Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:39 AM BST

PDB ID	:	1DLH
Title	:	CRYSTAL STRUCTURE OF THE HUMAN CLASS II MHC PROTEIN HLA-DR1 COMPLEXED WITH AN INFLUENZA VIRUS PEPTIDE
Authors	:	Stern, L.J.
Deposited on	:	1994-02-15
Resolution	:	2.80 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:

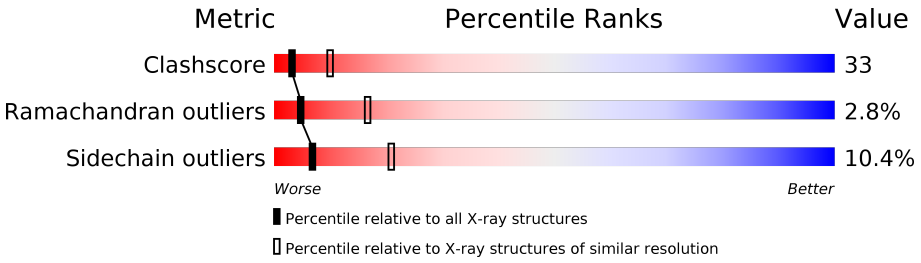
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	180	46% 48% 5% •
1	D	180	47% 46% 6% •
2	B	188	45% 45% 9% •
2	E	188	37% 55% 6% •
3	C	13	23% 77%
3	F	13	23% 69% 8%
4	G	2	100%
4	H	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	521	X	-	-	-
5	NAG	E	521	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6520 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 CLASS II HISTOCOMPATIBILITY ANTIGEN (HLA-DR1) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	10	0	0
			1478	957	240	276	5			
1	D	180	Total	C	N	O	S	10	0	0
			1478	957	240	276	5			

- Molecule 2 is a protein called CLASS II HISTOCOMPATIBILITY ANTIGEN (HLA-DR1) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	14	0	0
			1544	973	277	288	6			
2	E	188	Total	C	N	O	S	14	0	0
			1543	973	277	287	6			

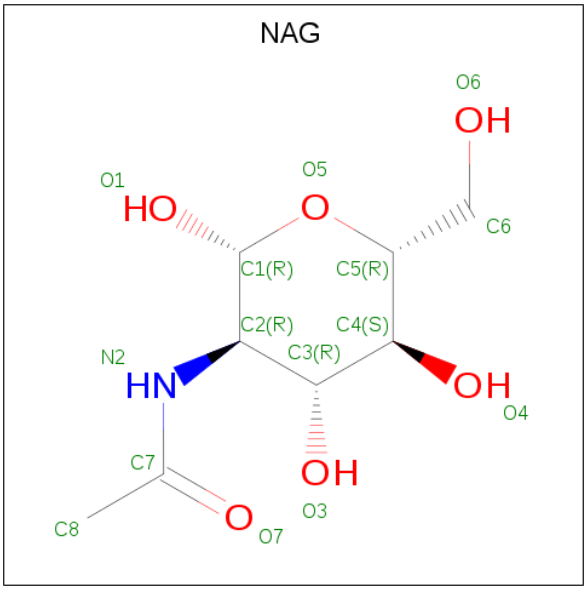
- Molecule 3 is a protein called ENTEROTOXIN TYPE B PRECURSOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			106	69	18	19			
3	F	13	Total	C	N	O	0	0	0
			106	69	18	19			

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

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

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	40	Total O 40 40	0	0
6	C	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	34	Total O 34 34	0	0
6	E	36	Total O 36 36	0	0
6	F	3	Total O 3 3	0	0

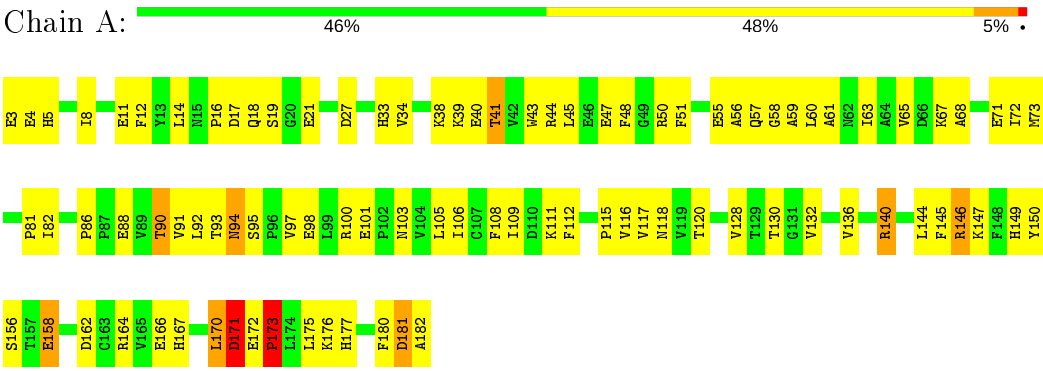
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

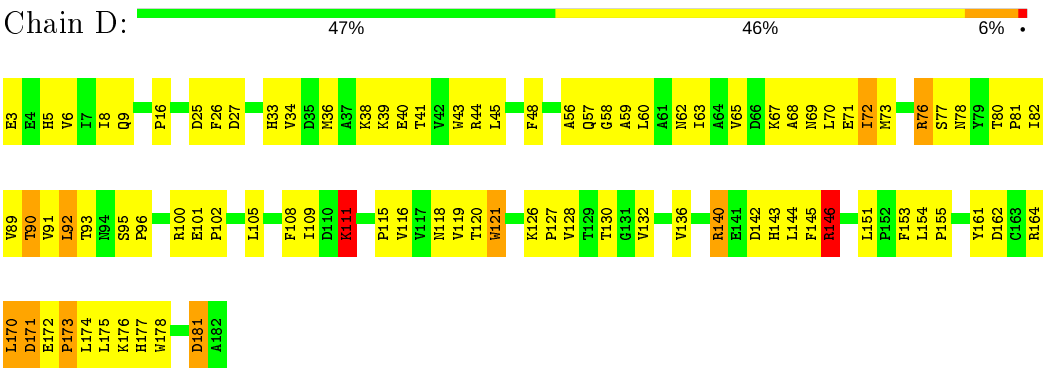
• Molecule 1: CLASS II HISTOCOMPATIBILITY ANTIGEN (HLA-DR1) (ALPHA CHAIN)

Chain A:



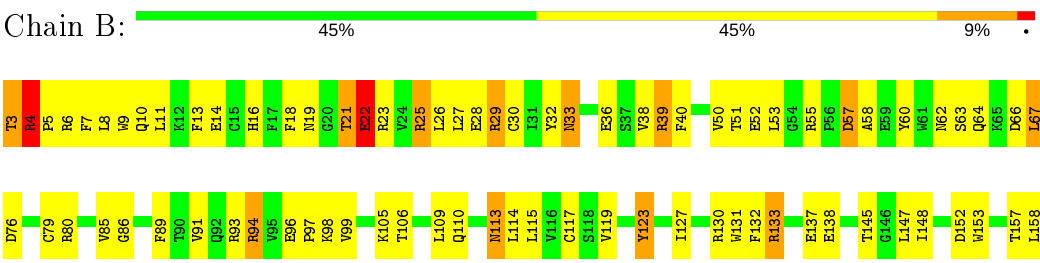
• Molecule 1: CLASS II HISTOCOMPATIBILITY ANTIGEN (HLA-DR1) (ALPHA CHAIN)

Chain D:



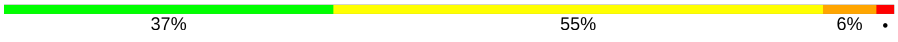
• Molecule 2: CLASS II HISTOCOMPATIBILITY ANTIGEN (HLA-DR1) (BETA CHAIN)

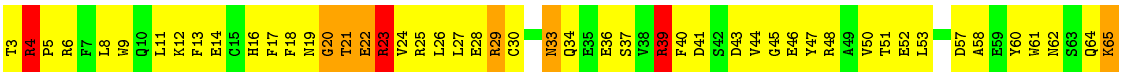
Chain B:



• Molecule 2: CLASS II HISTOCOMPATIBILITY ANTIGEN (HLA-DR1) (BETA CHAIN)

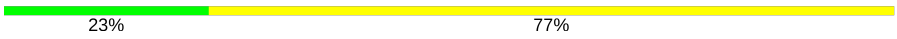
Chain E:

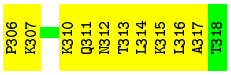




• Molecule 3: ENTEROTOXIN TYPE B PRECURSOR

Chain C:





• Molecule 3: ENTEROTOXIN TYPE B PRECURSOR

Chain F:

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

Chain G:

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

Chain H:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.60Å 94.60Å 247.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.205 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6520	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.96	2/1523 (0.1%)	1.03	2/2077 (0.1%)
1	D	1.01	1/1523 (0.1%)	1.04	3/2077 (0.1%)
2	B	0.98	2/1584 (0.1%)	1.06	2/2152 (0.1%)
2	E	0.96	0/1583	1.06	4/2150 (0.2%)
3	C	0.91	0/107	0.94	0/141
3	F	0.98	0/107	1.02	0/141
All	All	0.98	5/6427 (0.1%)	1.05	11/8738 (0.1%)

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
2	B	0	2
2	E	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	TYR	CD2-CE2	7.10	1.50	1.39
2	B	22	GLU	CG-CD	6.49	1.61	1.51
2	B	69	GLU	CG-CD	5.67	1.60	1.51
1	D	121	TRP	CB-CG	-5.51	1.40	1.50
1	A	158	GLU	CG-CD	5.20	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	146	ARG	NE-CZ-NH2	-7.08	116.76	120.30
2	E	39	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	D	92	LEU	CB-CG-CD2	-5.57	101.53	111.00
2	E	20	GLY	N-CA-C	-5.56	99.19	113.10
2	E	164	VAL	N-CA-C	-5.50	96.14	111.00
1	D	9	GLN	N-CA-C	-5.41	96.40	111.00
1	A	146	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	E	166	ARG	N-CA-C	-5.20	96.97	111.00
2	B	114	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	171	ASP	CB-CG-OD1	5.07	122.86	118.30
2	B	67	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	123	TYR	Sidechain
2	B	22	GLU	Mainchain
2	E	123	TYR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1478	0	1410	92	0
1	D	1478	0	1410	89	0
2	B	1544	0	1476	128	0
2	E	1543	0	1476	139	0
3	C	106	0	119	12	0
3	F	106	0	119	14	0
4	G	28	0	24	0	0
4	H	28	0	24	1	0
5	A	14	0	13	2	0
5	B	14	0	13	4	0
5	D	14	0	13	0	0
5	E	14	0	13	3	0
6	A	38	0	0	18	0
6	B	40	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2	0	0	0	0
6	D	34	0	0	17	0
6	E	36	0	0	14	0
6	F	3	0	0	1	0
All	All	6520	0	6110	413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (413) 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)
2:B:3:THR:HG22	2:B:6:ARG:NH2	1.67	1.07
1:D:164:ARG:HE	1:D:173:PRO:HB3	1.25	0.99
2:E:3:THR:HG22	2:E:6:ARG:NH2	1.76	0.99
1:A:164:ARG:HE	1:A:173:PRO:HB3	1.24	0.98
1:A:175:LEU:HG	6:A:534:HOH:O	1.67	0.94
2:E:23:ARG:HD3	6:E:524:HOH:O	1.68	0.94
1:D:132:VAL:HG12	1:D:151:LEU:HD12	1.51	0.92
2:B:70:GLN:HG2	6:B:532:HOH:O	1.72	0.90
1:A:90:THR:HG23	6:A:533:HOH:O	1.72	0.88
1:A:39:LYS:HG2	1:A:60:LEU:HD11	1.55	0.87
1:A:39:LYS:HB3	6:A:509:HOH:O	1.75	0.86
1:A:16:PRO:HG2	2:B:4:ARG:HD3	1.56	0.85
1:A:51:PHE:HD1	6:A:528:HOH:O	1.60	0.84
1:A:86:PRO:HB2	1:A:170:LEU:HD13	1.58	0.83
2:B:7:PHE:HA	6:B:558:HOH:O	1.78	0.82
2:E:29:ARG:HH11	2:E:29:ARG:HG2	1.43	0.82
1:D:39:LYS:HG2	1:D:60:LEU:HD11	1.61	0.82
1:A:76:ARG:HG3	2:B:53:LEU:HD22	1.63	0.80
1:A:50:ARG:N	6:A:528:HOH:O	2.14	0.80
6:D:524:HOH:O	2:E:34:GLN:HG2	1.80	0.79
1:D:86:PRO:HB2	1:D:170:LEU:HD13	1.62	0.79
2:E:96:GLU:HG2	2:E:97:PRO:HD2	1.65	0.79
2:B:3:THR:HG22	2:B:6:ARG:HH21	1.48	0.79
1:D:115:PRO:HD3	1:D:145:PHE:CE2	2.18	0.78
1:D:153:PHE:CE2	1:D:155:PRO:HG3	2.19	0.77
2:B:26:LEU:HD13	2:B:79:CYS:SG	2.25	0.77
1:D:132:VAL:HG12	1:D:151:LEU:CD1	2.15	0.76
1:A:180:PHE:HE1	1:A:182:ALA:HB2	1.51	0.76
1:A:164:ARG:NE	1:A:173:PRO:HB3	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:22:GLU:HG3	5:E:521:NAG:C1	2.16	0.76
1:D:36:MET:SD	1:D:63:ILE:HD12	2.26	0.75
1:A:3:GLU:HB3	2:B:18:PHE:CE2	2.21	0.75
1:A:90:THR:HA	1:A:176:LYS:HE3	1.69	0.74
1:A:51:PHE:N	6:A:528:HOH:O	2.19	0.74
2:E:36:GLU:HG2	2:E:50:VAL:HG21	1.70	0.74
2:B:119:VAL:HG11	2:B:127:ILE:CD1	2.18	0.73
1:D:164:ARG:NE	1:D:173:PRO:HB3	2.02	0.73
2:B:119:VAL:HG11	2:B:127:ILE:HD11	1.70	0.73
1:D:16:PRO:HG2	2:E:4:ARG:HD3	1.69	0.73
2:E:22:GLU:N	6:E:526:HOH:O	2.22	0.72
2:B:3:THR:HG22	2:B:6:ARG:HH22	1.54	0.72
1:A:14:LEU:HB3	6:A:535:HOH:O	1.88	0.71
2:E:141:GLY:HA2	6:E:532:HOH:O	1.89	0.71
2:B:4:ARG:NH1	2:B:6:ARG:HH22	1.89	0.71
1:D:178:TRP:O	6:D:530:HOH:O	2.09	0.71
2:B:29:ARG:HG2	2:B:29:ARG:HH11	1.55	0.70
2:B:105:LYS:HE2	1:D:181:ASP:OD2	1.91	0.70
2:E:85:VAL:HG13	3:F:306:PRO:HB2	1.72	0.70
2:B:23:ARG:HD3	6:B:535:HOH:O	1.91	0.70
2:B:67:LEU:HD11	3:C:314:LEU:HD22	1.73	0.70
2:B:69:GLU:HA	2:B:69:GLU:OE1	1.92	0.70
1:A:98:GLU:HB2	1:A:101:GLU:HB2	1.74	0.69
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.27	0.69
2:E:3:THR:HG22	2:E:6:ARG:HH21	1.54	0.68
2:E:9:TRP:CH2	2:E:30:CYS:HB3	2.28	0.68
2:E:105:LYS:NZ	6:E:539:HOH:O	2.27	0.68
2:E:29:ARG:NH1	2:E:29:ARG:HG2	2.09	0.68
1:D:140:ARG:HG3	1:D:144:LEU:O	1.93	0.68
2:E:3:THR:HG23	2:E:4:ARG:NH1	2.09	0.67
1:D:161:TYR:O	6:D:530:HOH:O	2.12	0.67
2:B:8:LEU:HD23	6:B:537:HOH:O	1.94	0.67
2:E:43:ASP:N	6:E:546:HOH:O	2.11	0.67
2:B:22:GLU:HG3	5:B:521:NAG:C1	2.24	0.67
2:B:109:LEU:HD21	2:B:190:ALA:HB1	1.78	0.66
1:D:142:ASP:O	6:D:524:HOH:O	2.14	0.66
1:D:105:LEU:HG	1:D:153:PHE:CE1	2.30	0.66
2:E:4:ARG:NH1	2:E:6:ARG:HH22	1.94	0.66
1:D:115:PRO:HD3	1:D:145:PHE:HE2	1.61	0.66
2:E:53:LEU:HD12	6:E:525:HOH:O	1.96	0.66
2:B:85:VAL:HG13	3:C:306:PRO:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:O	1:A:71:GLU:HG2	1.95	0.65
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.32	0.65
2:E:25:ARG:NH2	2:E:27:LEU:HD13	2.11	0.65
2:E:173:CYS:O	2:E:185:THR:HA	1.96	0.65
1:D:86:PRO:CB	1:D:170:LEU:HD13	2.27	0.65
1:A:132:VAL:HG12	1:A:151:LEU:CD1	2.27	0.65
2:B:16:HIS:N	6:B:550:HOH:O	2.30	0.64
2:E:3:THR:CG2	2:E:4:ARG:NH1	2.61	0.64
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.33	0.64
1:D:90:THR:HA	1:D:176:LYS:HE3	1.80	0.63
2:B:7:PHE:HD1	2:B:32:TYR:HH	1.45	0.63
1:D:96:PRO:HB2	6:D:513:HOH:O	1.99	0.63
2:E:3:THR:HG22	2:E:4:ARG:HH11	1.64	0.62
3:F:312:ASN:ND2	6:F:133:HOH:O	2.30	0.62
2:E:58:ALA:O	2:E:62:ASN:HB2	1.99	0.62
1:A:140:ARG:HG3	1:A:144:LEU:O	2.00	0.62
1:A:175:LEU:HD12	2:E:142:VAL:O	2.00	0.62
1:A:132:VAL:HG12	1:A:151:LEU:HD12	1.81	0.62
2:E:132:PHE:CE1	2:E:137:GLU:HB2	2.35	0.62
2:B:18:PHE:HB2	2:B:23:ARG:HB3	1.82	0.61
1:A:8:ILE:HG12	2:B:14:GLU:HB3	1.82	0.61
1:A:19:SER:N	6:A:535:HOH:O	2.26	0.61
1:A:82:ILE:HG22	2:B:6:ARG:HB2	1.82	0.61
2:E:133:ARG:HG3	2:E:171:TYR:CE2	2.36	0.61
1:A:44:ARG:O	1:A:45:LEU:HD23	2.01	0.60
2:E:99:VAL:HG12	2:E:186:VAL:HG11	1.82	0.60
1:A:166:GLU:HG2	6:A:527:HOH:O	2.00	0.60
2:E:107:GLN:HB2	2:E:108:PRO:CD	2.31	0.60
2:E:29:ARG:HH11	2:E:29:ARG:CG	2.13	0.60
2:E:26:LEU:HD13	2:E:79:CYS:SG	2.42	0.60
2:B:171:TYR:O	2:B:187:GLU:HA	2.02	0.59
2:B:19:ASN:ND2	5:B:521:NAG:C7	2.65	0.59
1:D:108:PHE:HE1	1:D:146:ARG:HG3	1.67	0.59
1:D:88:GLU:OE1	1:D:111:LYS:HE3	2.02	0.59
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.37	0.59
2:B:23:ARG:NH2	6:B:526:HOH:O	2.35	0.59
2:B:21:THR:HG23	2:B:80:ARG:HE	1.68	0.59
2:B:93:ARG:O	2:B:94:ARG:NH1	2.35	0.59
1:A:39:LYS:CG	1:A:60:LEU:HD11	2.31	0.59
2:B:85:VAL:O	2:B:85:VAL:HG12	2.02	0.59
2:E:65:LYS:O	2:E:69:GLU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:VAL:HG22	3:F:306:PRO:HB3	1.85	0.59
2:B:4:ARG:HD2	2:B:4:ARG:N	2.16	0.58
1:A:181:ASP:OD1	2:E:105:LYS:HE2	2.02	0.58
1:A:27:ASP:HB2	6:B:527:HOH:O	2.03	0.58
2:E:141:GLY:O	2:E:162:GLU:HG3	2.03	0.58
2:E:3:THR:CG2	2:E:4:ARG:HH11	2.15	0.58
2:E:41:ASP:OD1	6:E:546:HOH:O	2.17	0.58
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.37	0.58
2:B:99:VAL:HG12	2:B:186:VAL:HG11	1.85	0.58
2:B:4:ARG:HD2	2:B:4:ARG:H	1.69	0.57
2:B:3:THR:CG2	2:B:4:ARG:NH1	2.67	0.57
2:E:3:THR:HG22	2:E:6:ARG:HH22	1.66	0.57
2:B:29:ARG:HG2	2:B:29:ARG:NH1	2.18	0.57
1:D:143:HIS:HD2	2:E:12:LYS:NZ	2.03	0.57
1:A:38:LYS:HB2	1:A:40:GLU:HG2	1.87	0.57
2:B:3:THR:HG22	2:B:4:ARG:HH11	1.69	0.57
2:B:4:ARG:HH11	2:B:6:ARG:NH2	2.02	0.57
2:B:33:ASN:OD1	6:B:558:HOH:O	2.17	0.57
2:B:7:PHE:HD1	2:B:32:TYR:OH	1.87	0.56
2:E:116:VAL:HG22	2:E:160:MET:CE	2.35	0.56
2:E:26:LEU:CD1	2:E:79:CYS:SG	2.93	0.56
1:A:48:PHE:C	6:A:528:HOH:O	2.43	0.56
1:D:116:VAL:HG12	4:H:1:NAG:H82	1.87	0.56
1:D:65:VAL:HB	3:F:313:THR:OG1	2.06	0.56
2:B:26:LEU:CD1	2:B:79:CYS:SG	2.94	0.56
2:E:11:LEU:HD21	2:E:13:PHE:CZ	2.41	0.56
2:E:21:THR:N	6:E:526:HOH:O	2.38	0.56
1:A:34:VAL:HG22	1:A:41:THR:HG22	1.88	0.56
2:B:132:PHE:CE1	2:B:137:GLU:HB2	2.41	0.56
2:B:173:CYS:O	2:B:185:THR:HA	2.05	0.56
1:A:153:PHE:O	6:A:529:HOH:O	2.18	0.56
2:B:97:PRO:HG2	2:B:184:LEU:CD1	2.35	0.56
1:D:6:VAL:N	6:D:525:HOH:O	2.36	0.56
2:E:69:GLU:HA	2:E:69:GLU:OE1	2.05	0.56
1:A:103:ASN:N	6:A:529:HOH:O	2.35	0.56
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.86	0.56
1:A:73:MET:HG2	3:C:316:LEU:CD1	2.36	0.56
2:B:157:THR:O	2:B:158:LEU:HD12	2.05	0.55
2:B:33:ASN:ND2	6:B:558:HOH:O	2.38	0.55
2:E:67:LEU:HD11	3:F:314:LEU:HD22	1.87	0.55
1:A:128:VAL:HG11	1:A:151:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:TYR:N	6:D:530:HOH:O	2.36	0.55
1:D:87:PRO:HD2	1:D:170:LEU:HD22	1.88	0.55
1:D:38:LYS:HB2	1:D:40:GLU:HG2	1.88	0.55
2:B:10:GLN:NE2	6:B:541:HOH:O	2.38	0.55
1:D:5:HIS:HB3	6:D:525:HOH:O	2.06	0.55
2:E:123:TYR:O	2:E:177:HIS:HE1	1.89	0.55
2:E:96:GLU:CG	2:E:97:PRO:HD2	2.36	0.55
2:E:89:PHE:O	2:E:93:ARG:HB2	2.07	0.55
1:D:162:ASP:HB3	1:D:175:LEU:HD22	1.88	0.55
2:E:18:PHE:O	2:E:22:GLU:O	2.24	0.55
2:E:18:PHE:HB2	2:E:23:ARG:HB3	1.89	0.54
1:A:108:PHE:HE1	1:A:146:ARG:HG3	1.72	0.54
2:E:109:LEU:O	2:E:110:GLN:HB2	2.07	0.54
2:B:4:ARG:NH1	2:B:6:ARG:NH2	2.56	0.54
1:D:128:VAL:HG11	1:D:151:LEU:HD11	1.89	0.54
2:E:41:ASP:CG	6:E:546:HOH:O	2.45	0.54
2:B:11:LEU:HD21	2:B:13:PHE:CE1	2.42	0.54
2:B:85:VAL:HG21	3:C:307:LYS:O	2.07	0.54
2:E:152:ASP:O	2:E:153:TRP:HB2	2.07	0.54
1:D:3:GLU:OE1	2:E:16:HIS:HB3	2.07	0.54
2:E:28:GLU:HB3	2:E:40:PHE:HB3	1.88	0.54
5:A:501:NAG:H81	2:E:48:ARG:HH21	1.73	0.54
2:E:11:LEU:HD21	2:E:13:PHE:CE1	2.43	0.54
2:E:177:HIS:CD2	2:E:178:PRO:HD2	2.43	0.54
1:D:89:VAL:CG2	1:D:174:LEU:HD23	2.38	0.54
1:D:76:ARG:HG3	2:E:53:LEU:HD22	1.89	0.53
2:E:115:LEU:HD21	2:E:188:TRP:CE3	2.43	0.53
1:A:38:LYS:CB	1:A:40:GLU:HG2	2.39	0.53
2:E:116:VAL:HG22	2:E:160:MET:HE2	1.91	0.53
2:E:36:GLU:OE2	2:E:39:ARG:HD2	2.08	0.53
2:B:93:ARG:HG2	2:B:123:TYR:CD1	2.44	0.53
1:A:109:ILE:HG22	1:A:112:PHE:CE1	2.43	0.53
1:A:116:VAL:O	1:A:167:HIS:HD2	1.92	0.53
1:D:161:TYR:C	6:D:530:HOH:O	2.46	0.52
1:A:12:PHE:CE2	1:A:21:GLU:HB3	2.45	0.52
1:A:76:ARG:NH1	2:B:53:LEU:O	2.42	0.52
2:E:119:VAL:HG11	2:E:127:ILE:CD1	2.39	0.52
2:E:19:ASN:C	6:E:526:HOH:O	2.46	0.52
2:B:163:THR:HG21	2:B:171:TYR:CE1	2.45	0.52
1:D:70:LEU:HD13	2:E:9:TRP:HB2	1.90	0.52
1:A:98:GLU:OE1	1:A:101:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:PRO:HD2	2:E:6:ARG:HD3	1.91	0.52
2:B:29:ARG:CG	2:B:29:ARG:HH11	2.22	0.51
2:E:44:VAL:HG12	2:E:44:VAL:O	2.09	0.51
1:A:82:ILE:HB	2:B:33:ASN:OD1	2.10	0.51
2:E:4:ARG:HH11	2:E:6:ARG:NH2	2.07	0.51
2:E:147:LEU:HD21	2:E:155:PHE:CE2	2.45	0.51
1:D:8:ILE:HG12	2:E:14:GLU:HB3	1.92	0.51
2:E:74:ALA:O	2:E:78:TYR:HB3	2.10	0.51
2:E:22:GLU:CD	5:E:521:NAG:H4	2.30	0.51
1:A:65:VAL:O	1:A:68:ALA:HB3	2.11	0.51
2:E:97:PRO:HG2	2:E:184:LEU:CD1	2.40	0.51
1:A:86:PRO:CB	1:A:170:LEU:HD13	2.35	0.51
2:B:4:ARG:HH11	2:B:6:ARG:HH22	1.58	0.51
1:D:161:TYR:CA	6:D:530:HOH:O	2.58	0.51
1:A:65:VAL:HB	3:C:313:THR:OG1	2.11	0.51
2:E:171:TYR:O	2:E:187:GLU:HA	2.11	0.50
1:A:94:ASN:OD1	1:A:106:ILE:HD11	2.12	0.50
2:B:58:ALA:O	2:B:62:ASN:HB2	2.12	0.50
2:B:60:TYR:CE1	2:B:64:GLN:NE2	2.79	0.50
2:B:85:VAL:O	2:B:85:VAL:CG1	2.58	0.50
2:B:96:GLU:HG2	2:B:97:PRO:HD2	1.93	0.50
1:D:128:VAL:CG1	1:D:151:LEU:HD11	2.42	0.50
1:D:39:LYS:CG	1:D:60:LEU:HD11	2.37	0.50
1:A:91:VAL:HG23	1:A:176:LYS:HB3	1.93	0.50
1:A:58:GLY:O	1:A:61:ALA:HB3	2.11	0.50
2:E:4:ARG:H	2:E:4:ARG:HD2	1.76	0.50
1:D:109:ILE:CD1	1:D:119:VAL:HG21	2.42	0.50
2:E:4:ARG:HD2	2:E:4:ARG:N	2.26	0.50
2:B:3:THR:HG23	2:B:4:ARG:NH1	2.27	0.50
1:D:108:PHE:CE1	1:D:146:ARG:HG3	2.46	0.50
1:D:164:ARG:O	1:D:164:ARG:HG3	2.12	0.50
1:D:89:VAL:HG12	1:D:176:LYS:HG3	1.94	0.50
2:E:17:PHE:HD1	2:E:24:VAL:HG22	1.75	0.50
1:A:73:MET:HG3	2:B:9:TRP:CZ3	2.47	0.49
2:B:3:THR:HG22	2:B:4:ARG:NH1	2.25	0.49
2:E:110:GLN:HG2	2:E:166:ARG:HD3	1.93	0.49
1:D:3:GLU:HB3	2:E:18:PHE:CE2	2.48	0.49
2:E:4:ARG:NH1	2:E:6:ARG:NH2	2.61	0.49
2:E:78:TYR:CE1	3:F:311:GLN:HB2	2.47	0.49
2:E:127:ILE:HD11	2:E:175:VAL:CG1	2.43	0.49
1:D:34:VAL:HG11	1:D:59:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:THR:HG22	6:E:533:HOH:O	2.13	0.49
1:D:92:LEU:HD21	2:E:148:ILE:HG21	1.95	0.49
1:A:40:GLU:HG3	1:A:40:GLU:O	2.12	0.49
2:E:99:VAL:CG1	2:E:186:VAL:HG11	2.43	0.49
2:B:62:ASN:HA	2:B:68:LEU:HD21	1.95	0.49
2:B:99:VAL:CG1	2:B:186:VAL:HG11	2.42	0.49
2:E:180:VAL:HB	6:E:529:HOH:O	2.12	0.49
2:E:4:ARG:HH11	2:E:6:ARG:HH22	1.61	0.49
1:A:92:LEU:HD21	2:B:148:ILE:HG21	1.94	0.48
2:B:25:ARG:CZ	2:B:27:LEU:HD13	2.43	0.48
1:D:144:LEU:HD21	2:E:34:GLN:NE2	2.28	0.48
2:B:98:LYS:HE3	6:B:549:HOH:O	2.13	0.48
1:D:176:LYS:NZ	6:D:511:HOH:O	2.46	0.48
1:D:65:VAL:O	1:D:68:ALA:HB3	2.13	0.48
2:E:145:THR:HG23	2:E:158:LEU:O	2.13	0.48
1:D:178:TRP:N	6:D:530:HOH:O	2.42	0.48
2:E:81:HIS:CD2	3:F:309:VAL:CG2	2.96	0.48
1:A:72:ILE:HG22	1:A:73:MET:N	2.27	0.48
1:D:100:ARG:C	1:D:154:LEU:HD11	2.33	0.48
1:A:171:ASP:O	1:A:172:GLU:HB3	2.13	0.48
1:D:91:VAL:N	6:D:511:HOH:O	2.46	0.48
1:A:11:GLU:HA	1:A:21:GLU:O	2.14	0.48
2:B:25:ARG:NH2	2:B:27:LEU:HD13	2.29	0.48
1:D:34:VAL:HG12	1:D:36:MET:HE2	1.96	0.48
2:B:98:LYS:HD2	2:B:98:LYS:C	2.33	0.47
1:D:67:LYS:O	1:D:71:GLU:HG2	2.14	0.47
2:E:119:VAL:HG11	2:E:127:ILE:HD11	1.95	0.47
2:E:3:THR:HG23	2:E:4:ARG:HH12	1.78	0.47
2:B:166:ARG:HG3	2:B:166:ARG:HH11	1.79	0.47
2:E:104:SER:O	2:E:105:LYS:HB2	2.13	0.47
2:E:22:GLU:OE1	5:E:521:NAG:H4	2.14	0.47
2:B:51:THR:HG22	2:E:51:THR:HG22	1.96	0.47
2:E:18:PHE:HZ	6:E:534:HOH:O	1.96	0.47
1:A:81:PRO:CB	2:B:5:PRO:HB3	2.44	0.47
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.49	0.47
2:B:30:CYS:HB2	2:B:38:VAL:HG12	1.96	0.47
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.50	0.47
1:D:116:VAL:O	1:D:167:HIS:HD2	1.97	0.47
1:A:4:GLU:HB3	1:A:5:HIS:CD2	2.50	0.47
2:B:97:PRO:HG2	2:B:184:LEU:HD11	1.96	0.47
2:E:93:ARG:O	2:E:94:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:PRO:HG2	2:E:184:LEU:HD12	1.97	0.47
1:D:43:TRP:CE3	1:D:48:PHE:HB3	2.50	0.47
1:A:115:PRO:HD3	1:A:145:PHE:CE2	2.50	0.46
1:D:57:GLN:OE1	1:D:60:LEU:HD12	2.16	0.46
2:E:112:HIS:HA	2:E:163:THR:O	2.14	0.46
2:E:28:GLU:O	2:E:39:ARG:HA	2.16	0.46
2:E:93:ARG:HG2	2:E:123:TYR:CD1	2.50	0.46
2:E:96:GLU:HG3	2:E:180:VAL:HG23	1.98	0.46
1:A:86:PRO:HB2	1:A:170:LEU:CD1	2.38	0.46
2:E:166:ARG:HG3	2:E:166:ARG:HH11	1.80	0.46
1:D:101:GLU:OE1	1:D:101:GLU:HA	2.16	0.46
1:A:147:LYS:HD3	1:A:149:HIS:HE1	1.81	0.46
1:A:132:VAL:HG12	1:A:151:LEU:HD13	1.98	0.46
1:A:16:PRO:CD	2:B:6:ARG:HD3	2.46	0.46
2:E:147:LEU:HG	2:E:155:PHE:HD2	1.81	0.46
2:E:3:THR:CG2	2:E:6:ARG:NH2	2.65	0.46
1:A:19:SER:CA	6:A:535:HOH:O	2.63	0.46
1:D:89:VAL:HG23	1:D:174:LEU:HD23	1.98	0.46
1:A:33:HIS:CG	1:A:136:VAL:HG11	2.51	0.46
2:B:86:GLY:HA2	2:B:89:PHE:CE2	2.51	0.45
2:E:127:ILE:HD11	2:E:175:VAL:HG13	1.97	0.45
1:A:12:PHE:C	1:A:12:PHE:CD1	2.90	0.45
2:B:166:ARG:NE	6:B:536:HOH:O	2.28	0.45
2:B:23:ARG:CD	6:B:535:HOH:O	2.58	0.45
1:A:73:MET:HG2	3:C:316:LEU:HD11	1.98	0.45
1:A:73:MET:HG2	3:C:316:LEU:HD13	1.99	0.45
2:B:96:GLU:CG	2:B:97:PRO:HD2	2.47	0.45
2:E:37:SER:C	2:E:50:VAL:HG22	2.37	0.45
1:D:72:ILE:HG22	1:D:73:MET:N	2.31	0.45
1:A:81:PRO:HB3	2:B:5:PRO:HB3	1.98	0.45
2:B:110:GLN:HG2	6:B:536:HOH:O	2.16	0.45
1:A:3:GLU:HA	2:B:18:PHE:CD2	2.52	0.45
2:E:70:GLN:HE22	2:E:74:ALA:HB2	1.82	0.45
2:E:61:TRP:HA	2:E:64:GLN:NE2	2.32	0.45
1:A:77:SER:O	1:A:78:ASN:CB	2.65	0.44
2:E:92:GLN:NE2	6:E:549:HOH:O	2.49	0.44
2:B:36:GLU:OE2	2:B:39:ARG:NH1	2.51	0.44
1:D:121:TRP:O	1:D:127:PRO:HA	2.17	0.44
2:B:55:ARG:NH2	2:E:52:GLU:OE1	2.48	0.44
3:F:307:LYS:HD2	3:F:307:LYS:N	2.33	0.44
1:A:5:HIS:HE1	6:A:523:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LEU:HG	2:B:165:PRO:O	2.16	0.44
1:D:171:ASP:O	1:D:172:GLU:HB3	2.17	0.44
1:D:81:PRO:HB3	2:E:5:PRO:HB3	1.99	0.44
2:B:50:VAL:HG23	2:B:51:THR:HG23	1.99	0.44
2:E:60:TYR:CE1	2:E:64:GLN:NE2	2.86	0.44
2:E:70:GLN:NE2	2:E:74:ALA:HB2	2.33	0.44
1:A:115:PRO:HD2	2:B:8:LEU:HD13	2.00	0.44
1:A:177:HIS:CE1	2:E:162:GLU:OE2	2.71	0.44
2:E:36:GLU:O	2:E:50:VAL:HG23	2.17	0.44
2:E:47:TYR:CD2	2:E:61:TRP:HE3	2.36	0.43
2:B:67:LEU:CD1	3:C:314:LEU:HD22	2.46	0.43
1:A:153:PHE:C	6:A:529:HOH:O	2.56	0.43
1:D:27:ASP:N	6:D:514:HOH:O	2.50	0.43
1:D:5:HIS:ND1	1:D:26:PHE:CZ	2.86	0.43
2:B:33:ASN:CG	6:B:558:HOH:O	2.56	0.43
1:D:82:ILE:HG22	2:E:6:ARG:HB2	2.01	0.43
2:B:57:ASP:O	2:B:58:ALA:C	2.57	0.43
1:A:19:SER:O	6:A:535:HOH:O	2.21	0.43
1:A:16:PRO:HD2	2:B:6:ARG:HD3	2.00	0.43
2:E:44:VAL:CG1	2:E:44:VAL:O	2.66	0.43
2:B:133:ARG:HG2	2:B:171:TYR:CE1	2.54	0.43
2:B:36:GLU:O	2:B:50:VAL:CG2	2.67	0.43
2:B:145:THR:HG23	2:B:158:LEU:O	2.18	0.43
2:B:131:TRP:HE1	2:B:159:VAL:HG12	1.83	0.43
2:B:165:PRO:HA	2:B:169:GLU:OE1	2.18	0.43
2:B:11:LEU:CD2	3:C:313:THR:HG22	2.49	0.43
1:A:88:GLU:OE1	1:A:111:LYS:HE3	2.18	0.43
2:B:162:GLU:OE2	6:B:545:HOH:O	2.21	0.43
2:B:3:THR:HG23	2:B:4:ARG:HH12	1.84	0.43
2:B:60:TYR:CE2	3:C:317:ALA:HA	2.54	0.43
1:D:69:ASN:CG	3:F:316:LEU:HG	2.39	0.43
1:D:73:MET:HG2	3:F:316:LEU:CD1	2.48	0.43
1:D:77:SER:O	1:D:80:THR:HG23	2.19	0.43
2:E:89:PHE:CD1	2:E:90:THR:HG23	2.54	0.43
6:B:545:HOH:O	1:D:177:HIS:ND1	2.31	0.43
6:D:524:HOH:O	2:E:34:GLN:CG	2.54	0.43
2:B:99:VAL:CG2	2:B:175:VAL:HG21	2.49	0.42
1:D:38:LYS:CB	1:D:40:GLU:HG2	2.49	0.42
1:D:16:PRO:CD	2:E:6:ARG:HD3	2.49	0.42
1:D:115:PRO:HD2	2:E:8:LEU:HD13	2.00	0.42
1:A:14:LEU:O	1:A:18:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CD1	6:A:528:HOH:O	2.47	0.42
1:A:58:GLY:O	3:C:310:LYS:HE2	2.19	0.42
2:E:26:LEU:HD12	2:E:79:CYS:SG	2.59	0.42
1:A:108:PHE:CE1	1:A:146:ARG:HG3	2.53	0.42
2:B:52:GLU:O	2:B:55:ARG:HB2	2.19	0.42
1:A:43:TRP:HE3	1:A:48:PHE:HB3	1.83	0.42
1:D:178:TRP:HB3	6:D:530:HOH:O	2.19	0.42
2:E:147:LEU:HD21	2:E:155:PHE:CD2	2.54	0.42
2:E:44:VAL:O	2:E:46:GLU:N	2.52	0.42
2:B:170:VAL:HG12	6:B:525:HOH:O	2.19	0.42
1:D:100:ARG:O	1:D:154:LEU:HD11	2.20	0.42
2:E:17:PHE:HB3	2:E:20:GLY:O	2.20	0.42
2:B:152:ASP:O	2:B:153:TRP:HB2	2.20	0.42
2:B:130:ARG:NH1	2:B:176:GLU:OE2	2.53	0.42
2:E:166:ARG:CG	2:E:166:ARG:HH11	2.33	0.42
2:B:96:GLU:HG3	2:B:180:VAL:HG23	2.02	0.42
2:B:22:GLU:HG3	5:B:521:NAG:O5	2.19	0.42
1:A:162:ASP:HB3	1:A:175:LEU:HD22	2.02	0.41
2:B:109:LEU:O	2:B:110:GLN:HB2	2.20	0.41
2:E:13:PHE:CE2	3:F:311:GLN:HG2	2.54	0.41
1:D:126:LYS:HA	1:D:127:PRO:HD3	1.77	0.41
1:D:62:ASN:CG	3:F:313:THR:HG23	2.40	0.41
1:D:82:ILE:HB	2:E:33:ASN:OD1	2.19	0.41
2:B:170:VAL:HG12	2:B:170:VAL:O	2.19	0.41
2:B:94:ARG:HA	2:B:123:TYR:O	2.20	0.41
1:A:34:VAL:HG11	1:A:59:ALA:HB3	2.01	0.41
2:B:3:THR:CG2	2:B:4:ARG:HH11	2.30	0.41
2:B:91:VAL:HG23	2:B:91:VAL:H	1.68	0.41
2:E:131:TRP:HE1	2:E:159:VAL:HG12	1.86	0.41
1:A:14:LEU:CA	6:A:535:HOH:O	2.69	0.41
1:A:55:GLU:O	1:A:57:GLN:N	2.53	0.41
2:B:113:ASN:HA	2:B:113:ASN:HD22	1.69	0.41
2:B:147:LEU:HD12	2:B:147:LEU:HA	1.88	0.41
2:B:19:ASN:ND2	5:B:521:NAG:O7	2.54	0.41
2:B:28:GLU:O	2:B:39:ARG:HA	2.20	0.41
1:D:118:ASN:HB2	1:D:166:GLU:HB2	2.03	0.41
1:D:33:HIS:CD2	1:D:136:VAL:HG11	2.56	0.41
1:D:44:ARG:O	1:D:45:LEU:HD23	2.21	0.41
1:A:45:LEU:HB3	1:A:47:GLU:OE1	2.21	0.41
2:B:99:VAL:HG22	2:B:175:VAL:HG21	2.02	0.41
2:B:29:ARG:NH1	2:B:36:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:ARG:O	2:E:134:ASN:HB2	2.20	0.41
2:E:64:GLN:O	2:E:66:ASP:N	2.54	0.41
1:D:58:GLY:O	3:F:310:LYS:HE2	2.21	0.41
5:A:501:NAG:H81	2:E:48:ARG:NH2	2.35	0.40
2:B:13:PHE:CE2	3:C:311:GLN:HG2	2.56	0.40
1:D:178:TRP:CA	6:D:530:HOH:O	2.69	0.40
1:D:73:MET:HG3	2:E:9:TRP:CZ3	2.56	0.40
2:E:116:VAL:HG22	2:E:160:MET:HE3	2.02	0.40
2:E:81:HIS:HD2	3:F:309:VAL:HB	1.86	0.40
2:B:63:SER:OG	2:B:64:GLN:N	2.54	0.40
2:E:80:ARG:HG3	2:E:80:ARG:HH11	1.86	0.40
2:B:182:SER:HA	2:B:183:PRO:HD2	1.74	0.40
2:B:28:GLU:HB3	2:B:40:PHE:HB3	2.03	0.40
1:D:100:ARG:HA	1:D:100:ARG:HD3	1.85	0.40
1:D:140:ARG:HD2	1:D:140:ARG:HH11	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	178/180 (99%)	155 (87%)	18 (10%)	5 (3%)	5 17
1	D	178/180 (99%)	159 (89%)	13 (7%)	6 (3%)	3 13
2	B	186/188 (99%)	163 (88%)	19 (10%)	4 (2%)	6 22
2	E	186/188 (99%)	160 (86%)	20 (11%)	6 (3%)	4 13
3	C	11/13 (85%)	11 (100%)	0	0	100 100
3	F	11/13 (85%)	11 (100%)	0	0	100 100
All	All	750/762 (98%)	659 (88%)	70 (9%)	21 (3%)	5 17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	THR
1	D	78	ASN
1	D	111	LYS
2	E	45	GLY
1	A	17	ASP
1	A	78	ASN
2	B	106	THR
2	E	23	ARG
1	A	173	PRO
2	B	33	ASN
1	D	130	THR
2	E	4	ARG
2	E	33	ASN
1	A	56	ALA
2	B	4	ARG
1	D	56	ALA
1	D	72	ILE
1	D	173	PRO
2	E	186	VAL
2	E	135	GLY
2	B	186	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	164/164 (100%)	147 (90%)	17 (10%)	7 21
1	D	164/164 (100%)	150 (92%)	14 (8%)	10 31
2	B	170/170 (100%)	150 (88%)	20 (12%)	5 16
2	E	170/170 (100%)	153 (90%)	17 (10%)	7 22
3	C	12/12 (100%)	10 (83%)	2 (17%)	2 6
3	F	12/12 (100%)	10 (83%)	2 (17%)	2 6
All	All	692/692 (100%)	620 (90%)	72 (10%)	7 21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	63	ILE
1	A	90	THR
1	A	93	THR
1	A	94	ASN
1	A	95	SER
1	A	97	VAL
1	A	100	ARG
1	A	117	VAL
1	A	120	THR
1	A	140	ARG
1	A	156	SER
1	A	158	GLU
1	A	170	LEU
1	A	171	ASP
1	A	173	PRO
1	A	181	ASP
2	B	3	THR
2	B	4	ARG
2	B	21	THR
2	B	25	ARG
2	B	29	ARG
2	B	39	ARG
2	B	57	ASP
2	B	66	ASP
2	B	68	LEU
2	B	69	GLU
2	B	70	GLN
2	B	76	ASP
2	B	94	ARG
2	B	113	ASN
2	B	115	LEU
2	B	133	ARG
2	B	138	GLU
2	B	162	GLU
2	B	170	VAL
2	B	189	ARG
3	C	312	ASN
3	C	315	LYS
1	D	25	ASP
1	D	41	THR
1	D	76	ARG
1	D	90	THR

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Mol	Chain	Res	Type
1	D	93	THR
1	D	95	SER
1	D	102	PRO
1	D	111	LYS
1	D	120	THR
1	D	140	ARG
1	D	146	ARG
1	D	170	LEU
1	D	171	ASP
1	D	181	ASP
2	E	4	ARG
2	E	21	THR
2	E	22	GLU
2	E	23	ARG
2	E	29	ARG
2	E	39	ARG
2	E	57	ASP
2	E	65	LYS
2	E	66	ASP
2	E	68	LEU
2	E	106	THR
2	E	113	ASN
2	E	115	LEU
2	E	133	ARG
2	E	138	GLU
2	E	167	SER
2	E	189	ARG
3	F	312	ASN
3	F	315	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	143	HIS
1	A	149	HIS
1	A	167	HIS
2	B	64	GLN
2	B	70	GLN
2	B	113	ASN
2	B	150	ASN
3	C	311	GLN

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Mol	Chain	Res	Type
1	D	143	HIS
2	E	64	GLN
2	E	81	HIS
2	E	92	GLN
2	E	113	ASN
2	E	150	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	$\#\|Z\| > 2$
4	NAG	G	1	1,4	14,14,15	1.09	0	17,19,21	1.49	4 (23%)
4	NDG	G	2	4	14,14,15	1.19	1 (7%)	17,19,21	1.12	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	1.10	1 (5%)
4	NDG	H	2	4	14,14,15	1.17	1 (7%)	17,19,21	1.17	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NDG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NDG	H	2	4	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NDG	C1-C2	3.78	1.58	1.52
4	G	2	NDG	C1-C2	3.53	1.57	1.52
4	H	1	NAG	O4-C4	2.16	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	C4-C3-C2	-4.09	105.03	111.02
4	G	2	NDG	C4-C3-C2	3.74	116.50	111.02
4	H	2	NDG	C3-C4-C5	-2.86	105.14	110.24
4	G	1	NAG	O4-C4-C3	2.57	116.29	110.35
4	H	1	NAG	C1-C2-N2	-2.35	106.47	110.49
4	G	1	NAG	C2-N2-C7	-2.18	119.80	122.90
4	G	1	NAG	C6-C5-C4	-2.03	108.25	113.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NDG	C3-C2-N2-C7
4	H	2	NDG	C1-C2-N2-C7

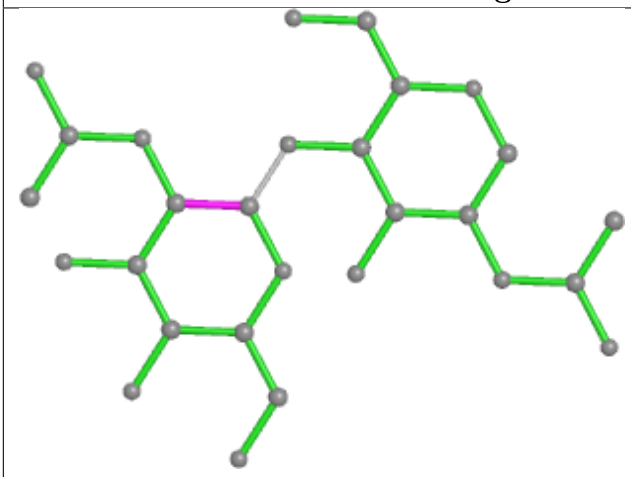
There are no ring outliers.

1 monomer is involved in 1 short contact:

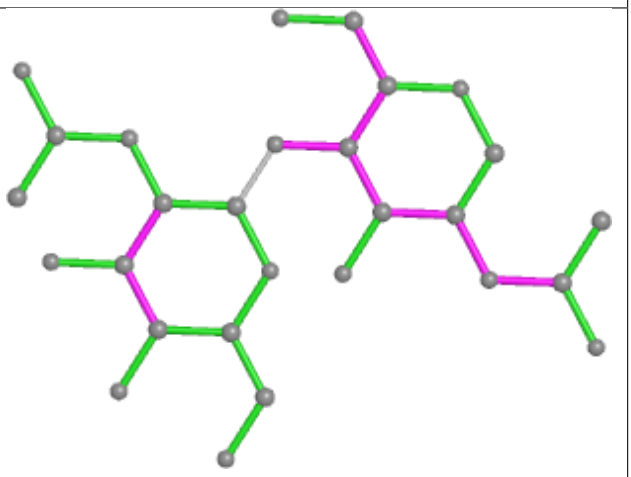
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0

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

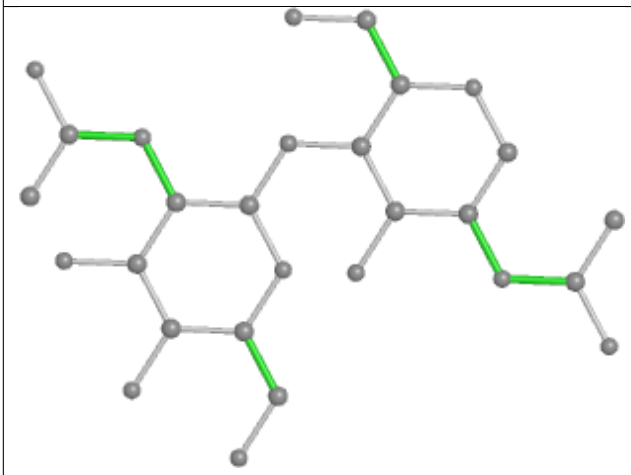
Oligosaccharide Chain G



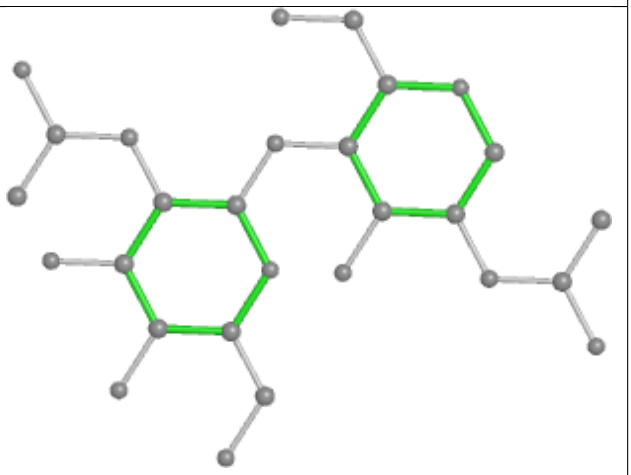
Bond lengths



Bond angles

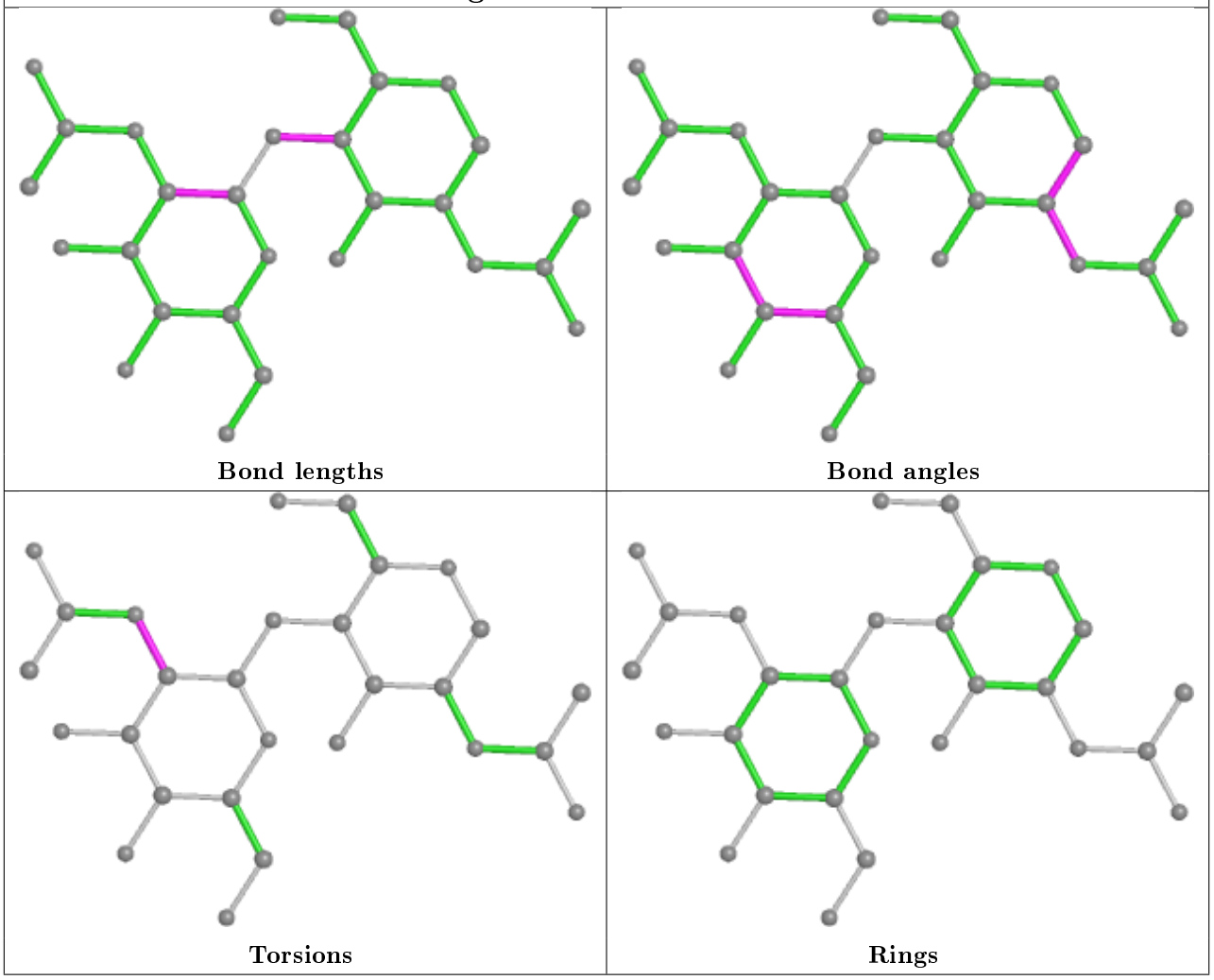


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	501	1	14,14,15	1.30	1 (7%)	17,19,21	1.35	1 (5%)
5	NAG	D	501	1	14,14,15	1.31	1 (7%)	17,19,21	1.18	2 (11%)
5	NAG	B	521	2	14,14,15	1.21	1 (7%)	17,19,21	1.71	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	E	521	2	14,14,15	1.26	2 (14%)	17,19,21	0.89	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	B	521	2	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	E	521	2	1/1/5/7	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	NAG	C1-C2	4.30	1.58	1.52
5	A	501	NAG	C1-C2	3.69	1.57	1.52
5	B	521	NAG	C1-C2	3.42	1.57	1.52
5	E	521	NAG	C1-C2	3.08	1.56	1.52
5	E	521	NAG	O5-C1	2.76	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	521	NAG	C1-O5-C5	5.33	119.42	112.19
5	A	501	NAG	C4-C3-C2	-3.54	105.83	111.02
5	E	521	NAG	C1-O5-C5	3.03	116.30	112.19
5	D	501	NAG	C1-O5-C5	2.78	115.96	112.19
5	B	521	NAG	O5-C1-C2	2.71	115.56	111.29
5	D	501	NAG	C4-C3-C2	-2.42	107.48	111.02
5	B	521	NAG	C6-C5-C4	2.11	117.95	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	521	NAG	C1
5	E	521	NAG	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	521	NAG	C4-C5-C6-O6
5	B	521	NAG	O5-C5-C6-O6
5	E	521	NAG	O5-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	E	521	NAG	C4-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	NAG	2	0
5	B	521	NAG	4	0
5	E	521	NAG	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.