



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:18 AM BST

PDB ID : 4EDA
Title : Structures of monomeric hemagglutinin and its complex with an Fab fragment of a neutralizing antibody that binds to H1 subtype influenza viruses: molecular basis of infectivity of 2009 pandemic H1N1 influenza A viruses
Authors : Kim, K.H.; Cho, K.J.; Lee, J.H.; Park, Y.H.; Khan, T.G.; Lee, J.Y.; Kang, S.H.; Alam, I.
Deposited on : 2012-03-27
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

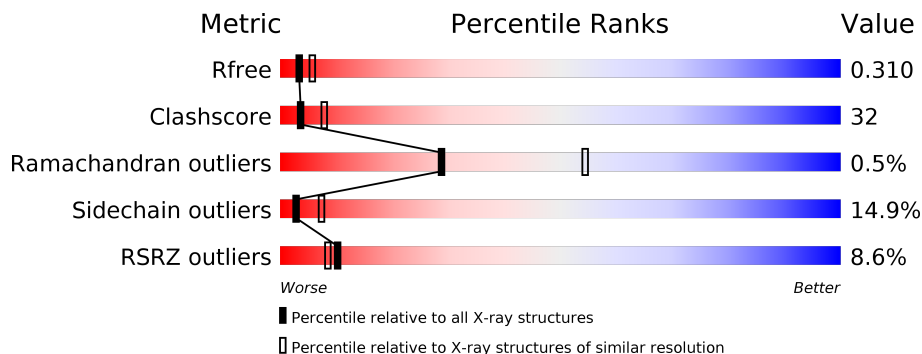
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	336	
1	C	336	
2	B	182	
2	D	182	
3	E	2	
3	F	2	

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
3	NAG	E	1	-	-	X	-
3	NAG	F	1	-	-	X	-
4	NAG	A	403	X	-	-	-
4	NAG	C	404	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7225 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2508	1585	433	479	11	0	0	0
1	C	311	2432	1538	420	464	10	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	expression tag	UNP C5MQE6
A	-7	ASP	-	expression tag	UNP C5MQE6
A	-6	PRO	-	expression tag	UNP C5MQE6
A	-5	GLY	-	expression tag	UNP C5MQE6
A	-4	TYR	-	expression tag	UNP C5MQE6
A	-3	LEU	-	expression tag	UNP C5MQE6
A	-2	LEU	-	expression tag	UNP C5MQE6
A	-1	GLU	-	expression tag	UNP C5MQE6
A	0	PHE	-	expression tag	UNP C5MQE6
C	-8	ALA	-	expression tag	UNP C5MQE6
C	-7	ASP	-	expression tag	UNP C5MQE6
C	-6	PRO	-	expression tag	UNP C5MQE6
C	-5	GLY	-	expression tag	UNP C5MQE6
C	-4	TYR	-	expression tag	UNP C5MQE6
C	-3	LEU	-	expression tag	UNP C5MQE6
C	-2	LEU	-	expression tag	UNP C5MQE6
C	-1	GLU	-	expression tag	UNP C5MQE6
C	0	PHE	-	expression tag	UNP C5MQE6

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	148	1200	748	200	246	6	0	0	0

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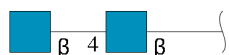
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	115	910	561	153	190	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP C5MQE6
B	178	SER	-	expression tag	UNP C5MQE6
B	179	LEU	-	expression tag	UNP C5MQE6
B	180	VAL	-	expression tag	UNP C5MQE6
B	181	PRO	-	expression tag	UNP C5MQE6
B	182	ARG	-	expression tag	UNP C5MQE6
D	177	ARG	-	expression tag	UNP C5MQE6
D	178	SER	-	expression tag	UNP C5MQE6
D	179	LEU	-	expression tag	UNP C5MQE6
D	180	VAL	-	expression tag	UNP C5MQE6
D	181	PRO	-	expression tag	UNP C5MQE6
D	182	ARG	-	expression tag	UNP C5MQE6

- 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	E	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

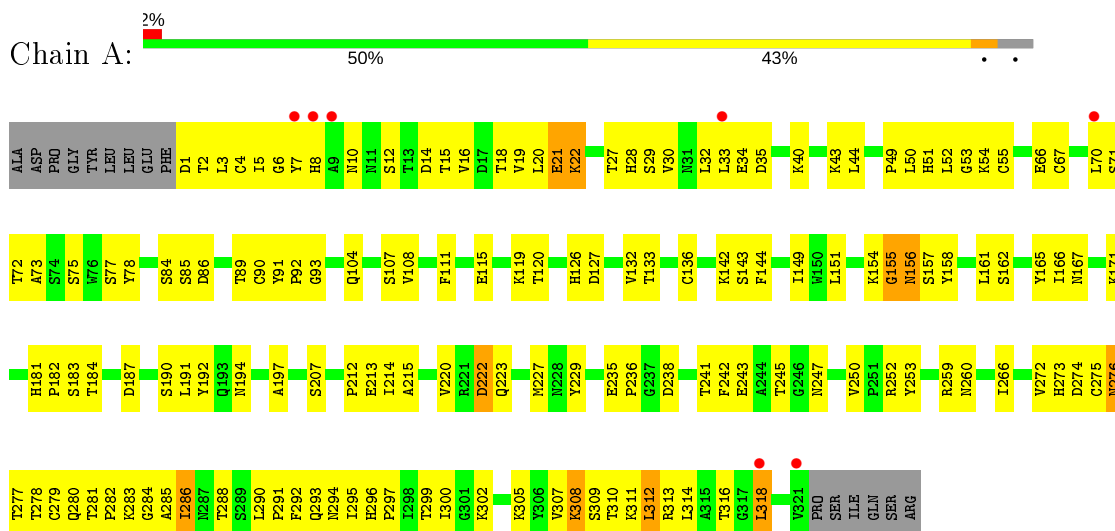
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	30	30	30	0	0
5	B	3	3	3	0	0
5	C	25	25	25	0	0
5	D	5	5	5	0	0

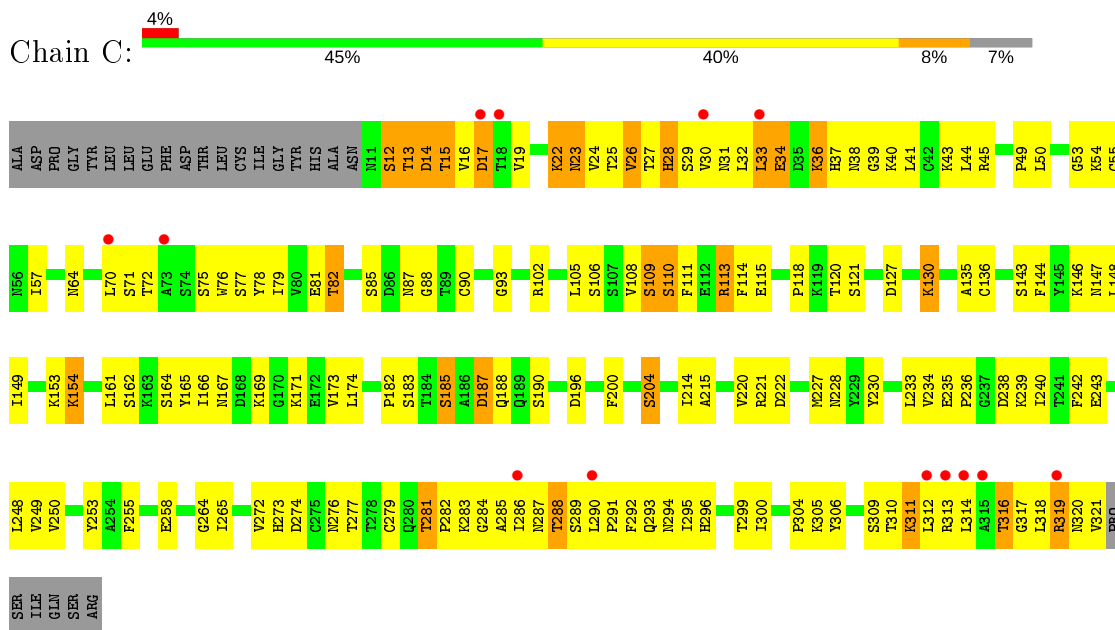
3 Residue-property plots

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.

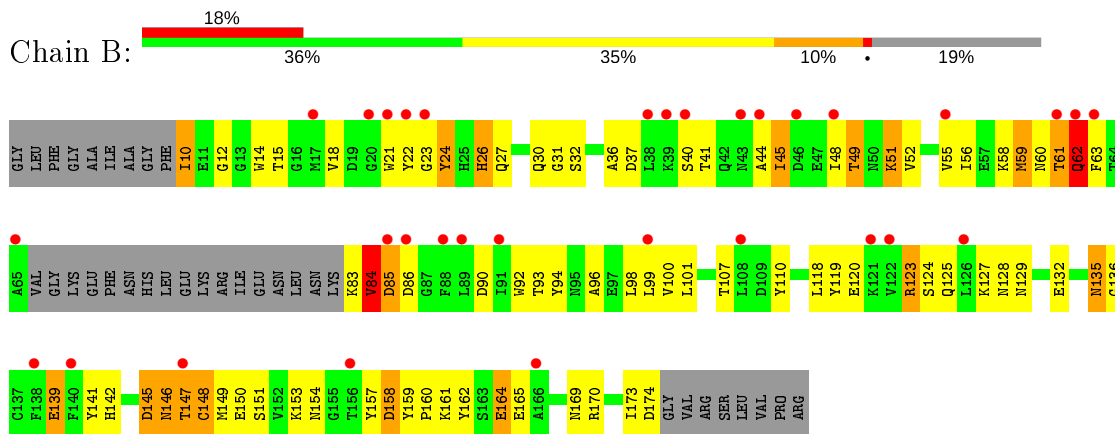
- Molecule 1: Hemagglutinin



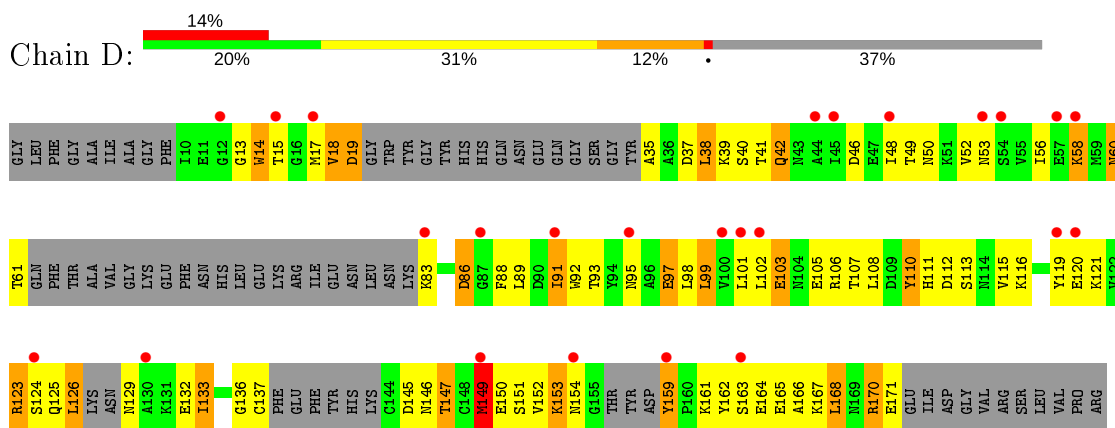
- Molecule 1: Hemagglutinin



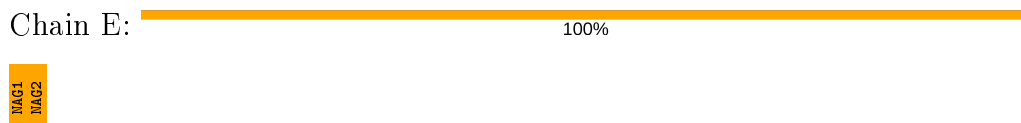
- Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	208.13Å 208.13Å 65.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.99 – 2.70 49.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.99-2.70) 99.5 (49.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.237 , 0.289 0.253 , 0.310	Depositor DCC
R_{free} test set	2260 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.085 for h,-h-k,-l	Depositor
Outliers	0 of 44808 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7225	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.42	1/2570 (0.0%)	0.65	1/3491 (0.0%)
1	C	0.42	0/2492	0.63	0/3384
2	B	0.31	0/1223	0.48	0/1650
2	D	0.29	0/916	0.57	0/1228
All	All	0.39	1/7201 (0.0%)	0.61	1/9753 (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	1
1	C	0	2
2	B	0	2
2	D	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	ASN	CA-C	-5.30	1.39	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ASN	N-CA-CB	-10.47	91.75	110.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	GLY	Peptide
2	B	62	GLN	Peptide
2	B	84	VAL	Peptide
1	C	154	LYS	Peptide
1	C	72	THR	Peptide
2	D	149	MET	Peptide
2	D	168	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2508	0	2457	147	0
1	C	2432	0	2387	153	0
2	B	1200	0	1112	77	0
2	D	910	0	871	87	0
3	E	28	0	25	8	0
3	F	28	0	25	8	0
4	A	28	0	26	0	0
4	C	28	0	26	1	0
5	A	30	0	0	0	0
5	B	3	0	0	1	0
5	C	25	0	0	4	0
5	D	5	0	0	0	0
All	All	7225	0	6929	444	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 32.

All (444) 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:90:CYS:HB3	3:E:1:NAG:H81	1.39	1.01
1:A:90:CYS:CB	3:E:1:NAG:H81	1.93	0.98
2:B:158:ASP:HB3	2:B:161:LYS:HB2	1.43	0.97
2:D:167:LYS:HD2	2:D:170:ARG:HB2	1.43	0.96
1:C:34:GLU:HG2	1:C:290:LEU:HD12	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:MET:HB2	2:B:92:TRP:CH2	2.10	0.87
2:B:123:ARG:NH2	2:B:124:SER:OG	2.08	0.86
2:B:59:MET:SD	2:B:60:ASN:N	2.48	0.86
2:B:56:ILE:O	2:B:59:MET:HG3	1.76	0.86
1:C:305:LYS:NZ	1:C:306:TYR:O	2.08	0.85
1:C:113:ARG:HH22	1:C:146:LYS:HE2	1.41	0.85
1:A:40:LYS:HZ2	1:A:273:HIS:HB2	1.44	0.83
1:C:115:GLU:OE1	1:C:118:PRO:HA	1.80	0.82
2:B:21:TRP:HZ3	2:B:45:ILE:HG12	1.45	0.81
2:D:151:SER:HB2	2:D:154:ASN:HB3	1.61	0.81
2:B:148:CYS:O	2:B:151:SER:OG	1.99	0.81
1:C:82:THR:HG23	1:C:85:SER:HB3	1.62	0.80
1:C:30:VAL:HG13	1:C:314:LEU:HB2	1.62	0.80
1:C:14:ASP:OD2	1:C:29:SER:OG	2.00	0.79
1:A:281:THR:HG22	1:A:283:LYS:H	1.47	0.78
1:A:40:LYS:NZ	1:A:273:HIS:HB2	1.98	0.77
1:C:43:LYS:HB2	1:C:276:ASN:OD1	1.85	0.76
2:D:153:LYS:H	2:D:153:LYS:HD2	1.51	0.76
1:C:64:ASN:HD21	3:F:1:NAG:H81	1.51	0.75
1:A:90:CYS:HB3	3:E:1:NAG:C8	2.16	0.75
2:B:147:THR:O	2:B:151:SER:HB3	1.87	0.75
1:C:90:CYS:HB3	3:F:1:NAG:H81	1.67	0.74
1:A:22:LYS:HB3	1:A:22:LYS:NZ	2.02	0.74
1:A:288:THR:HG22	1:A:290:LEU:HD12	1.69	0.74
1:A:3:LEU:HD13	2:B:26:HIS:HB3	1.70	0.74
1:A:280:GLN:HE21	1:A:281:THR:H	1.36	0.73
1:A:292:PHE:HE1	1:A:305:LYS:HD2	1.53	0.73
1:A:14:ASP:HB2	1:A:313:ARG:CZ	2.18	0.73
2:D:125:GLN:HG2	2:D:126:LEU:H	1.53	0.73
1:A:2:THR:HG22	2:B:139:GLU:HG3	1.70	0.73
2:B:21:TRP:CZ3	2:B:45:ILE:HG12	2.24	0.73
1:C:33:LEU:HD11	1:C:310:THR:O	1.88	0.73
1:A:5:ILE:HD13	2:B:118:LEU:HD23	1.72	0.72
2:B:44:ALA:O	2:B:48:ILE:HG12	1.88	0.72
1:A:281:THR:HG23	1:A:282:PRO:HD2	1.70	0.72
1:C:15:THR:HA	1:C:25:THR:HA	1.71	0.72
1:A:108:VAL:HG11	1:A:111:PHE:HB2	1.71	0.71
1:A:288:THR:HB	1:A:290:LEU:HB2	1.70	0.71
1:C:87:ASN:HD22	3:F:1:NAG:C7	2.03	0.71
1:C:320:ASN:ND2	1:C:321:VAL:H	1.89	0.71
1:C:93:GLY:HA3	1:C:227:MET:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:SER:HB3	1:C:109:SER:O	1.89	0.71
1:C:161:LEU:O	1:C:243:GLU:HA	1.91	0.70
1:A:314:LEU:HD23	2:B:100:VAL:HG13	1.74	0.70
1:C:40:LYS:HD2	1:C:273:HIS:CD2	2.27	0.70
1:A:133:THR:HG23	1:A:136:CYS:H	1.57	0.69
2:D:95:ASN:O	2:D:99:LEU:HD22	1.92	0.69
1:C:90:CYS:HB3	3:F:1:NAG:C8	2.22	0.69
1:C:33:LEU:HD22	1:C:312:LEU:H	1.58	0.69
1:C:319:ARG:HH21	2:D:108:LEU:HD22	1.58	0.69
2:B:164:GLU:N	2:B:164:GLU:OE1	2.24	0.69
1:C:27:THR:CG2	1:C:320:ASN:HB2	2.23	0.68
2:D:46:ASP:O	2:D:49:THR:OG1	2.10	0.68
1:C:38:ASN:HD21	1:C:285:ALA:HB3	1.59	0.67
1:C:281:THR:HG22	1:C:284:GLY:H	1.60	0.67
1:C:87:ASN:ND2	3:F:1:NAG:C7	2.57	0.67
1:A:299:THR:C	1:A:300:ILE:HD12	2.15	0.67
1:C:28:HIS:HB3	1:C:316:THR:OG1	1.94	0.67
1:A:132:VAL:HG12	1:A:143:SER:HA	1.77	0.66
1:C:167:ASN:ND2	1:C:173:VAL:HG23	2.10	0.66
1:C:183:SER:HA	1:C:215:ALA:O	1.95	0.66
2:D:126:LEU:HD12	2:D:159:TYR:CD1	2.29	0.66
2:D:14:TRP:O	2:D:14:TRP:HD1	1.79	0.66
1:A:292:PHE:CE1	1:A:305:LYS:HD2	2.31	0.66
2:D:37:ASP:CG	2:D:38:LEU:H	2.00	0.65
1:C:292:PHE:CD1	1:C:305:LYS:HB3	2.30	0.65
1:C:309:SER:OG	1:C:310:THR:N	2.30	0.65
2:D:149:MET:O	2:D:152:VAL:HG23	1.95	0.65
1:C:19:VAL:HG23	2:D:105:GLU:HB2	1.79	0.65
2:D:164:GLU:CD	2:D:164:GLU:H	2.00	0.64
1:A:154:LYS:O	1:A:157:SER:O	2.15	0.64
1:C:34:GLU:CG	1:C:290:LEU:HD12	2.27	0.64
2:D:167:LYS:CD	2:D:170:ARG:HB2	2.22	0.64
2:D:125:GLN:HG2	2:D:126:LEU:N	2.13	0.64
2:D:19:ASP:OD1	2:D:19:ASP:N	2.23	0.64
2:B:94:TYR:O	2:B:98:LEU:HG	1.96	0.64
1:A:292:PHE:CD1	1:A:305:LYS:HB2	2.33	0.64
2:D:161:LYS:O	2:D:165:GLU:HB2	1.98	0.64
1:C:321:VAL:C	2:D:13:GLY:HA3	2.19	0.63
1:C:64:ASN:ND2	3:F:1:NAG:H81	2.13	0.63
1:A:161:LEU:O	1:A:243:GLU:HA	1.98	0.63
2:B:23:GLY:HA3	2:B:36:ALA:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LEU:HA	1:C:233:LEU:HD23	1.81	0.63
1:C:49:PRO:HB3	1:C:78:TYR:CZ	2.34	0.63
2:B:26:HIS:ND1	2:B:26:HIS:O	2.29	0.63
1:C:110:SER:H	1:C:258:GLU:HG3	1.64	0.63
1:C:12:SER:HB3	1:C:27:THR:HA	1.80	0.63
2:B:107:THR:O	2:B:110:TYR:N	2.32	0.63
1:C:113:ARG:HG2	1:C:114:PHE:N	2.12	0.63
2:B:119:TYR:CE2	2:B:136:GLY:HA2	2.34	0.62
1:A:292:PHE:HD1	1:A:305:LYS:HB2	1.63	0.62
2:D:162:TYR:O	2:D:166:ALA:N	2.32	0.62
1:A:14:ASP:OD1	1:A:29:SER:OG	2.16	0.62
1:C:49:PRO:HB3	1:C:78:TYR:CE1	2.35	0.62
2:B:145:ASP:O	2:B:148:CYS:HB3	1.99	0.62
2:D:167:LYS:HD2	2:D:170:ARG:CB	2.25	0.62
1:C:113:ARG:HH22	1:C:146:LYS:CE	2.13	0.61
1:C:135:ALA:O	1:C:221:ARG:NH2	2.30	0.61
1:C:31:ASN:OD1	1:C:32:LEU:N	2.32	0.61
1:A:104:GLN:OE1	1:A:259:ARG:HD2	2.00	0.61
1:C:228:ASN:HB3	1:C:230:TYR:CE1	2.35	0.61
1:A:93:GLY:HA3	1:A:227:MET:O	2.01	0.61
1:C:79:ILE:HD11	1:C:105:LEU:O	2.01	0.61
1:A:281:THR:HG22	1:A:283:LYS:N	2.15	0.60
2:B:123:ARG:HG3	2:B:132:GLU:OE2	2.01	0.60
2:B:62:GLN:O	2:B:63:PHE:HB2	2.01	0.60
1:C:288:THR:O	1:C:289:SER:OG	2.19	0.59
1:A:288:THR:CG2	1:A:290:LEU:HD12	2.31	0.59
1:C:29:SER:HB2	1:C:313:ARG:HD2	1.85	0.59
1:A:136:CYS:HB2	1:A:143:SER:O	2.03	0.59
1:C:293:GLN:HG2	1:C:304:PRO:HG2	1.84	0.59
1:C:320:ASN:HD22	1:C:321:VAL:H	1.50	0.59
2:B:59:MET:SD	2:B:92:TRP:HZ2	2.25	0.59
1:C:185:SER:HA	1:C:214:ILE:HD13	1.83	0.59
1:C:22:LYS:HG3	1:C:23:ASN:N	2.18	0.59
1:A:90:CYS:SG	3:E:1:NAG:H81	2.42	0.59
1:C:318:LEU:HD21	2:D:111:HIS:HB3	1.85	0.58
1:A:280:GLN:NE2	1:A:284:GLY:O	2.37	0.58
1:A:14:ASP:HB2	1:A:313:ARG:NH2	2.17	0.58
1:C:113:ARG:NH2	1:C:146:LYS:HE2	2.17	0.58
2:D:120:GLU:OE1	2:D:123:ARG:HG2	2.04	0.58
1:A:213:GLU:OE1	1:C:230:TYR:OH	2.20	0.58
1:A:50:LEU:HD12	1:A:51:HIS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:H	1:A:318:LEU:HD23	1.67	0.57
2:D:52:VAL:HG13	2:D:53:ASN:H	1.70	0.57
1:A:183:SER:HA	1:A:215:ALA:O	2.03	0.57
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.86	0.57
2:D:108:LEU:O	2:D:108:LEU:HD23	2.04	0.57
2:B:124:SER:O	2:B:127:LYS:HG2	2.05	0.57
2:B:119:TYR:CD2	2:B:136:GLY:HA2	2.40	0.57
1:C:264:GLY:C	1:C:265:ILE:HD12	2.24	0.57
1:C:320:ASN:O	1:C:321:VAL:HB	2.05	0.57
2:D:113:SER:O	2:D:116:LYS:N	2.35	0.57
2:D:152:VAL:HB	2:D:153:LYS:HE3	1.87	0.57
2:B:59:MET:HB2	2:B:92:TRP:CZ2	2.39	0.57
2:D:60:ASN:H	2:D:92:TRP:HH2	1.52	0.57
1:C:31:ASN:C	1:C:32:LEU:HG	2.24	0.57
1:A:32:LEU:H	1:A:32:LEU:HD12	1.69	0.57
2:B:37:ASP:HB3	2:B:40:SER:OG	2.05	0.57
1:C:234:VAL:HG12	1:C:238:ASP:HB3	1.86	0.56
2:D:163:SER:O	2:D:166:ALA:HB3	2.05	0.56
2:B:169:ASN:O	2:B:173:ILE:HD13	2.05	0.56
2:D:167:LYS:HA	2:D:170:ARG:HG3	1.86	0.56
2:D:18:VAL:HG21	2:D:35:ALA:HA	1.87	0.56
1:A:86:ASP:HB2	3:E:1:NAG:O6	2.05	0.56
1:C:288:THR:O	1:C:289:SER:CB	2.54	0.56
1:C:17:ASP:OD2	1:C:22:LYS:HA	2.06	0.56
1:A:18:THR:OG1	1:A:21:GLU:O	2.19	0.55
1:C:57:ILE:HD12	1:C:102:ARG:HG2	1.87	0.55
1:A:151:LEU:HD12	1:A:250:VAL:HG11	1.87	0.55
2:B:129:ASN:HD21	2:B:159:TYR:HD1	1.54	0.55
2:B:59:MET:HB2	2:B:92:TRP:HH2	1.68	0.55
1:C:41:LEU:HB2	1:C:272:VAL:HA	1.88	0.55
1:C:31:ASN:HD21	1:C:311:LYS:NZ	2.04	0.55
1:C:14:ASP:N	1:C:14:ASP:OD1	2.39	0.55
1:A:16:VAL:HG12	1:A:313:ARG:HB3	1.88	0.55
1:A:53:GLY:O	1:A:85:SER:HB3	2.06	0.55
1:C:136:CYS:O	1:C:143:SER:HB3	2.07	0.55
1:A:54:LYS:HE3	1:A:66:GLU:O	2.07	0.55
1:A:308:LYS:HE3	2:B:90:ASP:HA	1.89	0.54
1:C:16:VAL:N	1:C:24:VAL:O	2.38	0.54
2:D:167:LYS:HE2	2:D:171:GLU:H	1.73	0.54
1:A:282:PRO:HG2	1:A:296:HIS:CG	2.42	0.54
1:C:292:PHE:CE1	1:C:305:LYS:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ASN:OD1	2:D:60:ASN:N	2.41	0.54
1:A:133:THR:HG23	1:A:136:CYS:N	2.21	0.54
2:D:125:GLN:O	2:D:159:TYR:OH	2.18	0.54
2:D:153:LYS:CD	2:D:153:LYS:H	2.09	0.54
1:A:91:TYR:CD1	1:A:227:MET:HB2	2.42	0.53
1:C:265:ILE:N	1:C:265:ILE:HD12	2.22	0.53
1:A:127:ASP:C	1:A:127:ASP:OD1	2.46	0.53
1:A:49:PRO:HB3	1:A:78:TYR:CE1	2.43	0.53
1:A:235:GLU:HB2	1:A:238:ASP:HB2	1.89	0.53
1:A:7:TYR:O	2:B:14:TRP:N	2.39	0.53
1:C:22:LYS:NZ	5:C:518:HOH:O	2.34	0.53
1:C:90:CYS:O	1:C:135:ALA:HB1	2.08	0.53
1:A:279:CYS:SG	1:A:286:ILE:HG13	2.49	0.53
2:B:30:GLN:NE2	2:B:145:ASP:OD2	2.41	0.53
2:B:61:THR:OG1	2:B:62:GLN:N	2.41	0.53
1:C:188:GLN:HB2	1:C:214:ILE:HD11	1.91	0.53
1:C:28:HIS:HB2	1:C:317:GLY:H	1.74	0.53
2:D:123:ARG:HG3	2:D:123:ARG:O	2.09	0.53
1:C:33:LEU:HD12	1:C:294:ASN:HB3	1.91	0.53
1:A:32:LEU:HD13	1:A:312:LEU:HB3	1.91	0.53
1:A:55:CYS:O	1:A:85:SER:HB2	2.08	0.53
1:C:167:ASN:O	1:C:236:PRO:O	2.27	0.53
2:D:103:GLU:O	2:D:107:THR:N	2.37	0.53
1:A:293:GLN:OE1	1:A:295:ILE:N	2.42	0.53
1:A:43:LYS:O	1:A:276:ASN:HA	2.08	0.53
1:A:10:ASN:ND2	1:A:28:HIS:NE2	2.58	0.52
1:A:288:THR:HB	1:A:290:LEU:H	1.73	0.52
2:B:173:ILE:HG22	2:B:174:ASP:OD1	2.09	0.52
1:C:41:LEU:HB2	1:C:272:VAL:HG22	1.91	0.52
1:A:92:PRO:HG3	1:A:223:GLN:HB2	1.91	0.52
1:C:235:GLU:HB2	1:C:238:ASP:HB2	1.92	0.52
2:D:37:ASP:CG	2:D:38:LEU:N	2.61	0.52
2:B:48:ILE:HD11	2:B:110:TYR:CD2	2.45	0.52
1:C:45:ARG:CZ	1:C:45:ARG:HB3	2.39	0.52
1:C:57:ILE:HG13	1:C:81:GLU:OE2	2.09	0.52
1:C:235:GLU:HA	5:C:523:HOH:O	2.09	0.52
1:C:37:HIS:HB2	1:C:285:ALA:O	2.09	0.52
1:C:79:ILE:HG13	1:C:106:SER:HA	1.92	0.52
1:A:162:SER:HA	1:A:242:PHE:O	2.10	0.52
1:C:33:LEU:CD2	1:C:312:LEU:H	2.21	0.52
1:A:3:LEU:CD1	2:B:26:HIS:HB3	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:HZ2	1:A:22:LYS:HB3	1.74	0.51
2:D:39:LYS:NZ	2:D:42:GLN:HE22	2.08	0.51
1:C:196:ASP:N	1:C:196:ASP:OD1	2.39	0.51
2:D:121:LYS:O	2:D:125:GLN:NE2	2.38	0.51
2:B:164:GLU:CD	2:B:165:GLU:H	2.13	0.51
1:C:30:VAL:CG1	1:C:314:LEU:HB2	2.39	0.51
1:A:136:CYS:O	1:A:143:SER:HB3	2.10	0.51
1:C:37:HIS:HD2	1:C:295:ILE:HG12	1.75	0.51
1:C:149:ILE:HB	1:C:250:VAL:CG2	2.41	0.51
1:C:32:LEU:HD12	1:C:312:LEU:C	2.32	0.50
1:C:64:ASN:ND2	1:C:88:GLY:O	2.43	0.50
1:A:266:ILE:HD11	1:A:300:ILE:HD13	1.93	0.50
1:A:90:CYS:CB	3:E:1:NAG:C8	2.78	0.50
1:C:26:VAL:HG22	1:C:28:HIS:H	1.75	0.50
1:C:31:ASN:HA	1:C:313:ARG:HD3	1.93	0.50
1:C:320:ASN:HD22	1:C:321:VAL:N	2.08	0.50
1:A:22:LYS:HZ3	1:A:22:LYS:HB3	1.75	0.50
1:A:10:ASN:HB2	1:A:27:THR:HB	1.94	0.50
1:A:49:PRO:HB3	1:A:78:TYR:CD1	2.46	0.50
1:C:162:SER:HA	1:C:242:PHE:O	2.12	0.50
1:C:316:THR:O	2:D:111:HIS:NE2	2.38	0.50
2:D:88:PHE:O	2:D:91:ILE:N	2.45	0.50
1:A:32:LEU:O	1:A:291:PRO:HG2	2.11	0.50
2:B:142:HIS:CD2	2:B:162:TYR:HB3	2.47	0.50
1:C:154:LYS:HD3	5:C:522:HOH:O	2.11	0.50
1:C:12:SER:CB	1:C:27:THR:HA	2.41	0.50
2:B:27:GLN:HA	2:B:31:GLY:O	2.11	0.49
1:C:53:GLY:H	1:C:70:LEU:HD21	1.78	0.49
1:A:158:TYR:HB3	1:A:192:TYR:O	2.12	0.49
1:C:147:ASN:O	1:C:148:LEU:HD23	2.12	0.49
1:C:281:THR:CG2	1:C:283:LYS:H	2.26	0.49
1:C:299:THR:O	1:C:300:ILE:HD13	2.13	0.49
2:D:112:ASP:C	2:D:115:VAL:HG12	2.33	0.49
2:D:58:LYS:HB3	2:D:58:LYS:NZ	2.28	0.49
1:A:161:LEU:HD23	1:A:161:LEU:O	2.13	0.49
1:C:14:ASP:O	1:C:26:VAL:N	2.44	0.49
1:C:165:TYR:CG	1:C:166:ILE:N	2.81	0.49
2:D:126:LEU:O	2:D:129:ASN:HB3	2.13	0.49
2:B:51:LYS:O	2:B:55:VAL:HG12	2.13	0.48
2:D:14:TRP:CD1	2:D:14:TRP:O	2.64	0.48
1:A:40:LYS:O	1:A:284:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ARG:O	2:B:173:ILE:HB	2.13	0.48
2:B:55:VAL:HG13	2:B:56:ILE:H	1.78	0.48
1:A:273:HIS:ND1	1:A:275:CYS:HB3	2.28	0.48
1:A:282:PRO:HG2	1:A:296:HIS:CD2	2.48	0.48
1:C:26:VAL:HG22	1:C:28:HIS:O	2.14	0.48
2:B:135:ASN:OD1	2:B:135:ASN:N	2.47	0.48
1:A:143:SER:OG	1:A:144:PHE:N	2.46	0.48
2:D:115:VAL:HG13	2:D:116:LYS:N	2.28	0.48
1:A:44:LEU:HD11	1:A:278:THR:O	2.13	0.48
1:C:234:VAL:CG1	1:C:238:ASP:HB3	2.43	0.48
1:A:308:LYS:HG3	2:B:93:THR:HG21	1.96	0.48
1:C:258:GLU:HA	5:C:509:HOH:O	2.14	0.48
1:C:39:GLY:O	1:C:40:LYS:HD3	2.14	0.48
2:D:40:SER:OG	2:D:41:THR:N	2.45	0.48
1:A:182:PRO:O	1:A:214:ILE:HA	2.14	0.47
2:B:129:ASN:ND2	2:B:159:TYR:HD1	2.12	0.47
1:A:296:HIS:ND1	1:A:297:PRO:HD2	2.28	0.47
2:B:59:MET:C	2:B:92:TRP:HH2	2.17	0.47
1:C:13:THR:O	1:C:15:THR:HG22	2.14	0.47
1:C:239:LYS:HG2	1:C:240:ILE:N	2.30	0.47
2:D:151:SER:HB2	2:D:154:ASN:CB	2.40	0.47
1:A:310:THR:OG1	1:A:311:LYS:N	2.47	0.47
2:B:154:ASN:OD1	5:B:201:HOH:O	2.21	0.47
1:A:15:THR:O	1:A:313:ARG:HD3	2.14	0.47
2:B:159:TYR:N	2:B:160:PRO:CD	2.78	0.47
2:D:149:MET:O	2:D:152:VAL:CG2	2.62	0.47
1:A:318:LEU:HD23	1:A:318:LEU:N	2.29	0.47
2:D:120:GLU:O	2:D:124:SER:OG	2.28	0.47
1:A:281:THR:HB	1:A:284:GLY:O	2.15	0.47
1:C:228:ASN:HB3	1:C:230:TYR:HE1	1.80	0.47
2:D:154:ASN:O	2:D:154:ASN:ND2	2.48	0.47
2:D:164:GLU:HG2	2:D:165:GLU:H	1.79	0.47
1:C:200:PHE:CD1	1:C:200:PHE:C	2.88	0.47
1:A:155:GLY:HA3	1:A:157:SER:H	1.79	0.46
1:A:165:TYR:CE1	1:A:167:ASN:HA	2.50	0.46
1:A:181:HIS:ND1	1:A:212:PRO:HA	2.30	0.46
1:A:183:SER:OG	1:A:184:THR:HG23	2.16	0.46
1:C:281:THR:HG23	1:C:283:LYS:H	1.80	0.46
1:C:320:ASN:ND2	1:C:321:VAL:N	2.61	0.46
1:C:64:ASN:OD1	3:F:1:NAG:C8	2.63	0.46
1:A:107:SER:HB3	1:A:260:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:LYS:HG2	2:D:83:LYS:O	2.15	0.46
1:A:50:LEU:HD12	1:A:51:HIS:N	2.30	0.46
2:B:127:LYS:HB2	2:B:128:ASN:H	1.42	0.46
1:C:127:ASP:OD2	1:C:130:LYS:HE3	2.16	0.46
1:C:31:ASN:HD21	1:C:311:LYS:HZ1	1.64	0.46
2:D:132:GLU:HG3	2:D:136:GLY:CA	2.44	0.46
2:B:150:GLU:OE1	2:B:150:GLU:N	2.47	0.46
2:D:37:ASP:OD2	2:D:38:LEU:N	2.49	0.45
2:D:56:ILE:N	2:D:56:ILE:HD12	2.32	0.45
1:A:197:ALA:HA	1:A:245:THR:OG1	2.17	0.45
2:B:119:TYR:HE2	2:B:136:GLY:HA2	1.81	0.45
1:C:31:ASN:ND2	1:C:311:LYS:NZ	2.64	0.45
1:A:161:LEU:HD23	1:A:161:LEU:C	2.36	0.45
1:A:181:HIS:CE1	1:A:212:PRO:HA	2.50	0.45
1:A:32:LEU:CD1	1:A:312:LEU:HB3	2.46	0.45
1:C:36:LYS:HD3	1:C:36:LYS:N	2.31	0.45
2:D:147:THR:HA	2:D:150:GLU:OE1	2.17	0.45
1:A:312:LEU:HA	1:A:312:LEU:HD22	1.72	0.45
1:A:3:LEU:HD11	2:B:24:TYR:HB2	1.98	0.45
1:C:32:LEU:O	1:C:291:PRO:HD2	2.17	0.45
2:D:161:LYS:O	2:D:165:GLU:CB	2.63	0.45
1:A:281:THR:HG23	1:A:282:PRO:CD	2.43	0.45
1:A:119:LYS:HD2	1:A:252:ARG:NH1	2.32	0.45
2:B:129:ASN:ND2	2:B:159:TYR:CD1	2.85	0.45
2:D:121:LYS:HD2	2:D:121:LYS:HA	1.55	0.45
2:D:14:TRP:CH2	2:D:17:MET:SD	3.10	0.45
2:D:89:LEU:HD23	2:D:89:LEU:O	2.17	0.45
2:D:93:THR:O	2:D:97:GLU:HG2	2.16	0.45
1:A:8:HIS:HE1	1:A:10:ASN:HA	1.81	0.44
1:C:108:VAL:HG21	1:C:111:PHE:HB2	1.99	0.44
1:C:204:SER:HB3	1:C:238:ASP:OD2	2.17	0.44
2:D:107:THR:O	2:D:110:TYR:N	2.45	0.44
1:A:273:HIS:CG	1:A:274:ASP:N	2.85	0.44
1:A:72:THR:OG1	1:A:73:ALA:N	2.51	0.44
2:B:24:TYR:CD1	2:B:153:LYS:HE2	2.52	0.44
1:C:319:ARG:HG2	1:C:319:ARG:H	1.24	0.44
2:D:165:GLU:O	2:D:168:LEU:HD22	2.16	0.44
1:A:166:ILE:HD12	1:A:166:ILE:N	2.32	0.44
1:A:34:GLU:HG2	1:A:286:ILE:HG21	2.00	0.44
2:B:148:CYS:HB2	2:B:162:TYR:OH	2.18	0.44
1:C:248:LEU:HD12	1:C:249:VAL:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:CYS:HA	1:C:87:ASN:HB2	1.99	0.44
2:D:86:ASP:OD1	2:D:86:ASP:N	2.50	0.44
1:A:241:THR:HG22	1:A:242:PHE:N	2.32	0.44
2:B:164:GLU:N	2:B:164:GLU:CD	2.70	0.44
2:B:60:ASN:HB3	2:B:61:THR:H	1.48	0.44
2:D:103:GLU:HA	2:D:106:ARG:HB2	1.99	0.44
2:D:56:ILE:HD12	2:D:56:ILE:H	1.83	0.44
1:A:192:TYR:C	1:A:194:ASN:H	2.21	0.44
1:A:296:HIS:CG	1:A:297:PRO:HD2	2.52	0.44
3:E:1:NAG:O4	3:E:2:NAG:C7	2.65	0.44
1:A:312:LEU:HD13	2:B:100:VAL:HG21	2.00	0.44
1:A:34:GLU:HG2	1:A:286:ILE:CG2	2.47	0.44
1:C:288:THR:OG1	1:C:289:SER:N	2.48	0.44
1:C:44:LEU:HD12	1:C:277:THR:HG23	1.99	0.44
1:C:161:LEU:HD23	1:C:161:LEU:C	2.39	0.44
1:C:173:VAL:HA	1:C:255:PHE:O	2.18	0.44
1:C:188:GLN:CB	1:C:214:ILE:HD11	2.47	0.44
2:D:14:TRP:C	2:D:14:TRP:CD1	2.92	0.44
2:D:110:TYR:CD1	2:D:110:TYR:C	2.92	0.43
2:D:39:LYS:HZ1	2:D:42:GLN:HE22	1.64	0.43
1:A:72:THR:O	1:A:73:ALA:HB2	2.17	0.43
2:B:45:ILE:O	2:B:49:THR:OG1	2.35	0.43
1:C:15:THR:HA	1:C:24:VAL:O	2.19	0.43
2:B:84:VAL:HB	2:B:85:ASP:H	1.71	0.43
1:C:64:ASN:OD1	3:F:1:NAG:H81	2.19	0.43
1:C:293:GLN:OE1	1:C:295:ILE:HG22	2.19	0.43
2:B:83:LYS:O	2:B:84:VAL:C	2.57	0.43
2:D:163:SER:HA	2:D:166:ALA:HB2	2.01	0.43
1:A:22:LYS:H	1:A:22:LYS:HG2	1.58	0.43
2:B:141:TYR:CZ	2:B:170:ARG:HG3	2.53	0.43
1:A:282:PRO:HG2	1:A:296:HIS:CE1	2.54	0.43
1:C:220:VAL:C	1:C:222:ASP:N	2.71	0.43
2:D:111:HIS:O	2:D:115:VAL:HG12	2.19	0.43
1:A:149:ILE:HB	1:A:250:VAL:CG2	2.49	0.43
1:A:32:LEU:N	1:A:32:LEU:HD12	2.34	0.43
1:C:182:PRO:HB3	1:C:187:ASP:HB3	2.01	0.43
2:B:10:ILE:HD11	2:B:12:GLY:O	2.19	0.42
2:B:48:ILE:HD11	2:B:110:TYR:CE2	2.54	0.42
2:B:146:ASN:N	2:B:146:ASN:OD1	2.52	0.42
1:A:281:THR:N	1:A:284:GLY:O	2.51	0.42
1:A:5:ILE:HD12	2:B:119:TYR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:TYR:OH	2:D:137:CYS:N	2.53	0.42
2:D:53:ASN:HA	2:D:56:ILE:HD13	2.00	0.42
2:D:98:LEU:HA	2:D:101:LEU:HD12	2.01	0.42
2:D:145:ASP:CG	2:D:146:ASN:H	2.22	0.42
2:D:153:LYS:HD2	2:D:153:LYS:N	2.27	0.42
1:A:192:TYR:CZ	1:A:247:ASN:HA	2.55	0.42
1:A:44:LEU:HD12	1:A:277:THR:O	2.19	0.42
1:A:55:CYS:C	1:A:85:SER:HB2	2.39	0.42
1:A:115:GLU:HB2	1:A:253:TYR:CE2	2.54	0.42
1:C:143:SER:OG	1:C:144:PHE:N	2.53	0.42
2:D:133:ILE:HD12	2:D:133:ILE:HA	1.90	0.42
2:D:88:PHE:O	2:D:91:ILE:HG22	2.19	0.42
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.89	0.42
1:C:28:HIS:HB2	1:C:317:GLY:N	2.35	0.42
2:B:125:GLN:NE2	2:B:157:TYR:HB3	2.34	0.42
1:C:31:ASN:CG	1:C:32:LEU:H	2.23	0.42
1:C:33:LEU:O	1:C:33:LEU:HD23	2.20	0.42
2:D:126:LEU:HG	2:D:129:ASN:ND2	2.34	0.42
2:D:91:ILE:O	2:D:95:ASN:HB2	2.20	0.42
1:C:292:PHE:HD1	1:C:305:LYS:HB3	1.80	0.42
1:A:126:HIS:CB	1:A:151:LEU:HD22	2.49	0.41
1:A:277:THR:HG21	1:A:285:ALA:HB1	2.01	0.41
1:A:294:ASN:HA	1:A:307:VAL:O	2.19	0.41
1:C:31:ASN:ND2	1:C:311:LYS:HZ3	2.17	0.41
1:C:34:GLU:OE2	1:C:36:LYS:HE2	2.20	0.41
1:A:273:HIS:CG	1:A:274:ASP:H	2.37	0.41
1:A:67:CYS:HB3	1:A:70:LEU:HD22	2.01	0.41
1:C:120:THR:OG1	1:C:121:SER:N	2.53	0.41
1:C:282:PRO:HG2	1:C:296:HIS:CE1	2.55	0.41
1:C:311:LYS:O	1:C:312:LEU:HD12	2.19	0.41
2:D:126:LEU:HD12	2:D:159:TYR:CE1	2.54	0.41
2:D:162:TYR:O	2:D:165:GLU:N	2.53	0.41
1:A:115:GLU:HA	1:A:253:TYR:HA	2.00	0.41
1:A:214:ILE:HD12	1:A:214:ILE:N	2.35	0.41
1:A:14:ASP:CB	1:A:313:ARG:NH2	2.83	0.41
1:A:16:VAL:HG11	1:A:314:LEU:O	2.19	0.41
1:C:90:CYS:HB2	1:C:135:ALA:O	2.20	0.41
1:A:213:GLU:CD	1:C:230:TYR:OH	2.58	0.41
1:A:126:HIS:HB2	1:A:151:LEU:HD22	2.03	0.41
1:A:220:VAL:C	1:A:222:ASP:N	2.72	0.41
1:A:6:GLY:HA2	2:B:10:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:LYS:CE	2:D:170:ARG:HB2	2.51	0.41
1:A:8:HIS:CE1	1:A:10:ASN:HA	2.56	0.41
1:C:36:LYS:HD3	1:C:36:LYS:H	1.84	0.41
1:A:307:VAL:CG1	1:A:309:SER:H	2.33	0.41
2:B:158:ASP:HB3	2:B:161:LYS:CB	2.30	0.41
1:C:293:GLN:O	1:C:306:TYR:HA	2.21	0.41
1:A:89:THR:HG21	1:A:229:TYR:CE2	2.56	0.41
1:C:114:PHE:C	1:C:253:TYR:HD1	2.24	0.41
1:C:319:ARG:NE	2:D:108:LEU:HD11	2.36	0.41
1:C:50:LEU:H	1:C:76:TRP:HB2	1.86	0.41
2:D:110:TYR:HD1	2:D:110:TYR:C	2.24	0.41
1:A:90:CYS:HB3	3:E:1:NAG:C7	2.51	0.41
1:A:132:VAL:HB	1:A:142:LYS:HB3	2.03	0.41
1:A:191:LEU:HB2	1:A:192:TYR:CD2	2.56	0.41
2:B:93:THR:O	2:B:96:ALA:N	2.54	0.41
1:C:114:PHE:O	1:C:253:TYR:HA	2.20	0.41
1:A:115:GLU:O	1:A:115:GLU:HG2	2.19	0.40
2:B:48:ILE:O	2:B:52:VAL:HG23	2.21	0.40
1:A:308:LYS:CE	2:B:90:ASP:HA	2.50	0.40
1:A:167:ASN:ND2	1:A:236:PRO:HA	2.35	0.40
1:A:182:PRO:HB2	1:A:187:ASP:HB3	2.02	0.40
1:A:280:GLN:NE2	1:A:284:GLY:C	2.74	0.40
1:C:153:LYS:HE2	1:C:190:SER:O	2.21	0.40
1:A:4:CYS:O	2:B:24:TYR:HB3	2.21	0.40
1:C:115:GLU:HB2	1:C:253:TYR:CE1	2.57	0.40
4:C:404:NAG:H3	4:C:404:NAG:H82	2.03	0.40
1:C:50:LEU:N	1:C:76:TRP:HB2	2.37	0.40
2:B:142:HIS:HB2	2:B:165:GLU:HG2	2.03	0.40
2:D:111:HIS:O	2:D:115:VAL:HB	2.21	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	319/336 (95%)	298 (93%)	19 (6%)	2 (1%)	25	50
1	C	309/336 (92%)	283 (92%)	26 (8%)	0	100	100
2	B	144/182 (79%)	120 (83%)	23 (16%)	1 (1%)	22	46
2	D	103/182 (57%)	80 (78%)	22 (21%)	1 (1%)	15	37
All	All	875/1036 (84%)	781 (89%)	90 (10%)	4 (0%)	29	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
2	B	84	VAL
2	D	18	VAL
1	A	19	VAL

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	281/294 (96%)	255 (91%)	26 (9%)	9	21
1	C	273/294 (93%)	238 (87%)	35 (13%)	4	10
2	B	130/157 (83%)	99 (76%)	31 (24%)	0	2
2	D	102/157 (65%)	77 (76%)	25 (24%)	0	2
All	All	786/902 (87%)	669 (85%)	117 (15%)	3	7

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	12	SER
1	A	20	LEU
1	A	21	GLU
1	A	22	LYS
1	A	30	VAL
1	A	33	LEU

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Mol	Chain	Res	Type
1	A	35	ASP
1	A	52	LEU
1	A	71	SER
1	A	75	SER
1	A	77	SER
1	A	84	SER
1	A	120	THR
1	A	156	ASN
1	A	171	LYS
1	A	190	SER
1	A	207	SER
1	A	222	ASP
1	A	272	VAL
1	A	286	ILE
1	A	302	LYS
1	A	308	LYS
1	A	312	LEU
1	A	316	THR
1	A	318	LEU
2	B	10	ILE
2	B	15	THR
2	B	18	VAL
2	B	22	TYR
2	B	24	TYR
2	B	26	HIS
2	B	32	SER
2	B	41	THR
2	B	45	ILE
2	B	49	THR
2	B	51	LYS
2	B	58	LYS
2	B	59	MET
2	B	61	THR
2	B	62	GLN
2	B	84	VAL
2	B	85	ASP
2	B	86	ASP
2	B	99	LEU
2	B	101	LEU
2	B	120	GLU
2	B	123	ARG
2	B	135	ASN

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Mol	Chain	Res	Type
2	B	139	GLU
2	B	145	ASP
2	B	146	ASN
2	B	147	THR
2	B	148	CYS
2	B	149	MET
2	B	158	ASP
2	B	164	GLU
1	C	12	SER
1	C	13	THR
1	C	14	ASP
1	C	15	THR
1	C	17	ASP
1	C	22	LYS
1	C	23	ASN
1	C	26	VAL
1	C	28	HIS
1	C	33	LEU
1	C	34	GLU
1	C	36	LYS
1	C	54	LYS
1	C	71	SER
1	C	77	SER
1	C	82	THR
1	C	109	SER
1	C	110	SER
1	C	113	ARG
1	C	130	LYS
1	C	164	SER
1	C	169	LYS
1	C	171	LYS
1	C	185	SER
1	C	187	ASP
1	C	204	SER
1	C	274	ASP
1	C	279	CYS
1	C	281	THR
1	C	286	ILE
1	C	287	ASN
1	C	288	THR
1	C	311	LYS
1	C	316	THR

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Mol	Chain	Res	Type
1	C	319	ARG
2	D	14	TRP
2	D	15	THR
2	D	19	ASP
2	D	38	LEU
2	D	42	GLN
2	D	48	ILE
2	D	50	ASN
2	D	58	LYS
2	D	60	ASN
2	D	61	THR
2	D	86	ASP
2	D	91	ILE
2	D	97	GLU
2	D	99	LEU
2	D	102	LEU
2	D	103	GLU
2	D	110	TYR
2	D	123	ARG
2	D	126	LEU
2	D	133	ILE
2	D	147	THR
2	D	149	MET
2	D	153	LYS
2	D	159	TYR
2	D	170	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	129	ASN
1	C	31	ASN
1	C	273	HIS
1	C	320	ASN

5.3.3 RNA

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](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.55	0	17,19,21	1.11	2 (11%)
3	NAG	E	2	3	14,14,15	0.68	0	17,19,21	1.28	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	1.76	4 (23%)
3	NAG	F	2	3	14,14,15	0.52	0	17,19,21	0.58	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
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-2.03	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	O5-C1-C2	-3.85	105.22	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O5-C1-C2	-3.73	105.40	111.29
3	F	1	NAG	C2-N2-C7	-3.43	118.02	122.90
3	F	1	NAG	C4-C3-C2	-2.64	107.15	111.02
3	E	1	NAG	C2-N2-C7	-2.33	119.58	122.90
3	E	2	NAG	C3-C4-C5	2.31	114.36	110.24
3	E	1	NAG	C4-C3-C2	-2.26	107.71	111.02
3	F	1	NAG	C3-C4-C5	2.21	114.18	110.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

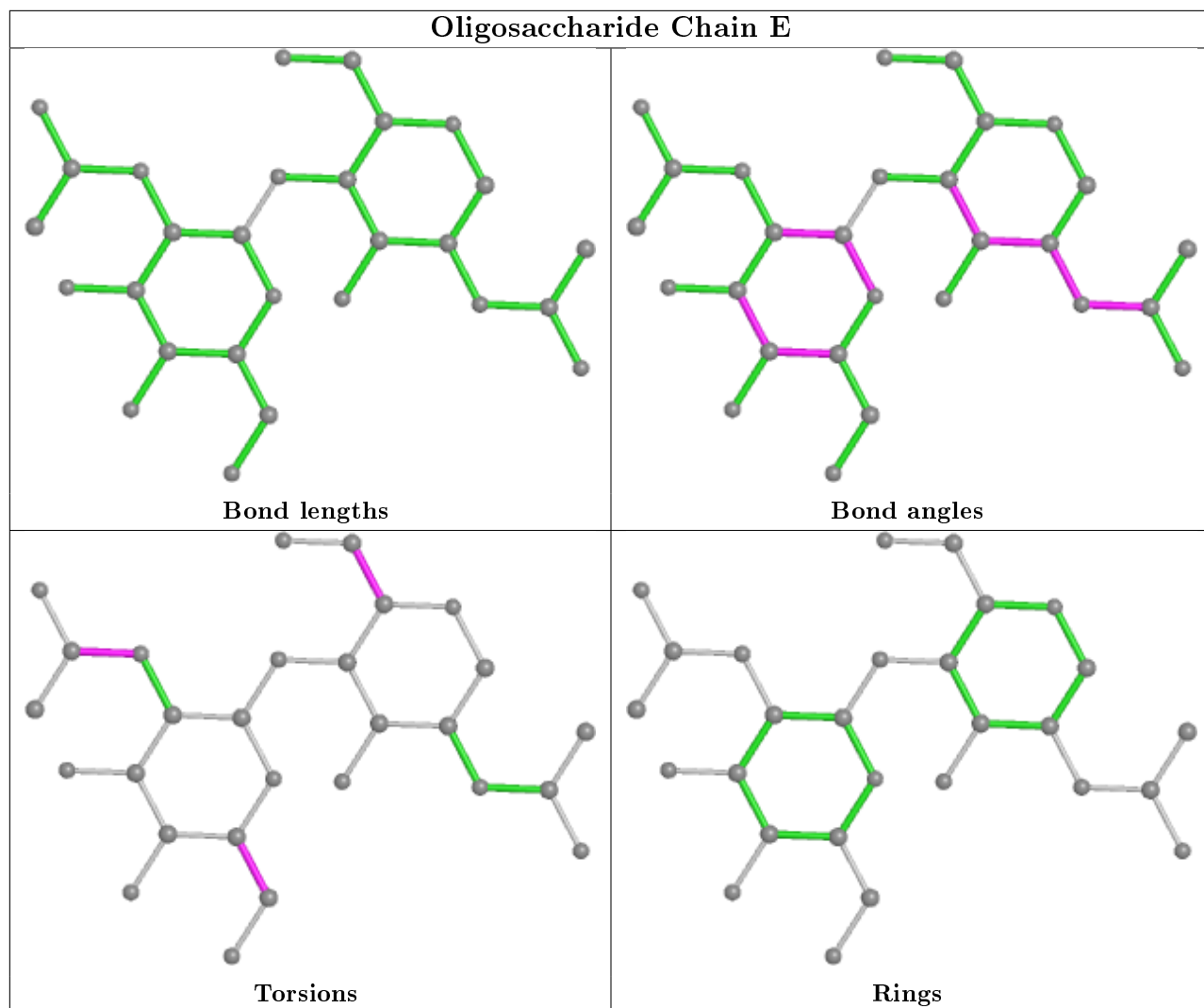
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2

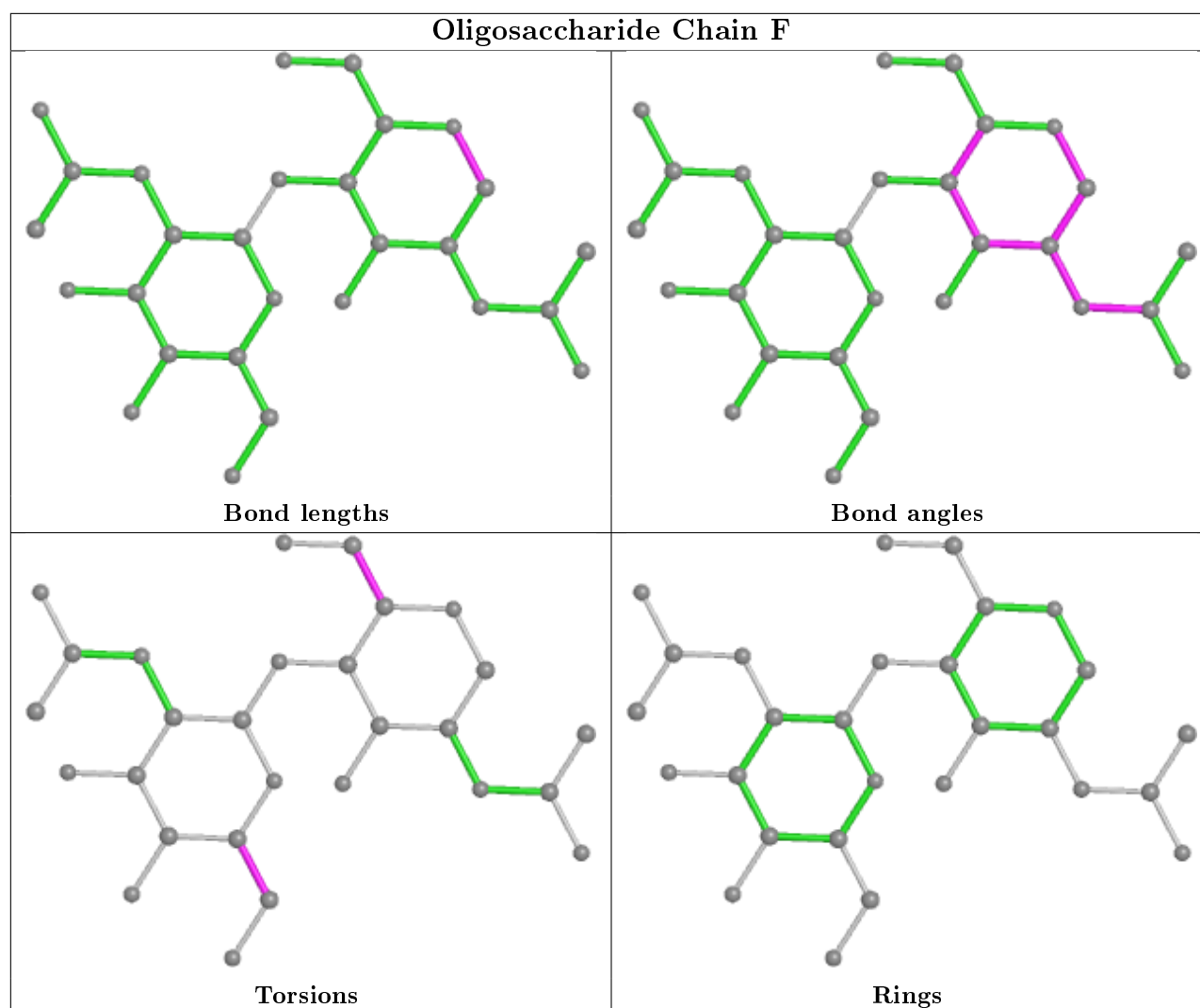
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
3	E	1	NAG	8	0
3	F	1	NAG	8	0

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





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$
4	NAG	A	403	1	14,14,15	0.77	1 (7%)	17,19,21	2.12	7 (41%)
4	NAG	C	404	1	14,14,15	0.45	0	17,19,21	0.88	1 (5%)
4	NAG	C	403	1	14,14,15	1.75	2 (14%)	17,19,21	3.59	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	404	1	14,14,15	0.52	0	17,19,21	1.09	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	403	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	C	404	1	-	4/6/23/26	0/1/1/1
4	NAG	C	403	1	-	1/6/23/26	0/1/1/1
4	NAG	A	404	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	NAG	O5-C1	-4.88	1.35	1.43
4	C	403	NAG	O5-C5	3.81	1.51	1.43
4	A	403	NAG	C1-C2	2.10	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	NAG	O5-C5-C6	-12.28	87.96	107.20
4	C	403	NAG	C1-O5-C5	6.53	121.05	112.19
4	A	403	NAG	C1-O5-C5	4.27	117.97	112.19
4	C	403	NAG	O5-C1-C2	3.48	116.78	111.29
4	A	403	NAG	C8-C7-N2	3.04	121.25	116.10
4	A	403	NAG	O5-C1-C2	3.00	116.03	111.29
4	C	403	NAG	O5-C5-C4	-2.94	103.67	110.83
4	A	403	NAG	O5-C5-C4	-2.88	103.82	110.83
4	A	403	NAG	C2-N2-C7	2.71	126.77	122.90
4	A	403	NAG	C3-C4-C5	-2.60	105.59	110.24
4	A	403	NAG	O5-C5-C6	2.59	111.27	107.20
4	C	404	NAG	O5-C5-C6	2.33	110.86	107.20
4	A	404	NAG	C4-C3-C2	-2.30	107.64	111.02
4	A	404	NAG	C1-O5-C5	2.19	115.15	112.19
4	A	404	NAG	C2-N2-C7	-2.09	119.92	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	403	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	404	NAG	C8-C7-N2-C2
4	C	404	NAG	O7-C7-N2-C2
4	A	403	NAG	C8-C7-N2-C2
4	A	403	NAG	O7-C7-N2-C2
4	A	403	NAG	O5-C5-C6-O6
4	C	404	NAG	C1-C2-N2-C7
4	A	403	NAG	C4-C5-C6-O6
4	A	404	NAG	O5-C5-C6-O6
4	C	404	NAG	C4-C5-C6-O6
4	C	403	NAG	O5-C5-C6-O6
4	A	404	NAG	C8-C7-N2-C2
4	A	404	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	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	321/336 (95%)	0.54	7 (2%) 62 63	38, 59, 119, 133	0
1	C	311/336 (92%)	0.56	13 (4%) 36 35	37, 62, 125, 134	0
2	B	148/182 (81%)	1.00	32 (21%) 0 0	98, 118, 137, 159	0
2	D	115/182 (63%)	1.11	25 (21%) 0 0	114, 137, 150, 153	0
All	All	895/1036 (86%)	0.70	77 (8%) 10 8	37, 82, 141, 159	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	58	LYS	6.6
2	B	121	LYS	5.7
2	D	119	TYR	4.9
1	A	318	LEU	4.8
2	B	21	TRP	4.7
2	D	163	SER	4.6
2	B	38	LEU	4.5
1	A	321	VAL	4.4
2	B	17	MET	4.1
2	B	65	ALA	4.0
2	D	130	ALA	3.8
1	C	314	LEU	3.8
2	B	62	GLN	3.7
2	B	22	TYR	3.4
1	C	70	LEU	3.3
2	B	63	PHE	3.2
2	B	85	ASP	3.2
2	D	57	GLU	3.2
2	B	43	ASN	3.1
1	C	30	VAL	3.1
2	B	61	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	108	LEU	3.1
2	D	124	SER	3.0
2	B	40	SER	2.9
1	A	9	ALA	2.9
2	D	53	ASN	2.9
2	D	12	GLY	2.8
2	D	15	THR	2.8
1	C	313	ARG	2.8
2	B	99	LEU	2.8
1	C	17	ASP	2.7
1	A	8	HIS	2.7
2	B	46	ASP	2.6
2	D	83	LYS	2.6
2	B	122	VAL	2.6
2	D	17	MET	2.5
2	B	86	ASP	2.5
1	A	70	LEU	2.5
2	D	48	ILE	2.5
1	C	33	LEU	2.5
2	B	126	LEU	2.5
1	C	286	ILE	2.5
2	B	20	GLY	2.5
2	B	147	THR	2.5
1	A	7	TYR	2.4
2	D	120	GLU	2.4
1	C	315	ALA	2.4
1	C	73	ALA	2.4
1	C	18	THR	2.4
1	C	319	ARG	2.4
1	C	290	LEU	2.4
1	A	33	LEU	2.4
2	D	44	ALA	2.4
2	B	48	ILE	2.4
2	B	23	GLY	2.3
2	B	89	LEU	2.3
2	D	91	ILE	2.3
2	D	87	GLY	2.3
2	D	54	SER	2.3
2	D	95	ASN	2.3
2	B	88	PHE	2.3
2	D	154	ASN	2.3
2	B	44	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	102	LEU	2.2
2	D	100	VAL	2.2
2	B	156	THR	2.2
2	B	140	PHE	2.2
2	D	159	TYR	2.2
2	D	101	LEU	2.2
2	D	149	MET	2.1
2	B	55	VAL	2.1
2	B	166	ALA	2.1
2	B	138	PHE	2.1
1	C	312	LEU	2.0
2	B	39	LYS	2.0
2	B	91	ILE	2.0
2	D	45	ILE	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](#)

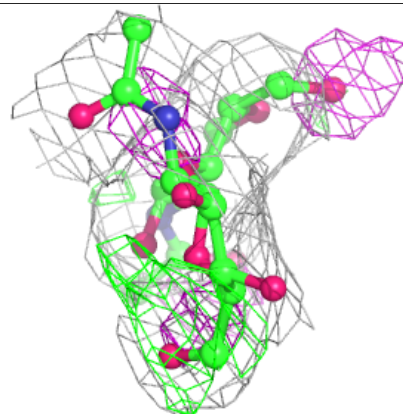
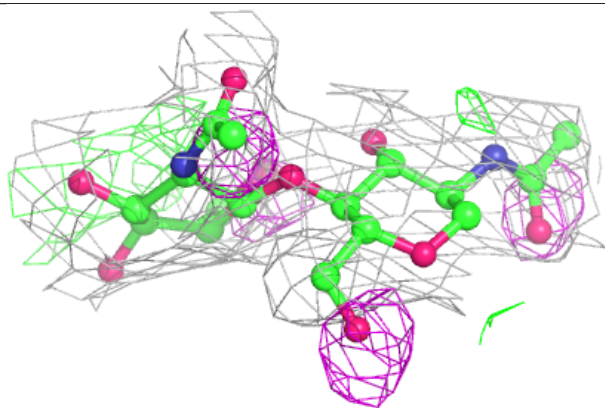
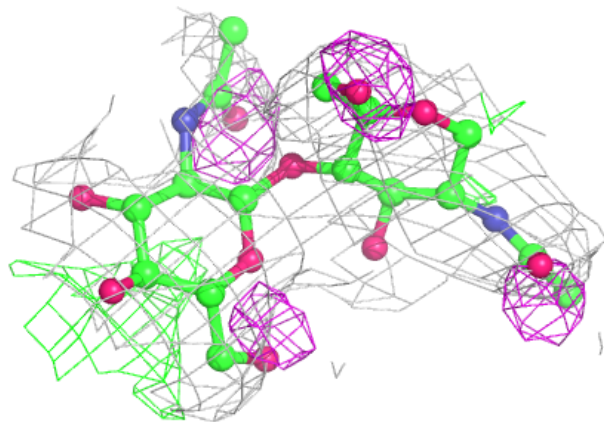
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.52	0.32	85,94,99,103	0
3	NAG	F	1	14/15	0.77	0.23	62,69,77,79	0
3	NAG	E	2	14/15	0.77	0.22	69,80,83,84	0
3	NAG	E	1	14/15	0.86	0.21	57,67,77,78	0

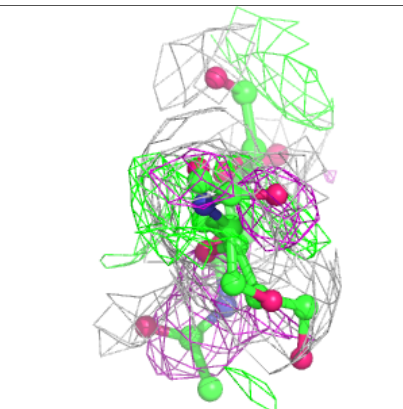
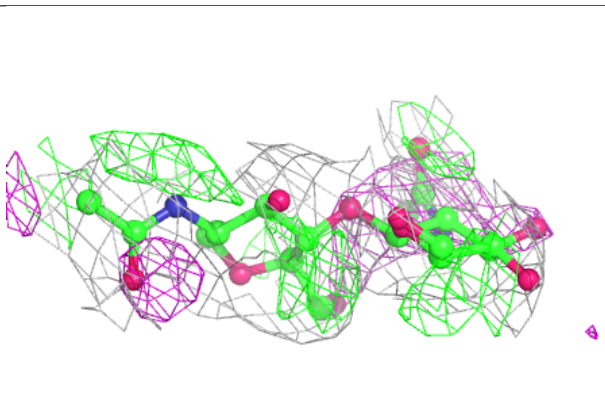
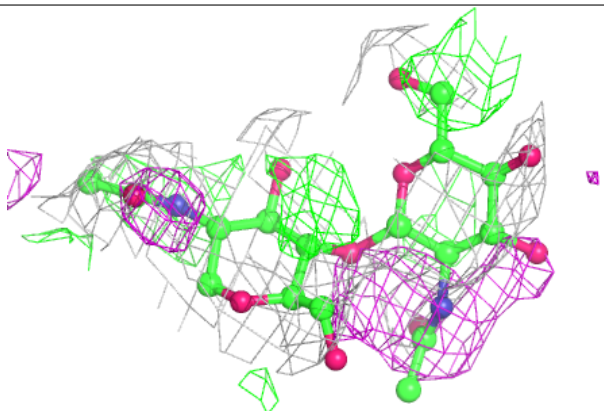
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain 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)



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
4	NAG	C	404	14/15	0.67	0.44	129,134,139,139	0
4	NAG	C	403	14/15	0.79	0.23	124,140,145,147	0
4	NAG	A	403	14/15	0.83	0.19	110,126,141,147	0
4	NAG	A	404	14/15	0.84	0.17	112,114,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.