48:SER:HB3	2.08	0.52
3:C:255:GLU:HG2	3:C:315:MET:CE	2.39	0.52
2:H:78:GLY:O	2:H:80:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:170:LEU:O	3:I:172:PRO:HD3	2.10	0.52
1:A:138:GLU:H	2:B:116:MET:HE3	1.74	0.52
2:B:247:LEU:H	2:B:248:PRO:HD2	1.74	0.52
2:B:215:TRP:CE2	2:B:227:ILE:HG21	2.45	0.52
3:C:229:PHE:CZ	3:C:254:GLN:HG2	2.44	0.52
2:H:231:VAL:C	2:H:233:ALA:H	2.13	0.52
1:A:138:GLU:H	2:B:116:MET:CE	2.23	0.52
2:B:57:HIS:CE1	2:B:195:ALA:HB1	2.45	0.52
3:C:77:PHE:HB2	3:C:325:ILE:HG21	1.91	0.52
2:B:143:ARG:NH1	2:B:192:GLN:HB2	2.24	0.52
3:C:51:LEU:HD11	3:C:119:ILE:HG13	1.92	0.52
2:H:180:MET:O	2:H:181:PHE:HB3	2.09	0.52
3:I:267:THR:HA	3:I:286:PRO:HA	1.92	0.52
3:I:414:GLU:O	3:I:418:ASN:HA	2.09	0.52
3:C:325:ILE:O	3:C:372:PHE:HA	2.11	0.52
3:C:376:ASN:ND2	3:C:378:GLU:HG3	2.24	0.52
1:L:131:PRO:HG2	1:L:134:LYS:CG	2.39	0.51
2:H:57:HIS:CE1	2:H:195:ALA:HB1	2.45	0.51
2:H:199:HIS:HB3	2:H:211:GLY:O	2.10	0.51
3:C:170:LEU:O	3:C:172:PRO:HD3	2.10	0.51
5:E:1:NAG:O7	5:E:1:NAG:O3	2.18	0.51
2:H:46:ILE:HA	2:H:52:ILE:HD13	1.91	0.51
2:B:51:TYR:CE1	2:B:107:ARG:HG3	2.44	0.51
3:I:51:LEU:HD11	3:I:119:ILE:HG13	1.92	0.51
3:C:415:VAL:HG12	3:C:416:PRO:HD3	1.91	0.51
2:H:47:LEU:O	2:H:48:SER:HB3	2.10	0.51
3:I:316:LEU:HB3	3:I:400:VAL:HB	1.92	0.51
3:I:317:VAL:HB	3:I:401:THR:HG23	1.92	0.51
2:H:209:VAL:CG2	2:H:231:VAL:HG21	2.38	0.51
3:I:148:GLY:N	3:I:170:LEU:HD21	2.26	0.51
3:C:99:LEU:O	3:C:100:GLN:C	2.49	0.51
2:H:188:GLU:O	2:H:189:ASP:HB2	2.11	0.51
2:B:188:GLU:O	2:B:189:ASP:HB2	2.11	0.51
3:I:316:LEU:HA	3:I:400:VAL:O	2.11	0.51
2:B:180:MET:O	2:B:181:PHE:HB3	2.11	0.51
3:C:317:VAL:HB	3:C:401:THR:HG23	1.92	0.51
2:H:241:SER:C	2:H:243:LYS:H	2.14	0.51
3:I:415:VAL:HG12	3:I:416:PRO:HD3	1.91	0.51
3:C:15:ILE:HD13	3:C:15:ILE:O	2.11	0.51
3:C:267:THR:HA	3:C:286:PRO:HA	1.92	0.51
2:H:222:ARG:HB2	2:H:224:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ARG:HB2	2:B:224:LYS:HG3	1.92	0.50
2:B:231:VAL:C	2:B:233:ALA:H	2.13	0.50
3:C:305:GLN:HE21	3:C:309:ASP:CB	2.24	0.50
3:C:207:ILE:HG23	3:C:211:THR:CB	2.41	0.50
2:H:47:LEU:HG	2:H:53:LEU:HB2	1.93	0.50
3:I:81:LEU:HD23	3:I:81:LEU:C	2.32	0.50
3:C:148:GLY:N	3:C:170:LEU:HD21	2.26	0.50
3:C:396:ASN:OD1	3:C:398:ASN:N	2.40	0.50
3:I:284:ILE:HB	3:I:409:LEU:HB2	1.93	0.50
3:I:346:PRO:HG3	3:I:363:TYR:CG	2.47	0.50
2:B:47:LEU:HG	2:B:53:LEU:HB2	1.93	0.50
2:B:181:PHE:HE2	2:B:211:GLY:HA3	1.75	0.50
2:B:199:HIS:HB3	2:B:211:GLY:O	2.11	0.50
2:H:151:GLN:OE1	3:I:399:ARG:NH1	2.31	0.50
2:H:181:PHE:HE2	2:H:211:GLY:HA3	1.75	0.50
2:H:238:ILE:O	2:H:241:SER:N	2.44	0.50
3:I:183:ARG:C	3:I:185:ALA:H	2.15	0.50
3:I:207:ILE:HG23	3:I:211:THR:CB	2.41	0.50
2:B:248:PRO:O	2:B:249:LYS:CB	2.59	0.50
3:C:316:LEU:HA	3:C:400:VAL:O	2.11	0.50
3:I:336:GLN:HA	3:I:340:LEU:O	2.11	0.50
1:A:130:TYR:N	1:A:130:TYR:CD2	2.79	0.50
2:H:191:CYS:O	2:H:194:ASP:HB2	2.12	0.50
3:I:70:LYS:HD2	3:I:76:ILE:HD12	1.94	0.50
3:I:99:LEU:O	3:I:100:GLN:C	2.49	0.50
3:I:305:GLN:HE21	3:I:309:ASP:CB	2.24	0.50
2:B:131(A):LEU:N	2:B:131(A):LEU:HD22	2.27	0.50
2:B:191:CYS:O	2:B:194:ASP:HB2	2.12	0.50
3:C:183:ARG:C	3:C:185:ALA:H	2.15	0.50
3:C:346:PRO:HG3	3:C:363:TYR:CG	2.47	0.50
2:H:61(A):ALA:HA	3:I:397:PRO:CB	2.42	0.50
2:B:135:THR:HG22	2:B:161:PRO:HA	1.94	0.50
3:C:45:ASN:HB3	3:C:48:VAL:HG23	1.94	0.50
3:C:284:ILE:HB	3:C:409:LEU:HB2	1.93	0.50
3:I:12:PRO:HG3	3:I:121:PHE:CG	2.46	0.49
3:I:206:ALA:HB1	3:I:368:PHE:CZ	2.47	0.49
3:C:102:LEU:HD23	3:C:340:LEU:CD1	2.42	0.49
2:H:141:PHE:CE1	2:H:155:LEU:HB2	2.47	0.49
3:I:183:ARG:O	3:I:185:ALA:N	2.45	0.49
2:B:141:PHE:CE1	2:B:155:LEU:HB2	2.46	0.49
2:H:131(A):LEU:HD22	2:H:131(A):LEU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:232:THR:CA	2:H:235:LEU:HD21	2.42	0.49
2:B:163:VAL:HB	2:B:182:CYS:HB3	1.93	0.49
3:C:49:TRP:CA	3:C:417:LEU:HD11	2.42	0.49
1:L:130:TYR:N	1:L:130:TYR:CD2	2.78	0.49
1:L:132:CYS:HA	2:H:120:PRO:HG2	1.94	0.49
3:I:113:GLU:O	3:I:114:LYS:C	2.50	0.49
3:I:238:LEU:HA	3:I:247:CYS:O	2.11	0.49
3:I:325:ILE:O	3:I:372:PHE:HA	2.10	0.49
3:C:113:GLU:O	3:C:114:LYS:C	2.50	0.49
3:C:144:ASN:ND2	9:C:905:HOH:O	2.41	0.49
3:C:336:GLN:HA	3:C:340:LEU:O	2.12	0.49
2:B:232:THR:CA	2:B:235:LEU:HD21	2.43	0.49
2:B:238:ILE:O	2:B:241:SER:N	2.46	0.49
2:B:241:SER:C	2:B:243:LYS:H	2.16	0.49
3:C:183:ARG:O	3:C:185:ALA:N	2.46	0.49
3:C:238:LEU:HA	3:C:247:CYS:O	2.12	0.49
3:I:108:PHE:O	3:I:111:ILE:HG12	2.13	0.49
3:C:81:LEU:C	3:C:81:LEU:HD23	2.32	0.49
3:C:408:PHE:CZ	3:C:426:VAL:HG21	2.48	0.49
3:C:324:ARG:O	3:C:325:ILE:HG13	2.13	0.49
2:H:103:ILE:HG12	2:H:104:ALA:H	1.74	0.49
3:I:79:SER:HB2	3:I:219:ILE:HD12	1.95	0.49
3:I:102:LEU:HD23	3:I:340:LEU:CD1	2.42	0.49
3:I:396:ASN:O	3:I:398:ASN:N	2.46	0.49
3:C:206:ALA:HB1	3:C:368:PHE:CZ	2.48	0.49
3:C:316:LEU:HB3	3:C:400:VAL:HB	1.93	0.49
1:L:135:GLN:HB3	2:H:25:GLY:O	2.13	0.49
2:B:20:GLN:O	2:B:156:LYS:HA	2.13	0.49
2:B:56:ALA:HB2	2:B:103:ILE:N	2.24	0.49
3:C:198:ILE:CD1	3:C:220:TYR:HB2	2.43	0.49
3:I:7:ILE:H	3:I:7:ILE:CD1	2.26	0.48
3:C:108:PHE:O	3:C:111:ILE:HG12	2.13	0.48
1:A:115:TYR:HE1	1:A:131:PRO:HB2	1.74	0.48
3:C:42:GLU:O	3:C:43:ALA:C	2.51	0.48
1:L:115:TYR:HE1	1:L:131:PRO:HB2	1.74	0.48
3:I:61:THR:O	3:I:64:GLN:HB2	2.13	0.48
3:I:171:GLN:HG3	3:I:173:LEU:HD21	1.95	0.48
2:H:135:THR:HG22	2:H:161:PRO:HA	1.94	0.48
2:H:163:VAL:HB	2:H:182:CYS:HB3	1.93	0.48
3:I:396:ASN:OD1	3:I:398:ASN:N	2.40	0.48
2:B:96:LYS:HG2	2:B:99:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:LEU:HD11	2:H:188:GLU:HB3	1.94	0.48
3:I:327:ASP:HB3	3:I:329:PHE:HE1	1.79	0.48
3:C:7:ILE:HD13	3:C:7:ILE:N	2.28	0.48
3:C:46:ARG:CD	3:C:46:ARG:C	2.82	0.48
3:I:45:ASN:HB3	3:I:48:VAL:HG23	1.94	0.48
3:I:49:TRP:CA	3:I:417:LEU:HD11	2.42	0.48
2:B:178:GLN:H	2:B:178:GLN:NE2	2.11	0.48
3:C:24:ARG:CZ	3:C:113:GLU:OE1	2.62	0.48
2:H:215:TRP:C	3:I:393:ARG:HD3	2.34	0.48
3:I:190:VAL:HG21	3:I:201:VAL:HG11	1.95	0.48
3:I:198:ILE:CD1	3:I:220:TYR:HB2	2.43	0.48
3:I:408:PHE:CZ	3:I:426:VAL:HG21	2.48	0.48
1:A:130:TYR:CE1	2:B:115:ARG:CA	2.88	0.48
3:C:100:GLN:O	3:C:103:MET:HB2	2.14	0.48
3:C:327:ASP:HB3	3:C:329:PHE:HE1	1.79	0.48
2:H:201:THR:CB	2:H:210:THR:HG21	2.43	0.48
2:H:231:VAL:C	2:H:233:ALA:N	2.67	0.48
3:I:86:ALA:C	3:I:88:ALA:H	2.17	0.48
3:I:202:ILE:HG12	3:I:368:PHE:CD2	2.49	0.48
3:I:258:PHE:CE1	3:I:272:LEU:HD22	2.49	0.48
2:B:158:LEU:HD11	2:B:188:GLU:HB3	1.94	0.48
2:B:177:THR:C	2:B:179:ASN:H	2.16	0.48
3:C:61:THR:O	3:C:64:GLN:HB2	2.13	0.48
3:C:340:LEU:CD2	3:C:343:LEU:HD23	2.32	0.48
3:I:42:GLU:O	3:I:43:ALA:C	2.51	0.48
2:B:151:GLN:CD	3:C:399:ARG:HH12	2.14	0.48
3:C:71:ASN:O	3:C:73:ASN:N	2.47	0.48
3:C:79:SER:HB3	3:C:82:SER:HB2	1.96	0.48
4:D:2:NAG:O3	4:D:2:NAG:C7	2.62	0.48
2:H:71:ARG:O	2:H:71:ARG:HG2	2.14	0.47
3:I:91:LYS:HG2	3:I:99:LEU:CD1	2.44	0.47
3:I:92:LEU:HD13	3:I:120:HIS:CD2	2.49	0.47
3:I:415:VAL:CG1	3:I:416:PRO:N	2.77	0.47
3:C:79:SER:HB2	3:C:219:ILE:HD12	1.96	0.47
3:I:50:GLU:OE1	3:I:111:ILE:HA	2.13	0.47
3:I:79:SER:HB3	3:I:82:SER:HB2	1.96	0.47
2:B:238:ILE:HG22	2:B:239:ASP:N	2.30	0.47
3:C:190:VAL:HG21	3:C:201:VAL:HG11	1.96	0.47
2:H:178:GLN:H	2:H:178:GLN:NE2	2.12	0.47
3:I:157:THR:O	3:I:158:TYR:C	2.53	0.47
3:I:218:THR:HG22	3:I:370:LYS:CB	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:THR:CB	2:B:210:THR:HG21	2.44	0.47
3:C:238:LEU:HD23	3:C:247:CYS:O	2.15	0.47
3:C:308:LEU:O	3:C:310:GLU:N	2.47	0.47
2:H:195:ALA:HA	2:H:213:VAL:O	2.14	0.47
3:I:193:LYS:C	3:I:195:GLU:H	2.17	0.47
2:B:61(A):ALA:HA	3:C:397:PRO:CB	2.43	0.47
2:B:195:ALA:HA	2:B:213:VAL:O	2.13	0.47
3:C:91:LYS:HG2	3:C:99:LEU:CD1	2.44	0.47
2:H:51:TYR:HE1	2:H:107:ARG:HB2	1.79	0.47
3:I:113:GLU:HB2	6:F:1:ZDO:OSB	2.15	0.47
2:B:231:VAL:C	2:B:233:ALA:N	2.68	0.47
2:B:231:VAL:HG12	2:B:235:LEU:CD1	2.45	0.47
2:B:234:PHE:C	2:B:236:LYS:N	2.67	0.47
3:C:92:LEU:HD13	3:C:120:HIS:CD2	2.49	0.47
3:C:157:THR:O	3:C:158:TYR:C	2.53	0.47
2:H:20:GLN:O	2:H:156:LYS:HA	2.13	0.47
3:I:46:ARG:C	3:I:46:ARG:CD	2.82	0.47
3:I:385:SER:O	3:I:387:ALA:N	2.47	0.47
2:H:96:LYS:HG2	2:H:99:TYR:CE1	2.49	0.47
3:I:198:ILE:HG23	3:I:370:LYS:HG2	1.96	0.47
2:B:133:GLN:HE21	2:B:133:GLN:HB2	1.60	0.47
3:C:50:GLU:OE1	3:C:111:ILE:HA	2.14	0.47
3:I:238:LEU:HD23	3:I:247:CYS:O	2.15	0.47
3:C:11:LYS:H	3:C:11:LYS:HE2	1.78	0.47
3:C:86:ALA:C	3:C:88:ALA:H	2.17	0.47
2:H:232:THR:HA	2:H:235:LEU:HD21	1.96	0.47
3:I:79:SER:CB	3:I:219:ILE:HD12	2.45	0.47
3:C:329:PHE:N	3:C:329:PHE:CD1	2.82	0.47
2:H:116:MET:O	2:H:118:VAL:HG23	2.15	0.47
2:B:29:TRP:HE3	2:B:120:PRO:O	1.98	0.47
3:C:396:ASN:O	3:C:398:ASN:N	2.47	0.47
2:H:231:VAL:HG12	2:H:235:LEU:CD1	2.45	0.46
3:I:225:TRP:HA	3:I:225:TRP:CE3	2.50	0.46
3:I:308:LEU:O	3:I:310:GLU:N	2.48	0.46
3:C:190:VAL:HG11	3:C:198:ILE:HG22	1.97	0.46
3:C:225:TRP:CE3	3:C:225:TRP:HA	2.50	0.46
3:I:100:GLN:O	3:I:103:MET:HB2	2.14	0.46
3:I:324:ARG:O	3:I:325:ILE:HG13	2.14	0.46
2:B:71:ARG:O	2:B:71:ARG:HG2	2.14	0.46
3:C:159:GLN:CD	3:C:170:LEU:H	2.18	0.46
2:H:182:CYS:HA	2:H:226:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:238:ILE:HG22	2:H:239:ASP:N	2.31	0.46
3:I:20:MET:O	3:I:21:CYS:O	2.34	0.46
3:I:71:ASN:O	3:I:73:ASN:N	2.48	0.46
2:B:214:SER:OG	2:B:215:TRP:HD1	1.98	0.46
3:C:121:PHE:O	3:C:124:ALA:HB3	2.15	0.46
3:C:130:LEU:HD11	3:C:419:THR:HG21	1.96	0.46
3:C:150:LYS:O	3:C:151:SER:C	2.54	0.46
3:C:258:PHE:CE1	3:C:272:LEU:HD22	2.49	0.46
2:H:234:PHE:C	2:H:236:LYS:N	2.67	0.46
3:I:71:ASN:C	3:I:73:ASN:N	2.69	0.46
3:I:121:PHE:O	3:I:124:ALA:HB3	2.15	0.46
3:I:159:GLN:CD	3:I:170:LEU:H	2.18	0.46
2:B:137:ILE:O	2:B:137:ILE:HG22	2.15	0.46
3:C:15:ILE:HD13	3:C:15:ILE:N	2.30	0.46
3:C:115:THR:C	3:C:117:ASP:N	2.68	0.46
3:C:193:LYS:C	3:C:195:GLU:H	2.17	0.46
3:I:329:PHE:N	3:I:329:PHE:CD1	2.84	0.46
3:I:346:PRO:HG3	3:I:363:TYR:CD1	2.51	0.46
2:B:78:GLY:O	2:B:79:GLY:C	2.53	0.46
2:B:182:CYS:HA	2:B:226:GLY:O	2.16	0.46
3:C:71:ASN:C	3:C:73:ASN:N	2.68	0.46
3:C:79:SER:CB	3:C:219:ILE:HD12	2.46	0.46
3:C:113:GLU:HB2	6:G:1:ZDO:OSB	2.15	0.46
3:C:157:THR:HG21	5:E:1:NAG:H62	1.98	0.46
3:C:334:GLN:O	3:C:335:LEU:C	2.54	0.46
2:H:211:GLY:CA	2:H:231:VAL:HG23	2.45	0.46
1:A:132:CYS:HA	2:B:120:PRO:HG2	1.98	0.46
3:C:346:PRO:HG3	3:C:363:TYR:CD1	2.51	0.46
2:H:177:THR:C	2:H:179:ASN:H	2.18	0.46
3:I:115:THR:C	3:I:117:ASP:N	2.67	0.46
3:I:130:LEU:HD11	3:I:419:THR:HG21	1.96	0.46
3:I:150:LYS:O	3:I:151:SER:C	2.55	0.46
1:A:115:TYR:HE2	9:A:27:HOH:O	1.99	0.46
2:B:99:TYR:CG	3:C:390:ILE:HG21	2.51	0.46
3:C:82:SER:OG	3:C:219:ILE:HD11	2.16	0.46
3:C:122:PHE:O	3:C:123:PHE:C	2.55	0.46
3:C:278:ASP:O	3:C:279:ILE:HD13	2.16	0.46
2:H:29:TRP:HE3	2:H:120:PRO:O	1.97	0.46
2:H:161:PRO:HD3	2:H:185:TYR:CE1	2.51	0.46
2:B:180:MET:CE	2:B:215:TRP:HE1	2.29	0.46
2:B:211:GLY:CA	2:B:231:VAL:HG23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:THR:HA	2:B:235:LEU:HD21	1.97	0.46
3:C:71:ASN:C	3:C:73:ASN:H	2.19	0.46
3:C:102:LEU:HD23	3:C:340:LEU:HD11	1.98	0.46
3:C:198:ILE:HG23	3:C:370:LYS:HG2	1.97	0.46
2:H:52:ILE:HB	2:H:106:LEU:HB2	1.98	0.46
3:I:349:SER:O	3:I:350:ALA:CB	2.64	0.46
1:A:134:LYS:CE	2:B:206:THR:HG23	2.42	0.46
2:B:183:ALA:HB3	2:B:228:TYR:HE1	1.76	0.46
2:H:180:MET:CE	2:H:215:TRP:HE1	2.29	0.45
3:I:11:LYS:H	3:I:11:LYS:HE2	1.81	0.45
3:I:15:ILE:HD13	3:I:15:ILE:N	2.31	0.45
3:I:255:GLU:HG2	3:I:315:MET:HE1	1.97	0.45
2:B:51:TYR:HE1	2:B:107:ARG:HB2	1.81	0.45
3:C:81:LEU:HD11	3:C:126:LEU:CD2	2.47	0.45
3:C:202:ILE:HG12	3:C:368:PHE:CD2	2.50	0.45
5:E:2:NAG:O3	5:E:2:NAG:C7	2.63	0.45
2:H:124:GLU:O	2:H:125:ARG:C	2.54	0.45
2:H:145:HIS:O	2:H:147:GLU:C	2.54	0.45
3:I:157:THR:HG21	4:D:1:NAG:H62	1.98	0.45
3:I:292:LEU:HD11	3:I:409:LEU:HG	1.98	0.45
2:B:50:PHE:CE1	2:B:111:PRO:HB3	2.51	0.45
3:C:146:LEU:HD11	3:C:215:LEU:CD1	2.47	0.45
3:C:220:TYR:OH	3:C:222:LYS:HE2	2.16	0.45
3:I:190:VAL:HG11	3:I:198:ILE:HG22	1.97	0.45
3:I:334:GLN:O	3:I:335:LEU:C	2.53	0.45
2:B:145:HIS:O	2:B:147:GLU:C	2.54	0.45
2:B:215:TRP:HA	3:C:393:ARG:HD3	1.97	0.45
3:C:222:LYS:CD	3:C:374:GLU:HG2	2.46	0.45
3:I:222:LYS:CD	3:I:374:GLU:HG2	2.46	0.45
3:I:430:CYS:O	3:I:431:VAL:CB	2.65	0.45
2:B:64:PHE:N	2:B:64:PHE:HD1	2.14	0.45
3:C:44:THR:HG21	3:C:417:LEU:HD13	1.99	0.45
3:C:65:HIS:NE2	3:C:338:MET:HG2	2.31	0.45
3:C:293:ALA:O	3:C:296:GLU:N	2.49	0.45
3:I:15:ILE:HD13	3:I:15:ILE:O	2.15	0.45
3:I:71:ASN:C	3:I:73:ASN:H	2.20	0.45
3:I:102:LEU:HD23	3:I:340:LEU:HD11	1.99	0.45
3:I:293:ALA:O	3:I:296:GLU:N	2.50	0.45
3:C:6:ASP:O	3:C:8:CYS:N	2.50	0.45
2:H:175:ILE:HG12	2:H:176:ILE:H	1.82	0.45
3:I:81:LEU:HD11	3:I:126:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:LEU:HD23	2:H:158:LEU:O	2.17	0.45
3:I:430:CYS:O	3:I:431:VAL:HG23	2.17	0.45
2:B:160:VAL:HA	2:B:161:PRO:HD3	1.81	0.45
2:B:161:PRO:HD3	2:B:185:TYR:CE1	2.51	0.45
3:C:270:LEU:HD23	3:C:283:LEU:HD12	1.98	0.45
3:C:430:CYS:O	3:C:431:VAL:CB	2.64	0.45
3:C:430:CYS:O	3:C:431:VAL:HG23	2.16	0.45
2:H:64:PHE:N	2:H:64:PHE:HD1	2.14	0.45
3:I:220:TYR:OH	3:I:222:LYS:HE2	2.17	0.45
1:A:125:ILE:O	1:A:126:PRO:O	2.35	0.45
2:B:124:GLU:O	2:B:125:ARG:C	2.55	0.45
2:B:202:ARG:NH2	2:B:204:LYS:O	2.46	0.45
3:C:183:ARG:NH2	3:C:204:SER:CA	2.77	0.45
3:C:395:LEU:O	3:C:397:PRO:HD3	2.16	0.45
3:I:65:HIS:NE2	3:I:338:MET:HG2	2.32	0.45
3:I:256:GLY:C	3:I:315:MET:HE3	2.38	0.45
3:C:225:TRP:HA	3:C:225:TRP:HE3	1.82	0.45
3:C:292:LEU:HD11	3:C:409:LEU:HG	1.98	0.45
1:L:125:ILE:O	1:L:126:PRO:O	2.35	0.45
2:H:50:PHE:CE1	2:H:111:PRO:HB3	2.52	0.45
2:H:137:ILE:O	2:H:137:ILE:HG22	2.17	0.45
2:H:214:SER:OG	2:H:215:TRP:HD1	1.97	0.45
3:I:192:ASN:O	3:I:192:ASN:OD1	2.35	0.45
3:I:395:LEU:O	3:I:397:PRO:HD3	2.17	0.45
2:B:116:MET:O	2:B:118:VAL:HG23	2.16	0.45
2:B:215:TRP:C	3:C:393:ARG:HD3	2.37	0.45
2:B:220:CYS:O	2:B:221:ALA:HB3	2.16	0.45
3:C:255:GLU:HG2	3:C:315:MET:HE2	1.99	0.45
3:I:291:SER:O	3:I:293:ALA:N	2.50	0.44
1:A:110:SER:O	1:A:111:CYS:SG	2.75	0.44
2:B:52:ILE:HB	2:B:106:LEU:HB2	1.98	0.44
2:B:63:ARG:HG2	2:B:63:ARG:HH21	1.82	0.44
2:B:175:ILE:HG12	2:B:176:ILE:H	1.82	0.44
3:C:80:PRO:HG2	3:C:81:LEU:H	1.82	0.44
3:C:300:THR:OG1	3:C:302:GLU:HB2	2.16	0.44
3:I:212:VAL:HG23	3:I:213:LEU:N	2.33	0.44
2:B:247:LEU:N	2:B:248:PRO:HD2	2.32	0.44
3:C:145:ARG:NE	3:C:171:GLN:HB2	2.32	0.44
3:I:12:PRO:C	3:I:14:ASP:N	2.70	0.44
3:C:12:PRO:C	3:C:14:ASP:N	2.69	0.44
3:I:204:SER:O	3:I:205:GLU:CB	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:396:ASN:O	3:I:397:PRO:C	2.55	0.44
2:B:230:LYS:HG2	2:B:232:THR:HG23	2.00	0.44
3:C:143:ALA:HB2	3:C:194:THR:CG2	2.48	0.44
1:L:130:TYR:HD1	2:H:114:PHE:HB3	1.81	0.44
3:I:143:ALA:HB2	3:I:194:THR:CG2	2.47	0.44
3:I:145:ARG:NE	3:I:171:GLN:HB2	2.32	0.44
3:I:146:LEU:HD11	3:I:215:LEU:CD1	2.47	0.44
3:C:106:PHE:HB3	3:C:108:PHE:CZ	2.52	0.44
1:L:130:TYR:N	1:L:130:TYR:HD2	2.15	0.44
2:H:195:ALA:HB2	3:I:393:ARG:C	2.38	0.44
3:I:122:PHE:O	3:I:125:LYS:N	2.51	0.44
3:I:225:TRP:HA	3:I:225:TRP:HE3	1.83	0.44
3:I:270:LEU:HD23	3:I:283:LEU:HD12	1.99	0.44
3:I:278:ASP:O	3:I:279:ILE:HD13	2.18	0.44
2:B:116:MET:O	2:B:117:ASN:HB2	2.17	0.44
3:C:192:ASN:OD1	3:C:192:ASN:O	2.36	0.44
3:C:291:SER:O	3:C:293:ALA:N	2.50	0.44
3:C:376:ASN:HD21	3:C:378:GLU:HG3	1.83	0.44
2:H:220:CYS:O	2:H:221:ALA:HB3	2.18	0.44
3:I:44:THR:HG21	3:I:417:LEU:HD13	1.99	0.44
3:C:12:PRO:HG3	3:C:121:PHE:CG	2.52	0.44
3:C:283:LEU:HD11	3:C:320:MET:CE	2.48	0.44
2:H:18:GLY:CA	2:H:188:GLU:OE2	2.66	0.43
3:I:147:PHE:O	3:I:213:LEU:HD12	2.18	0.43
3:I:183:ARG:NH2	3:I:204:SER:CA	2.77	0.43
3:I:402:PHE:CE1	3:I:404:ALA:HB2	2.53	0.43
2:B:127:TRP:CZ3	2:B:131(A):LEU:HD21	2.53	0.43
3:C:86:ALA:C	3:C:88:ALA:N	2.72	0.43
3:C:191:SER:C	3:C:193:LYS:H	2.21	0.43
1:L:86:ARG:O	1:L:87:LYS:CB	2.66	0.43
1:L:110:SER:O	1:L:111:CYS:SG	2.76	0.43
3:I:7:ILE:N	3:I:7:ILE:CD1	2.80	0.43
3:I:46:ARG:HD3	3:I:46:ARG:O	2.18	0.43
3:I:82:SER:OG	3:I:219:ILE:HD11	2.17	0.43
3:I:191:SER:C	3:I:193:LYS:H	2.21	0.43
1:A:130:TYR:HD1	2:B:114:PHE:HB3	1.83	0.43
1:A:138:GLU:CB	2:B:116:MET:HE1	2.48	0.43
3:C:131:TYR:CZ	3:C:135:ASN:ND2	2.87	0.43
3:C:187:ASN:O	3:C:188:LYS:C	2.57	0.43
3:C:212:VAL:HG23	3:C:213:LEU:N	2.33	0.43
1:L:95:ASP:O	1:L:122:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:80:PRO:HG2	3:I:81:LEU:H	1.83	0.43
3:I:187:ASN:O	3:I:188:LYS:C	2.57	0.43
3:I:355:VAL:CG2	3:I:356:ALA:H	2.21	0.43
2:B:239:ASP:C	2:B:239:ASP:OD2	2.57	0.43
3:C:77:PHE:CE1	3:C:373:LEU:HD22	2.53	0.43
3:C:127:ASN:O	3:C:131:TYR:N	2.51	0.43
3:C:349:SER:OG	3:C:350:ALA:N	2.51	0.43
2:H:127:TRP:CZ3	2:H:131(A):LEU:HD21	2.54	0.43
3:I:106:PHE:HB3	3:I:108:PHE:CZ	2.53	0.43
3:I:122:PHE:O	3:I:123:PHE:C	2.54	0.43
3:I:131:TYR:CZ	3:I:135:ASN:ND2	2.86	0.43
3:I:283:LEU:HD11	3:I:320:MET:CE	2.49	0.43
2:B:158:LEU:HD23	2:B:158:LEU:O	2.19	0.43
2:B:195:ALA:HB2	3:C:393:ARG:C	2.38	0.43
3:C:12:PRO:O	3:C:13:ARG:C	2.56	0.43
3:C:48:VAL:HG21	6:G:5:SGN:O5S	2.18	0.43
3:C:396:ASN:O	3:C:397:PRO:C	2.55	0.43
2:H:183:ALA:HB3	2:H:228:TYR:HE1	1.77	0.43
3:C:183:ARG:C	3:C:185:ALA:N	2.72	0.43
3:C:203:PRO:HG2	3:C:206:ALA:HB2	2.00	0.43
2:H:63:ARG:HG2	2:H:63:ARG:HH21	1.82	0.43
2:H:116:MET:O	2:H:117:ASN:HB2	2.18	0.43
2:H:239:ASP:OD2	2:H:239:ASP:C	2.56	0.43
3:I:7:ILE:HD13	3:I:7:ILE:H	1.81	0.43
3:I:200:ASP:O	3:I:201:VAL:C	2.56	0.43
3:I:203:PRO:HG2	3:I:206:ALA:HB2	2.00	0.43
3:C:147:PHE:CE2	3:C:186:ILE:HG23	2.54	0.43
1:L:86:ARG:O	1:L:86:ARG:HG3	2.18	0.43
2:H:77:GLU:OE1	2:H:80:GLU:OE1	2.36	0.43
3:I:271:GLU:HA	3:I:282:VAL:HA	2.01	0.43
3:I:300:THR:OG1	3:I:302:GLU:HB2	2.18	0.43
2:B:122:CYS:HB2	2:B:208:PHE:HD1	1.81	0.43
3:C:121:PHE:CD2	3:C:121:PHE:C	2.91	0.43
3:C:204:SER:O	3:C:205:GLU:CB	2.63	0.43
3:I:376:ASN:HD21	3:I:378:GLU:HG3	1.83	0.43
3:C:183:ARG:O	3:C:186:ILE:N	2.47	0.43
3:C:350:ALA:C	3:C:352:PRO:CD	2.87	0.43
3:I:75:ASN:OD1	3:I:427:ALA:N	2.50	0.43
3:I:183:ARG:C	3:I:185:ALA:N	2.71	0.43
3:I:260:TYR:HB2	3:I:316:LEU:HD21	2.00	0.43
3:C:349:SER:O	3:C:350:ALA:CB	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:GLU:C	2:H:75:GLN:HG3	2.38	0.43
3:I:121:PHE:CD2	3:I:121:PHE:C	2.91	0.43
3:I:350:ALA:C	3:I:352:PRO:CD	2.87	0.43
1:A:95:ASP:O	1:A:122:LYS:HB3	2.18	0.43
1:A:130:TYR:N	1:A:130:TYR:HD2	2.16	0.43
2:B:16:ILE:CG2	2:B:17:VAL:N	2.81	0.43
2:B:18:GLY:CA	2:B:188:GLU:OE2	2.67	0.43
1:L:138:GLU:H	2:H:116:MET:CE	2.32	0.42
3:I:430:CYS:O	3:I:431:VAL:HB	2.19	0.42
3:C:46:ARG:O	3:C:46:ARG:HD3	2.18	0.42
3:C:260:TYR:HB2	3:C:316:LEU:HD21	2.00	0.42
2:H:63:ARG:HG2	2:H:63:ARG:NH2	2.34	0.42
3:I:77:PHE:CE1	3:I:373:LEU:HD22	2.54	0.42
3:I:86:ALA:C	3:I:88:ALA:N	2.72	0.42
3:I:172:PRO:C	3:I:173:LEU:HD22	2.40	0.42
2:B:247:LEU:O	2:B:248:PRO:O	2.37	0.42
3:C:200:ASP:O	3:C:201:VAL:C	2.56	0.42
2:H:41:PHE:O	2:H:42:CYS:SG	2.77	0.42
3:I:47:ARG:CZ	3:I:114:LYS:HD3	2.49	0.42
3:I:127:ASN:O	3:I:131:TYR:N	2.53	0.42
3:I:349:SER:OG	3:I:350:ALA:N	2.52	0.42
2:H:150:ARG:HA	3:I:253:TYR:CE1	2.55	0.42
2:H:160:VAL:HA	2:H:161:PRO:HD3	1.82	0.42
3:I:12:PRO:O	3:I:13:ARG:C	2.58	0.42
3:I:22:ILE:HD13	3:I:24:ARG:CZ	2.50	0.42
3:C:47:ARG:CZ	3:C:114:LYS:HD3	2.50	0.42
3:C:81:LEU:HD11	3:C:126:LEU:HD21	2.00	0.42
3:I:48:VAL:HG21	6:F:5:SGN:O5S	2.19	0.42
3:I:326:GLU:HB3	3:I:372:PHE:CE2	2.51	0.42
2:B:41:PHE:HB2	3:C:395:LEU:HB2	2.02	0.42
3:C:92:LEU:HD23	3:C:158:TYR:CE1	2.54	0.42
3:C:147:PHE:O	3:C:213:LEU:HD12	2.19	0.42
3:C:354:ILE:O	3:C:354:ILE:HG22	2.19	0.42
3:C:430:CYS:O	3:C:431:VAL:HB	2.19	0.42
2:H:234:PHE:O	2:H:238:ILE:HG13	2.20	0.42
3:I:92:LEU:HD23	3:I:158:TYR:CE1	2.54	0.42
3:I:147:PHE:CE2	3:I:186:ILE:HG23	2.54	0.42
3:I:362:LEU:HD12	3:I:363:TYR:N	2.35	0.42
2:B:63:ARG:HG2	2:B:63:ARG:NH2	2.34	0.42
2:B:165:ARG:O	2:B:168:CYS:HB3	2.20	0.42
3:C:118:GLN:O	3:C:121:PHE:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:GLY:HA3	3:C:274:PHE:CE1	2.55	0.42
2:H:71:ARG:NH1	9:H:405:HOH:O	2.51	0.42
3:I:263:VAL:HG23	3:I:266:GLY:H	1.84	0.42
3:C:196:GLY:O	3:C:197:ARG:C	2.58	0.42
3:C:402:PHE:CE1	3:C:404:ALA:HB2	2.53	0.42
2:H:230:LYS:HG2	2:H:232:THR:HG23	2.01	0.42
3:I:50:GLU:C	3:I:52:SER:N	2.73	0.42
3:I:147:PHE:O	3:I:213:LEU:HA	2.20	0.42
3:I:155:ASN:OD1	3:I:156:GLU:N	2.53	0.42
2:H:165:ARG:O	2:H:168:CYS:HB3	2.20	0.42
3:I:285:LEU:HD11	3:I:406:ARG:CZ	2.49	0.42
2:H:16:ILE:CG2	2:H:17:VAL:N	2.82	0.42
3:I:101:GLN:HB3	3:I:340:LEU:HD12	2.02	0.42
3:I:354:ILE:HG22	3:I:354:ILE:O	2.19	0.42
3:C:96:ASN:O	3:C:97:ASP:C	2.58	0.42
3:C:230:SER:HA	3:C:231:PRO:HD3	1.87	0.42
3:C:122:PHE:O	3:C:125:LYS:N	2.52	0.41
3:C:101:GLN:O	3:C:103:MET:N	2.53	0.41
3:I:223:GLY:HA3	3:I:274:PHE:CE1	2.55	0.41
3:C:62:PHE:C	3:C:62:PHE:CD2	2.93	0.41
1:L:97:ASP:CB	1:L:123:ALA:HA	2.49	0.41
2:H:29:TRP:CE3	2:H:120:PRO:O	2.73	0.41
3:I:81:LEU:HD11	3:I:126:LEU:HD21	2.00	0.41
3:I:196:GLY:O	3:I:197:ARG:C	2.58	0.41
3:C:224:LEU:HD12	3:C:224:LEU:HA	1.90	0.41
3:C:285:LEU:HD11	3:C:406:ARG:CZ	2.50	0.41
3:C:308:LEU:O	3:C:309:ASP:C	2.59	0.41
2:H:86:GLU:OE1	2:H:107:ARG:NH2	2.53	0.41
3:I:346:PRO:HG3	3:I:363:TYR:CD2	2.56	0.41
2:B:50:PHE:CZ	2:B:111:PRO:HB3	2.55	0.41
3:C:149:ASP:HA	3:C:173:LEU:O	2.21	0.41
3:C:332:LYS:CG	3:C:333:GLU:N	2.81	0.41
2:H:21:GLU:CD	2:H:154:ARG:HD3	2.41	0.41
2:H:28:PRO:HG2	2:H:29:TRP:CZ3	2.56	0.41
3:I:15:ILE:O	3:I:16:PRO:C	2.58	0.41
3:I:40:ILE:HA	3:I:41:PRO:HD3	1.81	0.41
3:I:101:GLN:O	3:I:103:MET:N	2.53	0.41
3:I:143:ALA:HB2	3:I:194:THR:HG22	2.03	0.41
2:B:159:GLU:O	2:B:160:VAL:HG13	2.20	0.41
2:B:234:PHE:O	2:B:238:ILE:HG13	2.21	0.41
3:C:271:GLU:HA	3:C:282:VAL:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:360:ASP:O	3:C:361:ASP:CB	2.69	0.41
2:H:61(A):ALA:HA	3:I:397:PRO:HB2	2.02	0.41
3:I:80:PRO:HG2	3:I:81:LEU:N	2.36	0.41
3:I:224:LEU:HD12	3:I:224:LEU:HA	1.88	0.41
3:I:354:ILE:O	3:I:355:VAL:HG13	2.20	0.41
2:B:29:TRP:CE3	2:B:120:PRO:O	2.74	0.41
2:B:51:TYR:HB2	2:B:242:MET:HE3	2.03	0.41
2:B:124(A):PRO:HD3	2:B:208:PHE:HB3	2.03	0.41
3:C:286:PRO:O	3:C:406:ARG:NH2	2.54	0.41
3:C:350:ALA:C	3:C:352:PRO:HD3	2.41	0.41
2:H:52:ILE:HD13	2:H:52:ILE:HA	1.85	0.41
2:H:159:GLU:O	2:H:160:VAL:HG13	2.20	0.41
1:A:97:ASP:CB	1:A:123:ALA:HA	2.49	0.41
1:A:117:LEU:HD11	1:A:121:GLY:O	2.21	0.41
2:B:41:PHE:O	2:B:42:CYS:SG	2.78	0.41
3:C:147:PHE:O	3:C:213:LEU:HA	2.20	0.41
2:H:34:ILE:HG22	2:H:40:GLY:HA2	2.03	0.41
2:H:40:GLY:O	2:H:41:PHE:HB3	2.20	0.41
2:H:56:ALA:HB2	2:H:103:ILE:O	2.20	0.41
3:I:62:PHE:CD2	3:I:62:PHE:C	2.94	0.41
3:I:117:ASP:C	3:I:119:ILE:H	2.25	0.41
3:I:161:ILE:O	3:I:163:GLU:N	2.53	0.41
2:B:23:LYS:O	2:B:24:ASP:C	2.59	0.41
2:B:46:ILE:HG12	2:B:52:ILE:HD11	2.03	0.41
2:B:59:LEU:O	2:B:60:TYR:C	2.59	0.41
3:C:80:PRO:HG2	3:C:81:LEU:N	2.36	0.41
3:C:82:SER:O	3:C:83:ILE:C	2.58	0.41
3:C:123:PHE:O	3:C:127:ASN:ND2	2.54	0.41
3:C:152:LEU:HD13	3:C:362:LEU:HD12	2.02	0.41
3:C:161:ILE:O	3:C:163:GLU:N	2.54	0.41
3:C:239:PHE:CE2	3:C:429:PRO:HG3	2.56	0.41
3:C:263:VAL:HG23	3:C:266:GLY:H	1.84	0.41
1:L:132:CYS:CA	2:H:120:PRO:HG2	2.51	0.41
2:H:50:PHE:CZ	2:H:111:PRO:HB3	2.55	0.41
2:H:76:GLU:HA	2:H:80:GLU:OE1	2.21	0.41
2:H:78:GLY:C	2:H:80:GLU:N	2.72	0.41
3:I:123:PHE:O	3:I:127:ASN:ND2	2.53	0.41
3:I:402:PHE:HE1	3:I:404:ALA:HB2	1.86	0.41
2:B:21:GLU:CD	2:B:154:ARG:HD3	2.42	0.41
3:C:186:ILE:O	3:C:189:TRP:N	2.54	0.41
3:C:346:PRO:HG3	3:C:363:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:183:ARG:O	3:I:186:ILE:N	2.47	0.40
3:I:186:ILE:O	3:I:189:TRP:N	2.54	0.40
1:A:115:TYR:OH	1:A:134:LYS:HE2	2.21	0.40
2:B:96:LYS:HA	2:B:99:TYR:CE1	2.56	0.40
3:C:50:GLU:C	3:C:52:SER:N	2.74	0.40
3:C:118:GLN:O	3:C:121:PHE:HB3	2.21	0.40
3:C:332:LYS:O	3:C:333:GLU:C	2.59	0.40
1:L:138:GLU:CB	2:H:116:MET:HE1	2.52	0.40
3:I:350:ALA:C	3:I:352:PRO:HD3	2.41	0.40
3:C:316:LEU:HD12	3:C:316:LEU:O	2.21	0.40
3:C:326:GLU:HB3	3:C:372:PHE:CE2	2.51	0.40
1:L:99:PHE:HB2	1:L:110:SER:OG	2.21	0.40
1:L:114:GLY:O	1:L:127:THR:HB	2.22	0.40
3:I:149:ASP:HA	3:I:173:LEU:O	2.21	0.40
3:I:260:TYR:N	3:I:312:GLU:O	2.50	0.40
3:I:332:LYS:O	3:I:333:GLU:C	2.60	0.40
1:A:89:CYS:SG	1:A:101:HIS:O	2.79	0.40
3:C:23:TYR:CD1	3:C:23:TYR:C	2.94	0.40
3:C:101:GLN:HB3	3:C:340:LEU:HD12	2.02	0.40
3:C:187:ASN:ND2	3:C:200:ASP:HA	2.36	0.40
3:C:256:GLY:C	3:C:315:MET:HE3	2.41	0.40
2:H:96:LYS:HA	2:H:99:TYR:CE1	2.57	0.40
3:I:308:LEU:O	3:I:311:LEU:HG	2.21	0.40
1:L:86:ARG:O	1:L:90:SER:CB	2.70	0.40
1:L:115:TYR:OH	1:L:134:LYS:HE2	2.21	0.40
3:I:95:CYS:O	3:I:96:ASN:O	2.40	0.40
3:I:118:GLN:O	3:I:121:PHE:HB3	2.22	0.40
3:I:286:PRO:O	3:I:406:ARG:NH2	2.54	0.40
2:B:35:ASN:O	2:B:38:ASN:N	2.50	0.40
2:B:177:THR:HB	2:B:180:MET:HG3	2.04	0.40
3:C:4:PRO:O	3:C:5:VAL:CB	2.70	0.40
3:C:260:TYR:N	3:C:312:GLU:O	2.49	0.40
3:C:402:PHE:HE1	3:C:404:ALA:HB2	1.87	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	50/58 (86%)	36 (72%)	9 (18%)	5 (10%)	0	3
1	L	52/58 (90%)	37 (71%)	10 (19%)	5 (10%)	0	4
2	B	237/241 (98%)	174 (73%)	46 (19%)	17 (7%)	1	7
2	H	232/241 (96%)	174 (75%)	46 (20%)	12 (5%)	2	13
3	C	414/443 (94%)	290 (70%)	79 (19%)	45 (11%)	0	2
3	I	413/443 (93%)	294 (71%)	77 (19%)	42 (10%)	0	3
All	All	1398/1484 (94%)	1005 (72%)	267 (19%)	126 (9%)	1	4

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	87	LYS
1	L	102	GLU
1	L	126	PRO
2	H	125	ARG
2	H	144	THR
3	I	21	CYS
3	I	42	GLU
3	I	96	ASN
3	I	97	ASP
3	I	113	GLU
3	I	116	SER
3	I	177	GLU
3	I	228	LYS
3	I	245	GLU
3	I	350	ALA
3	I	359	ARG
3	I	386	THR
3	I	430	CYS
1	A	102	GLU
1	A	126	PRO

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Mol	Chain	Res	Type
2	B	79	GLY
2	B	125	ARG
2	B	144	THR
2	B	247	LEU
2	B	248	PRO
3	C	7	ILE
3	C	42	GLU
3	C	96	ASN
3	C	97	ASP
3	C	113	GLU
3	C	116	SER
3	C	177	GLU
3	C	228	LYS
3	C	245	GLU
3	C	350	ALA
3	C	355	VAL
3	C	361	ASP
3	C	385	SER
3	C	430	CYS
2	H	41	PHE
2	H	60	TYR
2	H	232	THR
2	H	242	MET
3	I	38	GLN
3	I	43	ALA
3	I	151	SER
3	I	162	SER
3	I	179	ALA
3	I	197	ARG
3	I	241	LYS
3	I	309	ASP
3	I	355	VAL
3	I	358	GLY
3	I	383	ALA
2	B	41	PHE
2	B	60	TYR
2	B	78	GLY
2	B	232	THR
2	B	238	ILE
2	B	244	THR
3	C	5	VAL
3	C	21	CYS

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Mol	Chain	Res	Type
3	C	38	GLN
3	C	43	ALA
3	C	151	SER
3	C	162	SER
3	C	197	ARG
3	C	241	LYS
3	C	309	ASP
3	C	356	ALA
3	C	386	THR
1	L	129	PRO
2	H	142	GLY
2	H	234	PHE
2	H	238	ILE
3	I	114	LYS
3	I	150	LYS
3	I	184	ALA
3	I	211	THR
3	I	357	GLU
3	I	407	PRO
3	I	429	PRO
1	A	88	LEU
1	A	129	PRO
2	B	142	GLY
2	B	234	PHE
2	B	242	MET
3	C	114	LYS
3	C	150	LYS
3	C	179	ALA
3	C	184	ALA
3	C	211	THR
3	C	381	GLU
3	C	407	PRO
3	C	429	PRO
1	L	95	ASP
3	I	183	ARG
3	I	292	LEU
3	I	378	GLU
1	A	95	ASP
3	C	132	ARG
3	C	183	ARG
3	C	292	LEU
3	C	378	GLU

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Mol	Chain	Res	Type
3	C	384	ALA
2	H	63	ARG
3	I	132	ARG
2	B	63	ARG
3	C	19	PRO
3	C	360	ASP
3	I	19	PRO
3	I	72	ASP
2	B	111	PRO
2	B	143	ARG
3	C	72	ASP
3	C	205	GLU
2	H	111	PRO
3	C	119	ILE
3	I	119	ILE
3	I	416	PRO
3	C	416	PRO
3	I	12	PRO
3	C	12	PRO
2	H	124(A)	PRO
3	I	161	ILE
3	I	421	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	33/50 (66%)	32 (97%)	1 (3%)	41	68
1	L	34/50 (68%)	32 (94%)	2 (6%)	19	49
2	B	189/203 (93%)	168 (89%)	21 (11%)	6	23
2	H	188/203 (93%)	169 (90%)	19 (10%)	7	27
3	C	331/389 (85%)	298 (90%)	33 (10%)	7	27
3	I	332/389 (85%)	298 (90%)	34 (10%)	7	27
All	All	1107/1284 (86%)	997 (90%)	110 (10%)	8	28

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	86	ARG
1	L	97	ASP
2	H	49	GLU
2	H	63	ARG
2	H	64	PHE
2	H	70	ASP
2	H	95	THR
2	H	115	ARG
2	H	118	VAL
2	H	133	GLN
2	H	144	THR
2	H	158	LEU
2	H	177	THR
2	H	178	GLN
2	H	181	PHE
2	H	185(B)	THR
2	H	205	ASP
2	H	206	THR
2	H	209	VAL
2	H	232	THR
2	H	235	LEU
3	I	7	ILE
3	I	11	LYS
3	I	15	ILE
3	I	46	ARG
3	I	82	SER
3	I	110	THR
3	I	115	THR
3	I	119	ILE
3	I	123	PHE
3	I	144	ASN
3	I	149	ASP
3	I	217	ASN
3	I	222	LYS
3	I	237	GLU
3	I	245	GLU
3	I	247	CYS
3	I	260	TYR
3	I	282	VAL
3	I	287	LYS
3	I	300	THR
3	I	315	MET

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Mol	Chain	Res	Type
3	I	316	LEU
3	I	317	VAL
3	I	327	ASP
3	I	329	PHE
3	I	332	LYS
3	I	342	ASP
3	I	361	ASP
3	I	366	ASP
3	I	393	ARG
3	I	407	PRO
3	I	414	GLU
3	I	415	VAL
3	I	430	CYS
1	A	97	ASP
2	B	49	GLU
2	B	63	ARG
2	B	64	PHE
2	B	70	ASP
2	B	80	GLU
2	B	95	THR
2	B	115	ARG
2	B	118	VAL
2	B	133	GLN
2	B	144	THR
2	B	158	LEU
2	B	177	THR
2	B	178	GLN
2	B	181	PHE
2	B	185(B)	THR
2	B	205	ASP
2	B	206	THR
2	B	209	VAL
2	B	232	THR
2	B	235	LEU
2	B	248	PRO
3	C	7	ILE
3	C	11	LYS
3	C	15	ILE
3	C	46	ARG
3	C	82	SER
3	C	110	THR
3	C	115	THR

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Mol	Chain	Res	Type
3	C	119	ILE
3	C	123	PHE
3	C	144	ASN
3	C	149	ASP
3	C	217	ASN
3	C	222	LYS
3	C	237	GLU
3	C	245	GLU
3	C	247	CYS
3	C	260	TYR
3	C	282	VAL
3	C	287	LYS
3	C	300	THR
3	C	315	MET
3	C	316	LEU
3	C	317	VAL
3	C	327	ASP
3	C	329	PHE
3	C	332	LYS
3	C	342	ASP
3	C	366	ASP
3	C	393	ARG
3	C	407	PRO
3	C	414	GLU
3	C	415	VAL
3	C	430	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	133	GLN
2	H	178	GLN
3	I	18	ASN
3	I	144	ASN
3	I	305	GLN
3	I	319	HIS
3	I	336	GLN
2	B	133	GLN
2	B	178	GLN
3	C	18	ASN
3	C	73	ASN
3	C	144	ASN

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Mol	Chain	Res	Type
3	C	305	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](#)

18 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
4	NAG	D	1	3,4	14,14,15	0.44	0	17,19,21	0.80	0
4	NAG	D	2	4	14,14,15	0.59	0	17,19,21	0.74	0
4	BMA	D	3	4	11,11,12	0.60	0	15,15,17	0.62	0
4	MAN	D	4	4	11,11,12	0.60	0	15,15,17	0.76	1 (6%)
4	MAN	D	5	4	10,10,12	0.62	0	13,13,17	0.52	0
4	MAN	D	6	4	11,11,12	0.64	0	15,15,17	0.76	1 (6%)
5	NAG	E	1	3,5	14,14,15	0.46	0	17,19,21	0.81	0
5	NAG	E	2	5	14,14,15	0.57	0	17,19,21	0.74	0
6	ZDO	F	1	6	20,21,21	2.74	5 (25%)	25,32,32	1.40	3 (12%)
6	IDS	F	2	6	16,16,17	1.50	2 (12%)	17,24,26	1.26	2 (11%)
6	SUS	F	3	6	22,23,24	2.78	5 (22%)	24,36,38	1.67	4 (16%)
6	BDP	F	4	6	12,12,13	0.68	0	14,17,19	0.66	0
6	SGN	F	5	6	18,19,20	2.82	4 (22%)	22,29,31	1.41	3 (13%)
6	ZDO	G	1	6	20,21,21	2.75	5 (25%)	25,32,32	1.38	3 (12%)
6	IDS	G	2	6	16,16,17	1.50	2 (12%)	17,24,26	1.26	2 (11%)
6	SUS	G	3	6	22,23,24	2.79	5 (22%)	24,36,38	1.68	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BDP	G	4	6	12,12,13	0.66	0	14,17,19	0.65	0
6	SGN	G	5	6	18,19,20	2.84	4 (22%)	22,29,31	1.40	3 (13%)

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
4	NAG	D	1	3,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/16/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	ZDO	F	1	6	-	4/13/33/33	0/1/1/1
6	IDS	F	2	6	-	0/9/26/29	0/1/1/1
6	SUS	F	3	6	-	8/16/33/36	0/1/1/1
6	BDP	F	4	6	-	1/4/21/24	0/1/1/1
6	SGN	F	5	6	-	2/11/28/31	0/1/1/1
6	ZDO	G	1	6	-	4/13/33/33	0/1/1/1
6	IDS	G	2	6	-	0/9/26/29	0/1/1/1
6	SUS	G	3	6	-	8/16/33/36	0/1/1/1
6	BDP	G	4	6	-	1/4/21/24	0/1/1/1
6	SGN	G	5	6	-	2/11/28/31	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	5	SGN	O1S-S1	7.36	1.50	1.42
6	G	5	SGN	O2S-S1	7.35	1.50	1.42
6	G	1	ZDO	OSB-S2	7.32	1.50	1.42
6	F	1	ZDO	OSA-S2	7.31	1.50	1.42
6	F	3	SUS	O1S-S1	7.31	1.50	1.42
6	G	5	SGN	O1S-S1	7.31	1.50	1.42
6	F	1	ZDO	OSB-S2	7.30	1.50	1.42
6	G	3	SUS	O1S-S1	7.30	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	3	SUS	O3S-S1	7.28	1.50	1.42
6	G	1	ZDO	OSA-S2	7.28	1.50	1.42
6	F	5	SGN	O2S-S1	7.27	1.50	1.42
6	F	3	SUS	O3S-S1	7.21	1.50	1.42
6	G	1	ZDO	O6-S6	-5.01	1.43	1.56
6	G	5	SGN	O6-S2	-5.00	1.43	1.56
6	F	1	ZDO	O6-S6	-4.97	1.43	1.56
6	F	5	SGN	O6-S2	-4.93	1.43	1.56
6	F	3	SUS	O6-S2	-4.87	1.43	1.56
6	G	3	SUS	O6-S2	-4.86	1.43	1.56
6	G	3	SUS	O3-S3	-4.66	1.43	1.57
6	F	3	SUS	O3-S3	-4.64	1.43	1.57
6	G	2	IDS	O2-S	-4.62	1.43	1.57
6	F	2	IDS	O2-S	-4.60	1.43	1.57
6	G	3	SUS	S1-N2	3.08	1.63	1.59
6	F	3	SUS	S1-N2	2.98	1.63	1.59
6	G	1	ZDO	S2-N2	2.94	1.63	1.59
6	F	1	ZDO	S2-N2	2.87	1.63	1.59
6	G	5	SGN	S1-N2	2.85	1.63	1.59
6	F	5	SGN	S1-N2	2.75	1.63	1.59
6	F	2	IDS	O2-C2	-2.37	1.43	1.47
6	G	2	IDS	O2-C2	-2.37	1.43	1.47
6	G	1	ZDO	O1-C1	2.28	1.44	1.40
6	F	1	ZDO	O1-C1	2.21	1.43	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3	SUS	O1S-S1-O3S	-4.94	108.47	120.16
6	F	3	SUS	O1S-S1-O3S	-4.89	108.61	120.16
6	F	3	SUS	C3-O3-S3	-4.60	109.99	118.88
6	G	3	SUS	C3-O3-S3	-4.58	110.03	118.88
6	F	1	ZDO	OSA-S2-OSB	-4.58	109.34	120.16
6	G	5	SGN	O1S-S1-O2S	-4.56	109.39	120.16
6	G	1	ZDO	OSA-S2-OSB	-4.51	109.49	120.16
6	F	5	SGN	O1S-S1-O2S	-4.48	109.56	120.16
6	G	2	IDS	C2-O2-S	-3.97	112.73	117.91
6	F	2	IDS	C2-O2-S	-3.94	112.77	117.91
6	F	1	ZDO	C1M-O1-C1	-3.19	108.34	113.27
6	F	5	SGN	C6-C5-C4	-3.07	105.69	112.09
6	G	1	ZDO	C1M-O1-C1	-3.05	108.56	113.27
6	G	5	SGN	C6-C5-C4	-3.02	105.78	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3	SUS	O6-C6-C5	2.56	112.39	107.62
6	F	2	IDS	O2-C2-C3	2.51	110.46	106.95
6	G	2	IDS	O2-C2-C3	2.48	110.42	106.95
6	G	3	SUS	O6-C6-C5	2.46	112.22	107.62
4	D	6	MAN	C1-O5-C5	2.44	115.50	112.19
6	G	3	SUS	O5-C1-C2	-2.36	107.56	111.29
6	G	1	ZDO	C3-C4-C5	-2.21	106.30	110.24
6	F	1	ZDO	C3-C4-C5	-2.19	106.33	110.24
4	D	4	MAN	C1-O5-C5	2.18	115.14	112.19
6	F	3	SUS	O5-C1-C2	-2.17	107.87	111.29
6	F	5	SGN	O6-C6-C5	2.15	111.63	107.62
6	G	5	SGN	O6-C6-C5	2.07	111.48	107.62

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
6	F	1	ZDO	C2-N2-S2-OSA
6	F	3	SUS	C2-N2-S1-O2S
6	G	1	ZDO	C2-N2-S2-OSA
6	G	3	SUS	C2-N2-S1-O2S
4	D	6	MAN	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	6	MAN	C4-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
5	E	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
6	F	3	SUS	C6-O6-S2-O4S
6	G	3	SUS	C6-O6-S2-O4S
4	D	3	BMA	C4-C5-C6-O6
6	F	1	ZDO	C6-O6-S6-OS3
6	F	3	SUS	C6-O6-S2-O6S
6	G	1	ZDO	C6-O6-S6-OS3
6	G	3	SUS	C6-O6-S2-O6S
4	D	2	NAG	C1-C2-N2-C7

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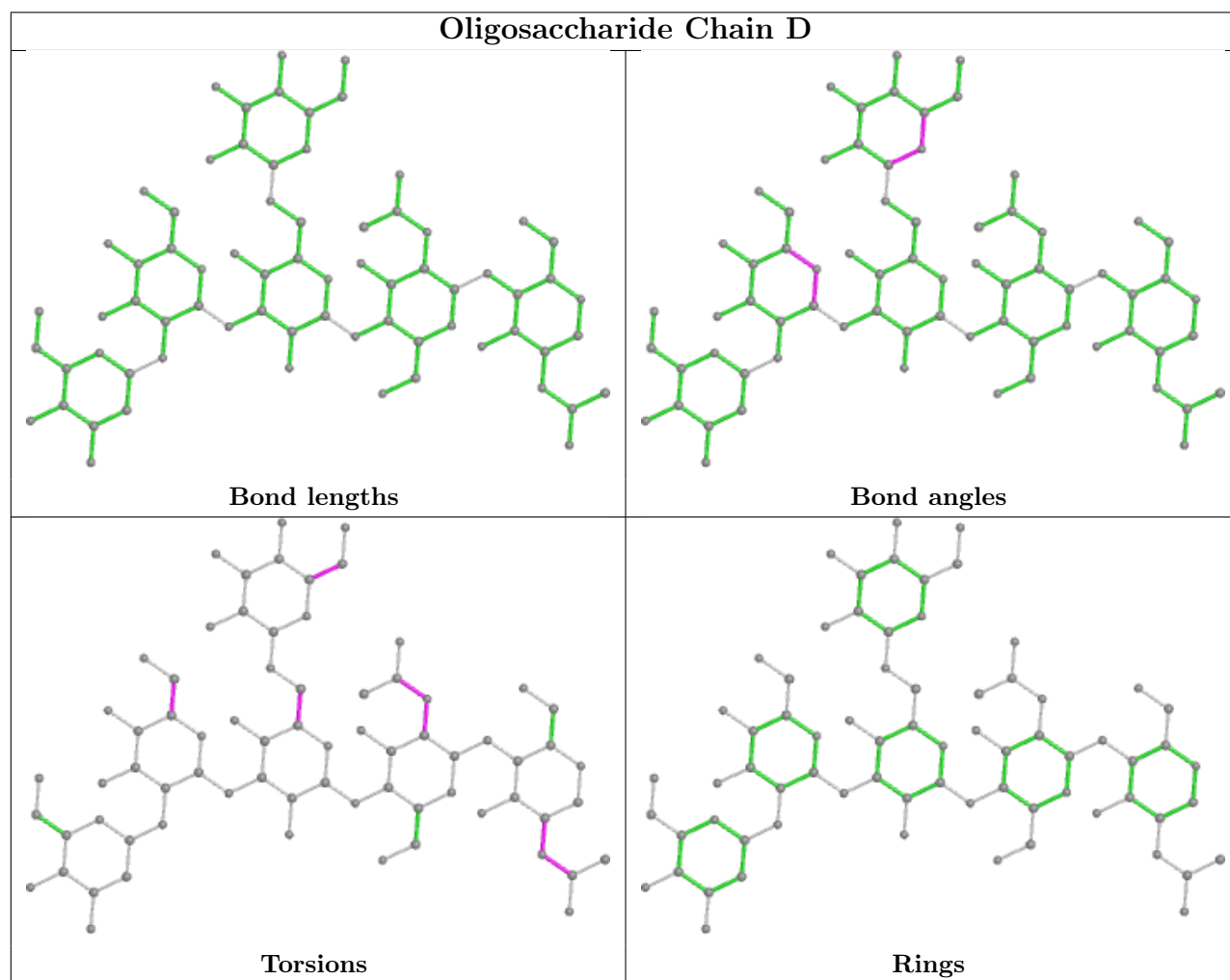
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C1-C2-N2-C7
4	D	4	MAN	O5-C5-C6-O6
6	F	1	ZDO	C6-O6-S6-OS2
6	G	1	ZDO	C6-O6-S6-OS2
4	D	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C3-C2-N2-C7
6	F	3	SUS	C2-N2-S1-O1S
6	G	3	SUS	C2-N2-S1-O1S
6	F	1	ZDO	C6-O6-S6-OS1
6	F	3	SUS	C6-O6-S2-O5S
6	F	5	SGN	C6-O6-S2-O5S
6	G	1	ZDO	C6-O6-S6-OS1
6	G	3	SUS	C6-O6-S2-O5S
6	G	5	SGN	C6-O6-S2-O5S
6	F	3	SUS	C1-C2-N2-S1
6	G	3	SUS	C1-C2-N2-S1
6	F	3	SUS	C3-C2-N2-S1
6	G	3	SUS	C3-C2-N2-S1
4	D	1	NAG	C3-C2-N2-C7
5	E	1	NAG	C3-C2-N2-C7
6	G	5	SGN	C6-O6-S2-O4S
6	F	5	SGN	C6-O6-S2-O4S
6	F	4	BDP	O5-C5-C6-O6B
6	G	4	BDP	O5-C5-C6-O6B
6	F	3	SUS	C2-N2-S1-O3S
6	G	3	SUS	C2-N2-S1-O3S

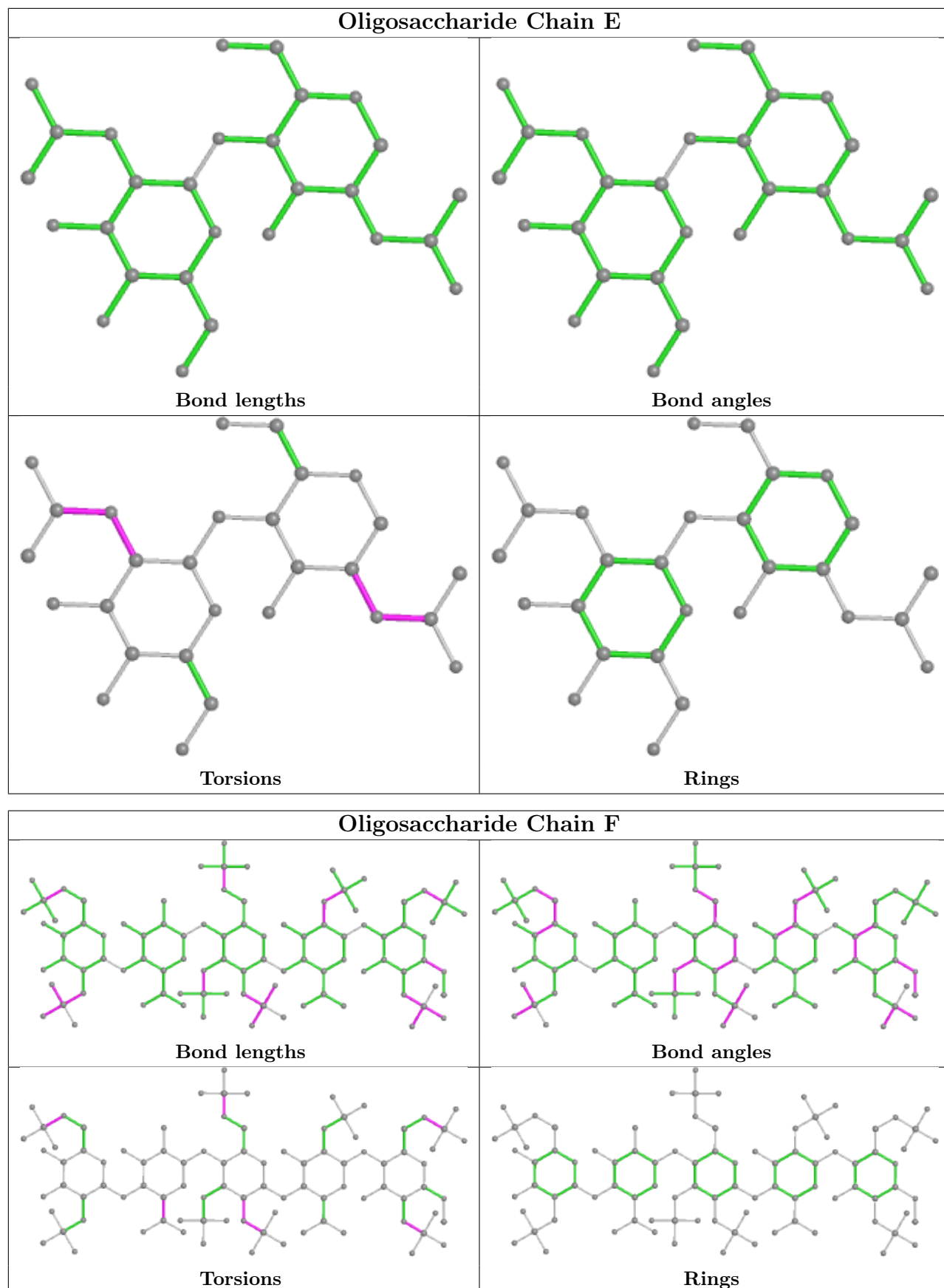
There are no ring outliers.

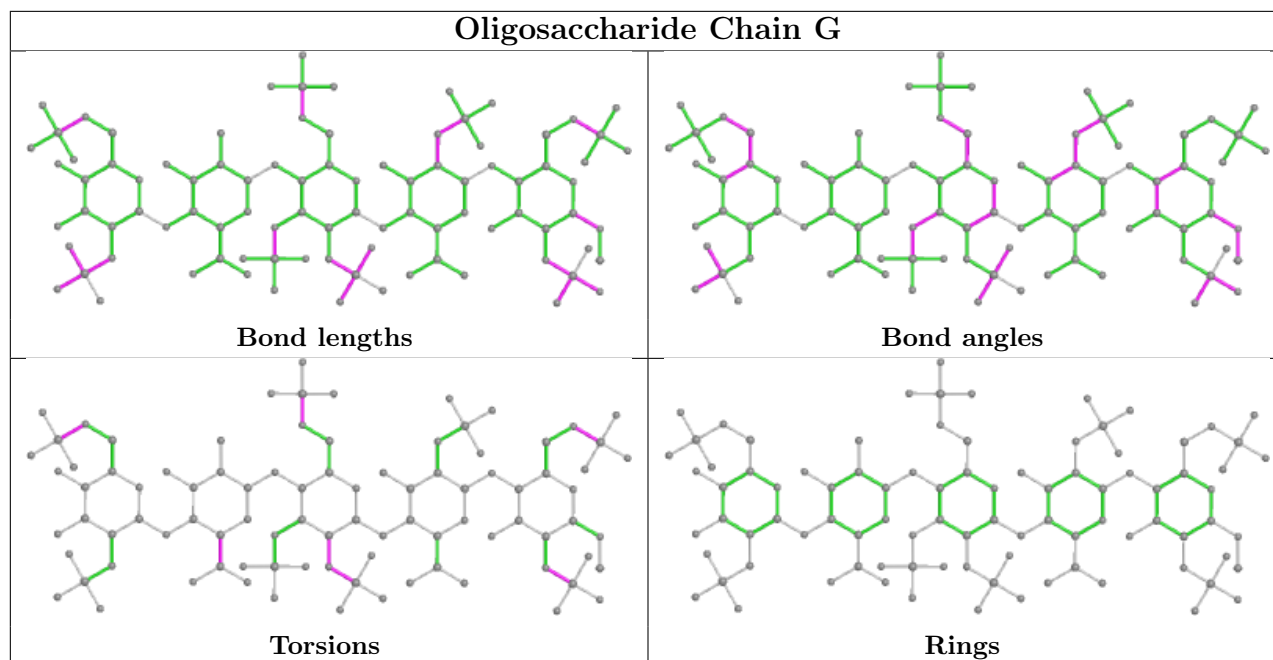
10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	5	SGN	1	0
4	D	3	BMA	3	0
4	D	1	NAG	5	0
6	F	1	ZDO	1	0
6	F	5	SGN	1	0
5	E	1	NAG	5	0
6	G	1	ZDO	1	0
4	D	2	NAG	4	0
4	D	4	MAN	3	0
5	E	2	NAG	6	0

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







5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
8	NAG	I	501	3	14,14,15	0.95	1 (7%)	17,19,21	2.15	3 (17%)
8	NAG	C	501	3	14,14,15	0.95	1 (7%)	17,19,21	2.15	3 (17%)
8	NAG	I	701	3	14,14,15	0.63	0	17,19,21	0.61	0
8	NAG	C	701	3	14,14,15	0.63	0	17,19,21	0.61	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
8	NAG	I	501	3	-	4/6/23/26	0/1/1/1
8	NAG	C	501	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	I	701	3	-	6/6/23/26	0/1/1/1
8	NAG	C	701	3	-	6/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	NAG	O5-C5	2.29	1.48	1.43
8	I	501	NAG	O5-C5	2.11	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	NAG	C1-O5-C5	6.21	120.61	112.19
8	I	501	NAG	C1-O5-C5	6.13	120.50	112.19
8	C	501	NAG	C4-C3-C2	-4.48	104.45	111.02
8	I	501	NAG	C4-C3-C2	-4.44	104.51	111.02
8	I	501	NAG	O5-C1-C2	3.50	116.82	111.29
8	C	501	NAG	O5-C1-C2	3.45	116.73	111.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	501	NAG	C8-C7-N2-C2
8	I	501	NAG	O7-C7-N2-C2
8	I	701	NAG	C8-C7-N2-C2
8	I	701	NAG	O7-C7-N2-C2
8	C	501	NAG	C8-C7-N2-C2
8	C	501	NAG	O7-C7-N2-C2
8	C	701	NAG	C8-C7-N2-C2
8	C	701	NAG	O7-C7-N2-C2
8	I	701	NAG	C1-C2-N2-C7
8	C	701	NAG	C1-C2-N2-C7
8	I	701	NAG	C4-C5-C6-O6
8	C	701	NAG	C4-C5-C6-O6
8	I	701	NAG	O5-C5-C6-O6
8	C	501	NAG	C4-C5-C6-O6
8	I	501	NAG	C4-C5-C6-O6
8	I	501	NAG	C3-C2-N2-C7
8	I	701	NAG	C3-C2-N2-C7
8	C	501	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	C	701	NAG	C3-C2-N2-C7
8	C	701	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	501	NAG	1	0
8	C	501	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	52/58 (89%)	0.44	1 (1%) 66 65	29, 65, 82, 83	1 (1%)
1	L	54/58 (93%)	-0.01	0 100 100	29, 65, 81, 83	0
2	B	239/241 (99%)	-0.44	1 (0%) 92 93	1, 19, 45, 80	3 (1%)
2	H	234/241 (97%)	-0.49	0 100 100	1, 19, 38, 53	3 (1%)
3	C	418/443 (94%)	-0.15	8 (1%) 66 65	1, 41, 87, 99	6 (1%)
3	I	417/443 (94%)	-0.14	8 (1%) 66 65	1, 39, 85, 103	3 (0%)
All	All	1414/1484 (95%)	-0.23	18 (1%) 77 77	1, 31, 83, 103	16 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	387	ALA	4.0
3	I	387	ALA	3.8
3	C	388	VAL	3.7
3	C	358	GLY	3.3
3	C	386	THR	3.1
3	C	382	ALA	2.7
3	C	16	PRO	2.6
2	B	117	ASN	2.6
1	A	118	ALA	2.5
3	I	384	ALA	2.5
3	I	82	SER	2.5
3	I	360	ASP	2.4
3	I	38	GLN	2.4
3	C	381	GLU	2.2
3	I	386	THR	2.1
3	I	359	ARG	2.1
3	C	385	SER	2.1
3	I	388	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

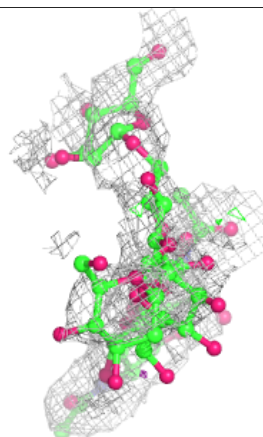
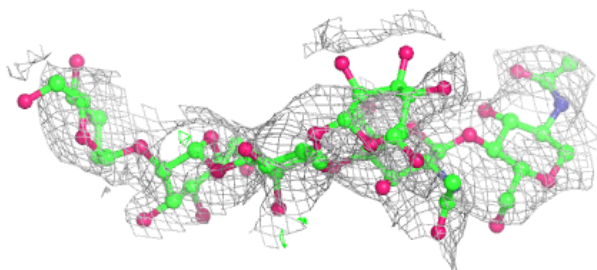
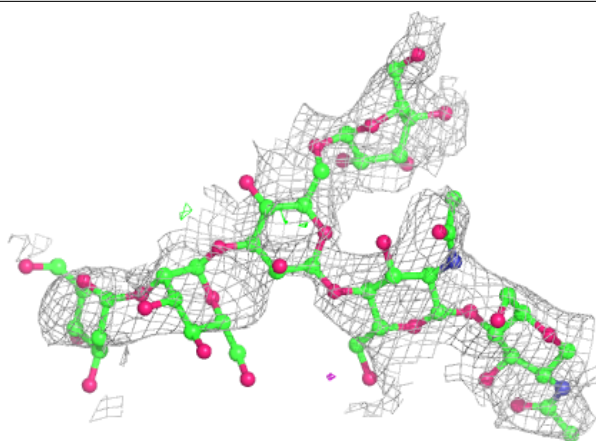
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	6	11/12	0.40	0.34	135,136,137,137	0
4	BMA	D	3	11/12	0.60	0.37	129,134,135,139	0
4	MAN	D	5	10/12	0.66	0.40	148,149,150,150	0
4	NAG	D	2	14/15	0.71	0.32	107,110,117,121	0
4	MAN	D	4	11/12	0.74	0.42	143,145,147,147	0
5	NAG	E	1	14/15	0.82	0.22	85,87,93,100	0
5	NAG	E	2	14/15	0.84	0.30	106,110,114,115	0
6	IDS	G	2	16/17	0.84	0.18	49,55,65,66	0
6	ZDO	G	1	21/21	0.88	0.17	50,54,56,58	0
4	NAG	D	1	14/15	0.89	0.19	84,88,94,101	0
6	IDS	F	2	16/17	0.90	0.15	50,55,65,65	0
6	BDP	G	4	12/13	0.92	0.18	28,32,34,34	0
6	BDP	F	4	12/13	0.93	0.13	27,31,34,34	0
6	ZDO	F	1	21/21	0.93	0.17	50,52,56,59	0
6	SUS	G	3	23/24	0.94	0.14	37,43,49,50	0
6	SUS	F	3	23/24	0.95	0.15	39,43,48,48	0
6	SGN	G	5	19/20	0.95	0.12	28,32,36,36	0
6	SGN	F	5	19/20	0.96	0.13	29,32,36,36	0

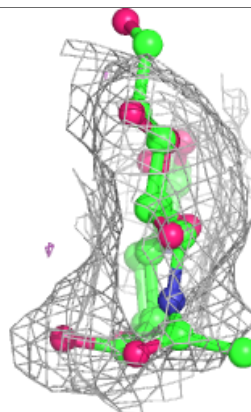
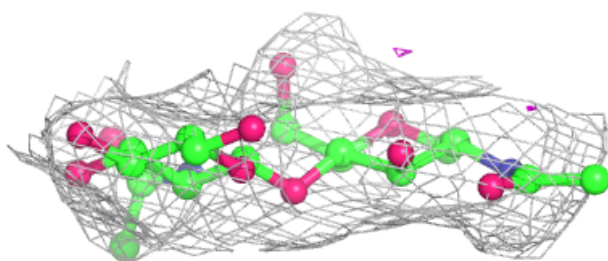
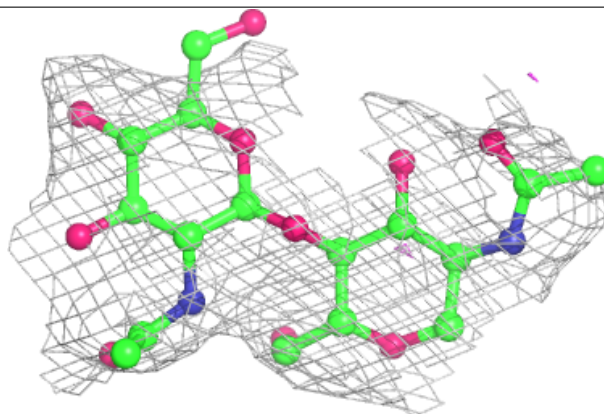
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

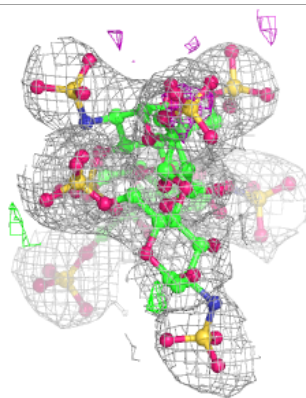
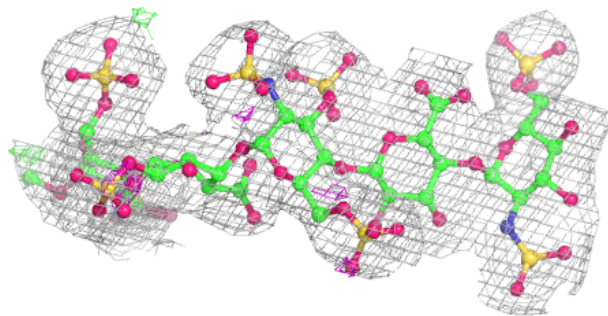
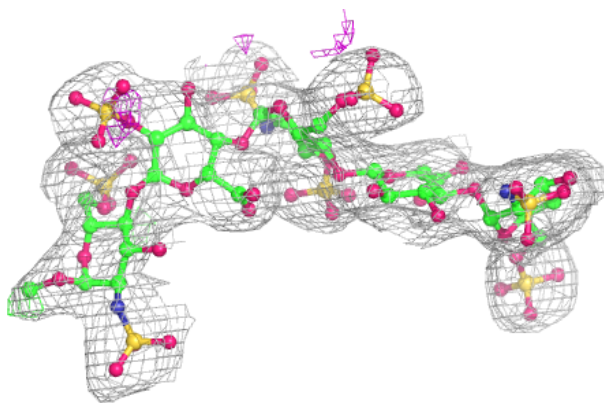
**Electron density around Chain E:**

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

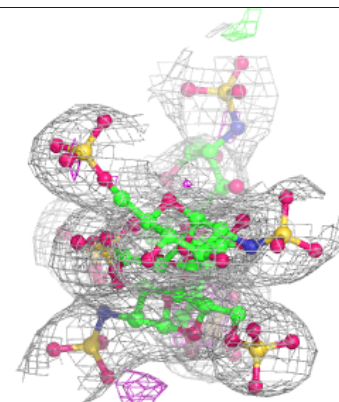
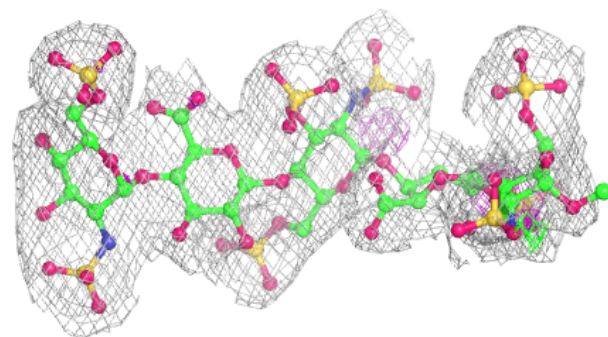
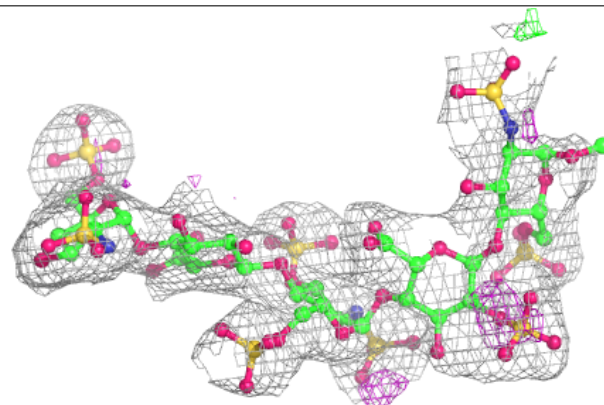


Electron density around Chain F:

$2mF_o-DF_c$ (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)



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
8	NAG	I	501	14/15	0.64	0.26	103,108,110,110	0
8	NAG	I	701	14/15	0.64	0.50	92,94,97,97	0
8	NAG	C	501	14/15	0.67	0.26	102,109,110,110	0
8	NAG	C	701	14/15	0.69	0.47	92,94,97,97	0
7	CA	B	401	1/1	0.96	0.04	12,12,12,12	0
7	CA	H	401	1/1	0.98	0.09	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.