Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2023 – 07:09 PM EDT

PDB ID	:	1R9N
Title	:	Crystal Structure of human dipeptidyl peptidase IV in complex with a decapeptide (tNPY) at 2.3 Ang. Resolution
Authors	:	Aertgeerts, K.; Ye, S.; Tennant, M.G.; Collins, B.; Rogers, J.; Sang, B.-C.; Skene, R.; Webb, D.R.; Prasad, G.S.
Deposited on	:	2003-10-30
Resolution	:	2.30 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 (i) symbol.

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

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

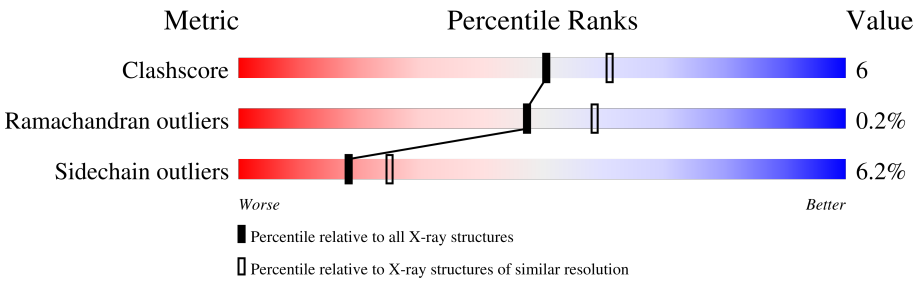
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	739	81% 15% • •
1	B	739	81% 16% • •
1	C	739	86% 11% • •
1	D	739	78% 19% • •
2	E	10	40% 60%
2	F	10	20% 40% 40%
2	G	10	40% 60%
2	H	10	30% 20% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	2	100%
3	J	2	50% 50%
3	K	2	100%
3	L	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	2811	X	-	-	-
4	NAG	A	6851	X	-	-	-
4	NAG	D	2811	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25627 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 Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5963	3827	982	1128	26	0	0	0
1	B	731	5993	3845	991	1131	26	0	0	0
1	C	727	5957	3824	981	1126	26	0	0	0
1	D	727	5957	3824	981	1126	26	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	-	cloning artifact	UNP P27487
A	29	ASP	-	cloning artifact	UNP P27487
A	30	PRO	-	cloning artifact	UNP P27487
A	31	GLY	-	cloning artifact	UNP P27487
A	32	GLY	-	cloning artifact	UNP P27487
A	33	SER	-	cloning artifact	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	28	ALA	-	cloning artifact	UNP P27487
B	29	ASP	-	cloning artifact	UNP P27487
B	30	PRO	-	cloning artifact	UNP P27487
B	31	GLY	-	cloning artifact	UNP P27487
B	32	GLY	-	cloning artifact	UNP P27487
B	33	SER	-	cloning artifact	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487

Continued on next page...

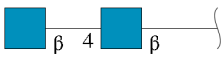
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	HIS	-	expression tag	UNP P27487
C	28	ALA	-	cloning artifact	UNP P27487
C	29	ASP	-	cloning artifact	UNP P27487
C	30	PRO	-	cloning artifact	UNP P27487
C	31	GLY	-	cloning artifact	UNP P27487
C	32	GLY	-	cloning artifact	UNP P27487
C	33	SER	-	cloning artifact	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	28	ALA	-	cloning artifact	UNP P27487
D	29	ASP	-	cloning artifact	UNP P27487
D	30	PRO	-	cloning artifact	UNP P27487
D	31	GLY	-	cloning artifact	UNP P27487
D	32	GLY	-	cloning artifact	UNP P27487
D	33	SER	-	cloning artifact	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- Molecule 2 is a protein called Neuropeptide Y.

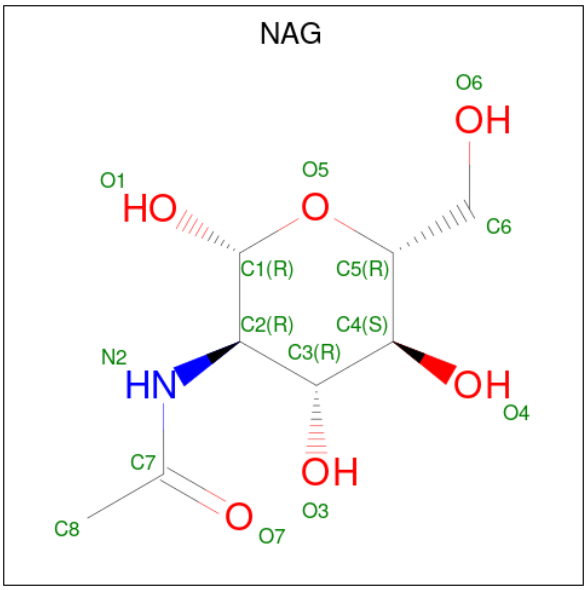
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	4	34	23	5	6	0	0	0
			Total	C	N	O			
2	F	6	49	32	7	10	0	0	0
			Total	C	N	O			
2	G	4	34	23	5	6	0	0	0
			Total	C	N	O			
2	H	5	41	28	6	7	0	0	0

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	342	342	342	0	0
			Total	O		
5	E	3	3	3	0	0
			Total	O		
5	B	361	361	361	0	0
			Total	O		
5	F	4	4	4	0	0
			Total	O		
5	C	277	277	277	0	0
			Total	O		
5	G	6	6	6	0	0
			Total	O		
5	D	254	254	254	0	0
			Total	O		
5	H	2	2	2	0	0

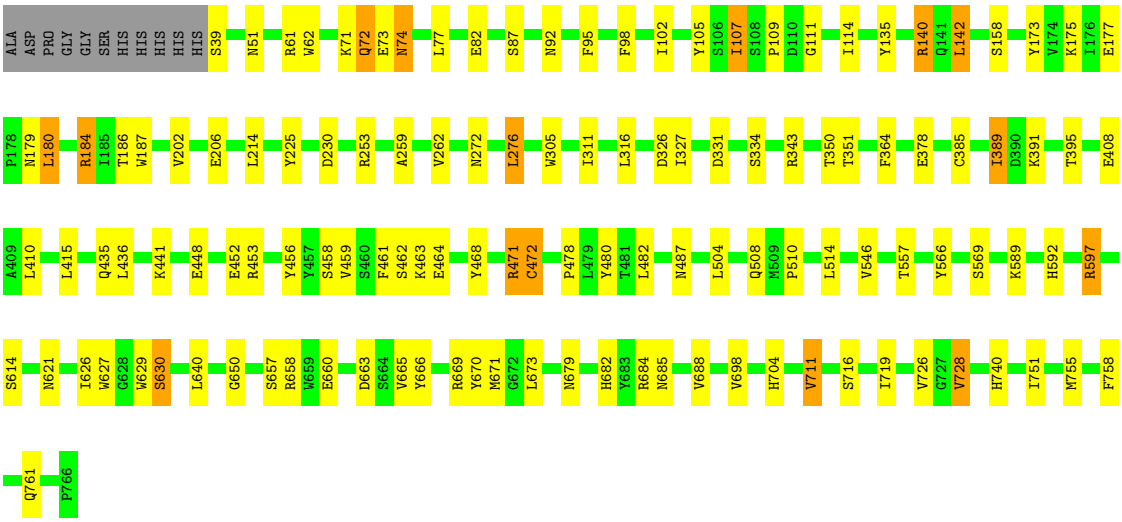
3 Residue-property plots (i)

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.

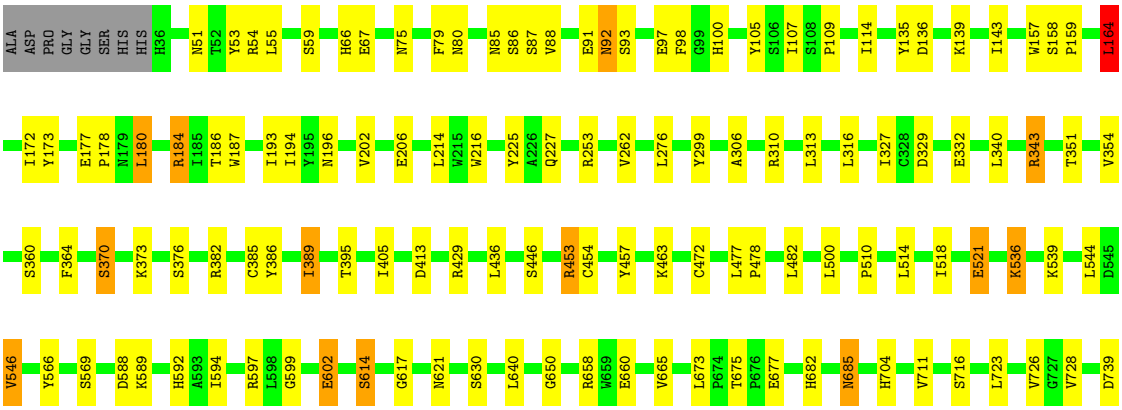
• Molecule 1: Dipeptidyl peptidase IV

Chain A: 81% 15% • •



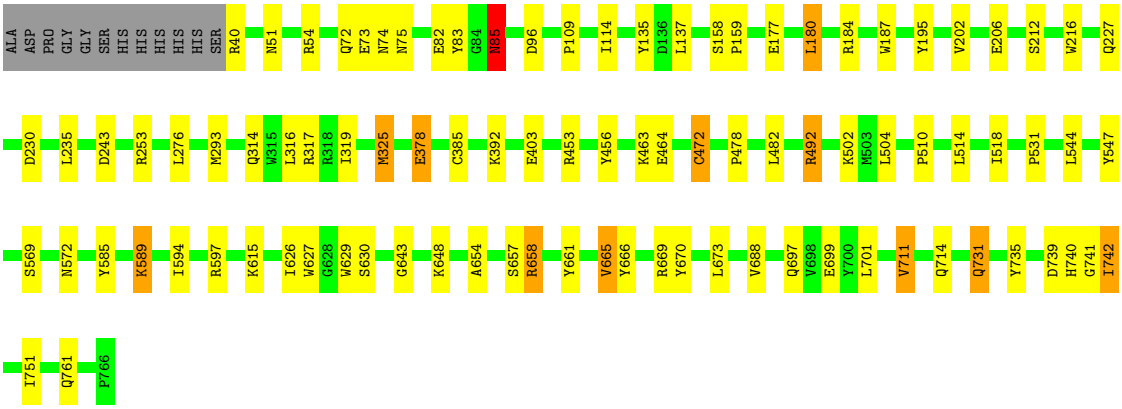
• Molecule 1: Dipeptidyl peptidase IV

Chain B: 81% 16% • •



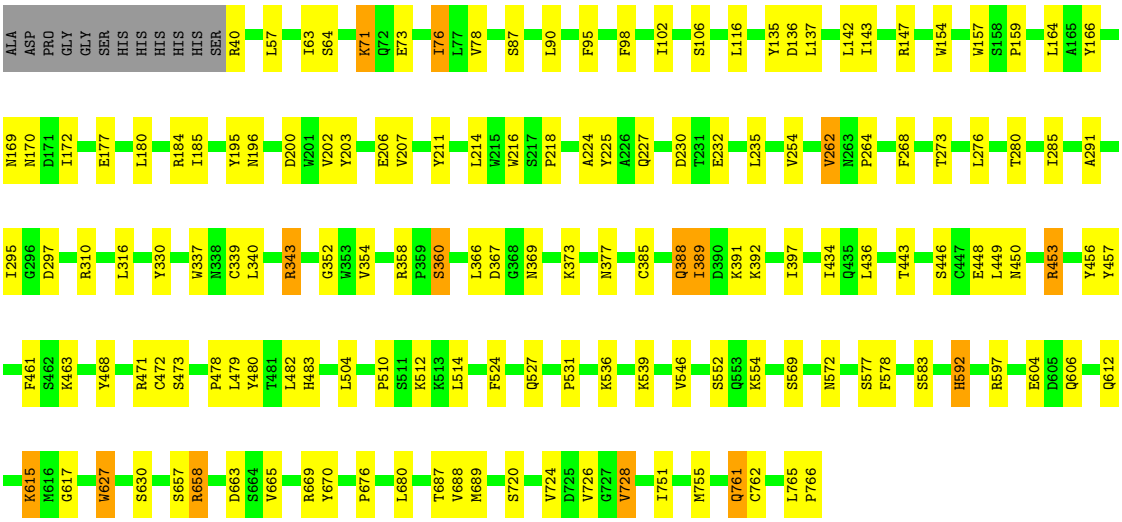
• Molecule 1: Dipeptidyl peptidase IV

Chain C:



• Molecule 1: Dipeptidyl peptidase IV

Chain D:

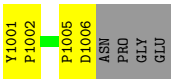


• Molecule 2: Neuropeptide Y

Chain E:

• Molecule 2: Neuropeptide Y

Chain F:

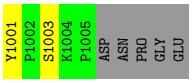


• Molecule 2: Neuropeptide Y

Chain G:

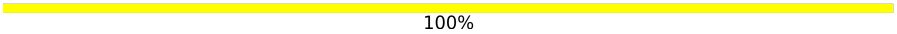
• Molecule 2: Neuropeptide Y

Chain H:



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

Chain I:

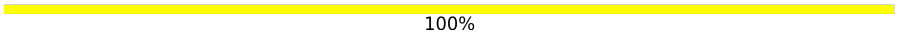


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

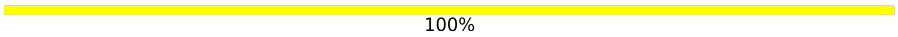
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.61Å 122.70Å 145.41Å 90.00° 114.88° 90.00°	Depositor
Resolution (Å)	41.17 – 2.30	Depositor
% Data completeness (in resolution range)	100.0 (41.17-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.211 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25627	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

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	0.52	0/6135	0.65	0/8344
1	B	0.49	0/6168	0.63	2/8389 (0.0%)
1	C	0.49	0/6129	0.61	0/8336
1	D	0.48	0/6129	0.60	0/8336
2	E	0.77	0/35	0.64	0/46
2	F	0.76	0/51	0.73	0/69
2	G	0.62	0/35	0.78	0/46
2	H	0.61	0/43	0.71	0/58
All	All	0.50	0/24725	0.62	2/33624 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	739	ASP	CB-CG-OD2	6.74	124.37	118.30
1	B	164	LEU	CA-CB-CG	5.20	127.27	115.30

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	5963	0	5677	80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5993	0	5700	70	0
1	C	5957	0	5674	45	0
1	D	5957	0	5677	72	0
2	E	34	0	33	6	0
2	F	49	0	44	4	0
2	G	34	0	33	5	0
2	H	41	0	40	1	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
4	A	84	0	78	3	0
4	B	70	0	65	1	0
4	C	56	0	52	0	0
4	D	28	0	26	0	0
5	A	342	0	0	0	0
5	B	361	0	0	0	0
5	C	277	0	0	2	0
5	D	254	0	0	0	0
5	E	3	0	0	0	0
5	F	4	0	0	0	0
5	G	6	0	0	0	0
5	H	2	0	0	0	0
All	All	25627	0	23199	269	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 6.

All (269) 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:253:ARG:HH21	1:B:253:ARG:HH21	1.08	0.97
1:C:711:VAL:HG13	1:C:740:HIS:CE1	2.03	0.93
1:A:711:VAL:HG13	1:A:740:HIS:CE1	2.04	0.93
1:C:589:LYS:HD3	5:C:5477:HOH:O	1.70	0.90
1:A:74:ASN:HD21	1:A:92:ASN:HD22	1.17	0.88
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.55	0.87
1:B:599:GLY:N	1:B:602:GLU:OE2	2.08	0.86
1:D:230:ASP:OD1	1:D:264:PRO:HB3	1.78	0.83
1:A:458:SER:OG	1:A:471:ARG:NH1	2.15	0.79
1:A:327:ILE:HD13	1:A:389:ILE:HG13	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.66	0.78
1:A:614:SER:HB2	1:A:621:ASN:OD1	1.87	0.74
1:A:704:HIS:ND1	1:A:716:SER:OG	2.19	0.73
1:A:73:GLU:O	1:A:74:ASN:ND2	2.21	0.72
1:D:539:LYS:HE3	1:D:617:GLY:O	1.89	0.72
1:B:594:ILE:HG21	1:B:602:GLU:HG2	1.73	0.71
1:C:206:GLU:HB3	1:C:665:VAL:HG22	1.71	0.71
1:A:711:VAL:CG1	1:A:740:HIS:CE1	2.74	0.70
1:A:107:ILE:HD11	1:A:111:GLY:HA2	1.71	0.69
1:A:343:ARG:HD2	1:A:389:ILE:HG23	1.74	0.69
1:B:88:VAL:HG11	1:B:91:GLU:HG3	1.75	0.69
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.28	0.69
1:C:711:VAL:CG1	1:C:740:HIS:CE1	2.76	0.69
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.57	0.68
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.74	0.68
1:D:471:ARG:HG3	1:D:480:TYR:CE1	2.29	0.67
1:A:177:GLU:HB2	1:A:180:LEU:HD23	1.76	0.67
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.30	0.67
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.76	0.66
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.61	0.66
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.78	0.65
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.27	0.63
1:D:232:GLU:HB3	1:D:262:VAL:HG21	1.79	0.63
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.90	0.63
1:A:688:VAL:HG22	1:A:719:ILE:HG12	1.81	0.63
1:D:71:LYS:HE2	1:D:71:LYS:O	1.99	0.63
1:C:319:ILE:HD12	1:C:319:ILE:H	1.64	0.63
1:D:154:TRP:O	1:D:166:TYR:HA	1.99	0.62
1:C:643:GLY:HA2	1:C:697:GLN:HE22	1.64	0.62
1:C:648:LYS:NZ	1:C:699:GLU:OE2	2.32	0.62
1:C:293:MET:HE2	1:C:317:ARG:HG2	1.82	0.62
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.91	0.62
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.64	0.62
1:D:196:ASN:ND2	1:D:227:GLN:HG3	2.15	0.61
1:C:456:TYR:O	1:C:472:CYS:HA	1.99	0.61
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.65	0.61
1:A:74:ASN:ND2	1:A:92:ASN:HB3	2.17	0.60
1:A:72:GLN:HB2	1:A:77:LEU:HD22	1.83	0.60
1:A:184:ARG:HD3	1:A:186:THR:O	2.02	0.60
1:B:206:GLU:OE2	2:F:1001:TYR:N	2.35	0.59
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:SER:HB3	4:B:851:NAG:H81	1.82	0.59
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.37	0.59
1:B:675:THR:HB	1:B:677:GLU:OE1	2.03	0.58
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.69	0.58
1:D:751:ILE:O	1:D:755:MET:HG3	2.03	0.58
1:A:758:PHE:O	1:A:761:GLN:HG3	2.05	0.57
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.86	0.57
1:A:173:TYR:CE1	1:A:184:ARG:HG3	2.40	0.57
1:B:677:GLU:CD	1:B:677:GLU:H	2.08	0.56
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.21	0.56
1:D:206:GLU:OE2	1:D:663:ASP:OD2	2.23	0.56
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.88	0.55
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.89	0.55
1:C:109:PRO:HG2	1:C:158:SER:O	2.06	0.55
1:B:630:SER:OG	2:F:1002:PRO:C	2.45	0.54
1:D:360:SER:HB3	1:D:373:LYS:HG3	1.89	0.54
1:A:109:PRO:HG2	1:A:158:SER:O	2.08	0.54
1:A:87:SER:HB3	4:A:851:NAG:H81	1.90	0.54
1:A:206:GLU:CB	1:A:665:VAL:HG22	2.37	0.54
1:B:214:LEU:HD23	1:B:225:TYR:HB3	1.89	0.54
1:A:74:ASN:ND2	1:A:92:ASN:HD22	1.98	0.54
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.73	0.54
1:B:453:ARG:HG3	1:B:454:CYS:SG	2.47	0.53
1:A:378:GLU:CD	1:A:378:GLU:H	2.11	0.53
1:A:630:SER:OG	2:E:1002:PRO:C	2.47	0.53
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.24	0.53
1:C:85:ASN:C	1:C:85:ASN:HD22	2.12	0.52
1:B:79:PHE:CE2	1:B:86:SER:HB3	2.45	0.52
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.90	0.52
1:B:177:GLU:HB2	1:B:180:LEU:CD2	2.34	0.52
1:D:726:VAL:HG23	1:D:728:VAL:HG13	1.91	0.52
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.92	0.52
1:A:726:VAL:HG23	1:A:728:VAL:HG12	1.92	0.51
1:B:360:SER:O	1:B:373:LYS:NZ	2.43	0.51
1:D:172:ILE:HB	1:D:185:ILE:HB	1.92	0.51
1:A:472:CYS:O	1:A:478:PRO:HA	2.09	0.51
1:C:544:LEU:HD23	1:C:626:ILE:HD12	1.91	0.51
1:A:364:PHE:CE2	1:A:389:ILE:HD11	2.43	0.51
1:D:397:ILE:HD12	1:D:434:ILE:HD13	1.91	0.51
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.91	0.51
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLU:OE2	2:G:1001:TYR:N	2.44	0.51
1:C:643:GLY:HA2	1:C:697:GLN:NE2	2.26	0.50
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.46	0.50
1:D:291:ALA:O	1:D:295:ILE:HG23	2.11	0.50
1:B:196:ASN:ND2	1:B:227:GLN:HG3	2.27	0.50
1:C:547:TYR:OH	2:G:1003:SER:HB2	2.11	0.50
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.92	0.50
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.45	0.50
1:B:343:ARG:HD2	1:B:389:ILE:HG23	1.92	0.50
1:C:629:TRP:CD1	2:G:1004:LYS:HB2	2.46	0.50
1:B:544:LEU:HG	1:B:546:VAL:HG12	1.93	0.50
1:B:299:TYR:N	1:B:316:LEU:O	2.39	0.50
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.94	0.50
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.95	0.50
1:C:741:GLY:O	1:C:742:ILE:C	2.51	0.50
1:C:701:LEU:HD13	1:C:731:GLN:HB3	1.94	0.49
1:B:682:HIS:HA	1:B:685:ASN:HB2	1.93	0.49
1:B:370:SER:OG	1:B:386:TYR:CE2	2.66	0.49
1:B:184:ARG:HD3	1:B:186:THR:O	2.13	0.49
2:G:1001:TYR:CE1	2:G:1003:SER:HB3	2.47	0.49
1:C:51:ASN:ND2	1:C:54:ARG:HH11	2.11	0.49
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.48	0.49
1:D:453:ARG:NH2	1:D:479:LEU:HB2	2.28	0.49
1:D:95:PHE:HB3	1:D:98:PHE:HB2	1.95	0.49
1:B:136:ASP:OD2	1:B:139:LYS:HE2	2.12	0.49
1:A:471:ARG:HH11	1:A:471:ARG:HB3	1.78	0.48
1:D:159:PRO:HD3	1:D:216:TRP:HB2	1.95	0.48
1:A:666:TYR:CE1	2:E:1002:PRO:HD3	2.47	0.48
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.79	0.48
1:B:472:CYS:O	1:B:478:PRO:HA	2.13	0.48
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.44	0.48
2:F:1005:PRO:O	2:F:1006:ASP:CB	2.61	0.48
1:D:76:ILE:HG23	1:D:90:LEU:HB2	1.94	0.48
1:B:453:ARG:NH2	1:B:477:LEU:O	2.38	0.48
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.43	0.48
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.95	0.47
1:D:456:TYR:HB3	1:D:473:SER:HB2	1.95	0.47
1:C:472:CYS:O	1:C:478:PRO:HA	2.14	0.47
1:B:184:ARG:NH1	1:B:187:TRP:HA	2.28	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG13	1.96	0.47
1:A:175:LYS:NZ	1:A:180:LEU:O	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:SER:HB2	1:D:457:TYR:CE2	2.50	0.47
1:B:539:LYS:NZ	1:B:617:GLY:O	2.34	0.47
1:C:518:ILE:HG22	1:C:518:ILE:O	2.14	0.47
1:D:468:TYR:CZ	1:D:483:HIS:HB2	2.50	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.96	0.46
1:D:340:LEU:HB2	1:D:343:ARG:HG2	1.98	0.46
1:B:92:ASN:HD22	1:B:93:SER:N	2.14	0.46
1:D:235:LEU:HA	1:D:254:VAL:O	2.15	0.46
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.51	0.46
1:C:73:GLU:C	1:C:75:ASN:H	2.19	0.46
1:D:195:TYR:O	1:D:227:GLN:HA	2.16	0.46
1:B:446:SER:HB2	1:B:457:TYR:CE2	2.51	0.46
1:D:657:SER:OG	1:D:689:MET:SD	2.73	0.46
1:B:143:ILE:HD13	1:B:178:PRO:HB2	1.97	0.46
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.97	0.46
1:A:751:ILE:O	1:A:755:MET:HG3	2.15	0.46
1:B:518:ILE:HG22	1:B:521:GLU:HA	1.97	0.46
1:C:666:TYR:CE1	2:G:1002:PRO:HD3	2.50	0.46
1:D:310:ARG:HH21	1:D:389:ILE:HD13	1.80	0.46
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.16	0.45
1:D:78:VAL:HG12	1:D:87:SER:O	2.17	0.45
1:A:688:VAL:CG2	1:A:719:ILE:HG12	2.46	0.45
1:D:136:ASP:HB2	1:D:143:ILE:HD11	1.97	0.45
1:D:546:VAL:HG12	1:D:606:GLN:OE1	2.16	0.45
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.51	0.45
1:A:206:GLU:OE1	2:E:1001:TYR:N	2.50	0.45
1:A:471:ARG:HD2	1:A:480:TYR:OH	2.17	0.45
1:B:53:TYR:HB3	1:B:500:LEU:HD11	1.98	0.45
1:B:75:ASN:HD22	1:B:91:GLU:HA	1.82	0.45
1:C:51:ASN:HD21	1:C:54:ARG:HD3	1.81	0.45
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.46	0.45
1:B:105:TYR:CE2	1:B:107:ILE:HD12	2.52	0.45
1:C:630:SER:HA	1:C:654:ALA:O	2.16	0.45
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.17	0.45
1:D:367:ASP:OD2	1:D:369:ASN:HB2	2.17	0.45
1:D:472:CYS:O	1:D:478:PRO:HA	2.17	0.45
1:C:206:GLU:CB	1:C:665:VAL:HG22	2.44	0.45
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.52	0.45
1:D:177:GLU:HB2	1:D:180:LEU:HB2	1.98	0.45
1:D:546:VAL:HG22	1:D:627:TRP:O	2.16	0.45
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.35	0.44
1:A:546:VAL:HG12	1:A:627:TRP:O	2.17	0.44
1:A:206:GLU:HB3	1:A:665:VAL:HG22	1.99	0.44
1:A:657:SER:HA	1:A:688:VAL:HG13	1.99	0.44
1:D:135:TYR:HD1	1:D:142:LEU:HD13	1.82	0.44
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.99	0.44
1:D:676:PRO:HG3	1:D:680:LEU:HD22	1.99	0.44
2:H:1001:TYR:CE1	2:H:1003:SER:HB3	2.53	0.44
1:A:179:ASN:OD1	1:A:180:LEU:HD22	2.18	0.44
1:A:408:GLU:HG3	1:A:459:VAL:CG1	2.47	0.44
1:A:629:TRP:CD1	2:E:1004:LYS:HB2	2.52	0.44
1:A:684:ARG:CB	4:A:6851:NAG:HN2	2.30	0.44
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.00	0.44
1:B:614:SER:HB3	1:B:621:ASN:OD1	2.18	0.44
1:D:177:GLU:HB2	1:D:180:LEU:HD13	1.99	0.44
1:A:435:GLN:OE1	1:A:441:LYS:HE2	2.18	0.44
1:B:206:GLU:CB	1:B:665:VAL:HG22	2.48	0.44
1:C:492:ARG:HE	1:C:492:ARG:HB3	1.66	0.44
1:D:106:SER:HG	1:D:157:TRP:HD1	1.66	0.44
1:C:735:TYR:OH	1:C:751:ILE:HA	2.18	0.43
1:D:64:SER:HA	1:D:463:LYS:HD3	2.00	0.43
1:B:376:SER:HA	1:B:382:ARG:HA	2.00	0.43
1:A:114:ILE:HG23	1:A:135:TYR:HB3	2.00	0.43
1:A:74:ASN:HD22	1:A:74:ASN:C	2.21	0.43
1:D:330:TYR:HB2	1:D:337:TRP:CH2	2.53	0.43
1:D:612:GLN:HA	1:D:615:LYS:HE3	2.00	0.43
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.54	0.43
1:D:102:ILE:HG21	1:D:116:LEU:HD22	1.99	0.43
1:D:388:GLN:HB3	1:D:391:LYS:HG2	2.00	0.43
1:A:343:ARG:CD	1:A:389:ILE:HG23	2.46	0.43
1:B:536:LYS:H	1:B:536:LYS:HG3	1.66	0.43
1:B:640:LEU:HD11	1:B:650:GLY:HA3	2.00	0.43
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.49	0.43
1:D:524:PHE:HB3	1:D:578:PHE:CZ	2.54	0.43
1:B:588:ASP:O	1:B:592:HIS:HB2	2.19	0.43
1:C:82:GLU:HG2	1:C:83:TYR:CZ	2.53	0.43
1:B:109:PRO:HG2	1:B:158:SER:O	2.19	0.43
1:D:207:VAL:O	1:D:358:ARG:NE	2.51	0.43
1:A:626:ILE:O	1:A:650:GLY:HA2	2.18	0.43
1:D:446:SER:HA	1:D:449:LEU:HD12	1.99	0.43
1:A:206:GLU:OE2	2:E:1001:TYR:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:HD22	1:C:253:ARG:HB3	2.02	0.42
1:D:159:PRO:CD	1:D:216:TRP:HB3	2.49	0.42
1:D:200:ASP:OD1	1:D:264:PRO:HG3	2.19	0.42
1:D:726:VAL:HG23	1:D:728:VAL:CG1	2.49	0.42
1:B:723:LEU:HB3	1:B:728:VAL:HG22	2.01	0.42
1:D:169:ASN:O	1:D:170:ASN:HB2	2.20	0.42
1:A:640:LEU:HB3	1:A:698:VAL:HG21	2.01	0.42
1:C:378:GLU:CD	1:C:378:GLU:H	2.22	0.42
1:A:456:TYR:HB2	1:A:557:THR:OG1	2.19	0.42
1:A:487:ASN:OD1	1:A:487:ASN:N	2.52	0.42
1:A:62:TRP:CG	1:A:462:SER:HA	2.55	0.42
1:C:177:GLU:HB2	1:C:180:LEU:HB2	2.01	0.42
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.54	0.42
1:A:410:LEU:HD13	1:A:415:LEU:HD12	2.02	0.42
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.85	0.42
1:D:512:LYS:HE2	1:D:527:GLN:OE1	2.19	0.42
1:D:720:SER:O	1:D:724:VAL:HG23	2.20	0.42
1:B:172:ILE:HD13	1:B:214:LEU:HD21	2.02	0.42
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.02	0.42
1:B:405:ILE:HG13	1:B:429:ARG:CD	2.50	0.42
1:D:206:GLU:HB3	1:D:665:VAL:HG22	2.02	0.42
1:D:446:SER:HB2	1:D:457:TYR:CD2	2.55	0.42
1:A:435:GLN:HB3	1:A:441:LYS:HB2	2.00	0.41
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.55	0.41
1:B:67:GLU:HA	1:B:79:PHE:O	2.20	0.41
1:B:351:THR:OG1	1:B:592:HIS:HD2	2.03	0.41
1:C:195:TYR:O	1:C:227:GLN:HA	2.20	0.41
1:D:552:SER:O	1:D:583:SER:HB2	2.20	0.41
1:D:554:LYS:HB3	1:D:577:SER:HB3	2.02	0.41
1:A:471:ARG:HD3	1:A:480:TYR:CE1	2.56	0.41
1:A:272:ASN:O	1:A:276:LEU:HD13	2.20	0.41
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.03	0.41
1:C:739:ASP:HB2	5:C:5202:HOH:O	2.19	0.41
1:D:63:ILE:HG13	1:D:64:SER:N	2.35	0.41
1:A:331:ASP:HB3	1:A:334:SER:HB2	2.03	0.41
1:A:684:ARG:HB2	4:A:6851:NAG:HN2	1.86	0.41
1:B:206:GLU:HB3	1:B:665:VAL:HG22	2.03	0.41
1:D:200:ASP:OD2	1:D:203:TYR:HB2	2.21	0.41
1:A:671:MET:O	1:A:679:ASN:ND2	2.46	0.41
1:B:405:ILE:HG13	1:B:429:ARG:HD2	2.02	0.41
2:F:1005:PRO:O	2:F:1006:ASP:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:CB	1:A:180:LEU:HD23	2.48	0.40
1:C:630:SER:HG	1:C:740:HIS:CE1	2.39	0.40
1:D:216:TRP:CZ3	1:D:273:THR:HG21	2.56	0.40
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.55	0.40
1:B:741:GLY:O	1:B:742:ILE:C	2.59	0.40
1:D:765:LEU:HA	1:D:766:PRO:HD3	1.95	0.40
2:E:1001:TYR:CD2	2:E:1003:SER:HB3	2.56	0.40
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.03	0.40
1:D:159:PRO:HB2	1:D:218:PRO:O	2.21	0.40
1:D:352:GLY:HA3	1:D:592:HIS:CD2	2.56	0.40
1:A:39:SER:HB3	1:A:508:GLN:HG2	2.03	0.40
1:A:408:GLU:HG3	1:A:459:VAL:HG12	2.04	0.40
1:D:761:GLN:HG3	1:D:762:CYS:N	2.36	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	726/739 (98%)	695 (96%)	29 (4%)	2 (0%)	41	50
1	B	729/739 (99%)	695 (95%)	34 (5%)	0	100	100
1	C	725/739 (98%)	688 (95%)	33 (5%)	4 (1%)	25	31
1	D	725/739 (98%)	683 (94%)	41 (6%)	1 (0%)	51	64
2	E	2/10 (20%)	2 (100%)	0	0	100	100
2	F	4/10 (40%)	3 (75%)	1 (25%)	0	100	100
2	G	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
2	H	3/10 (30%)	3 (100%)	0	0	100	100
All	All	2916/2996 (97%)	2770 (95%)	139 (5%)	7 (0%)	47	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	C	85	ASN
1	A	630	SER
1	C	74	ASN
1	D	630	SER
1	C	714	GLN
1	C	742	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	653/661 (99%)	612 (94%)	41 (6%)	18	24
1	B	656/661 (99%)	614 (94%)	42 (6%)	17	23
1	C	652/661 (99%)	616 (94%)	36 (6%)	21	30
1	D	652/661 (99%)	607 (93%)	45 (7%)	15	20
2	E	4/9 (44%)	4 (100%)	0	100	100
2	F	6/9 (67%)	6 (100%)	0	100	100
2	G	4/9 (44%)	4 (100%)	0	100	100
2	H	5/9 (56%)	5 (100%)	0	100	100
All	All	2632/2680 (98%)	2468 (94%)	164 (6%)	18	25

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	61	ARG
1	A	71	LYS
1	A	74	ASN
1	A	82	GLU
1	A	102	ILE
1	A	107	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	140	ARG
1	A	142	LEU
1	A	180	LEU
1	A	184	ARG
1	A	202	VAL
1	A	230	ASP
1	A	262	VAL
1	A	276	LEU
1	A	316	LEU
1	A	326	ASP
1	A	350	THR
1	A	385	CYS
1	A	389	ILE
1	A	391	LYS
1	A	395	THR
1	A	436	LEU
1	A	448	GLU
1	A	452	GLU
1	A	453	ARG
1	A	463	LYS
1	A	464	GLU
1	A	471	ARG
1	A	472	CYS
1	A	482	LEU
1	A	504	LEU
1	A	514	LEU
1	A	566	TYR
1	A	589	LYS
1	A	597	ARG
1	A	658	ARG
1	A	673	LEU
1	A	685	ASN
1	A	711	VAL
1	A	728	VAL
1	B	51	ASN
1	B	54	ARG
1	B	55	LEU
1	B	59	SER
1	B	66	HIS
1	B	92	ASN
1	B	97	GLU
1	B	164	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	180	LEU
1	B	184	ARG
1	B	202	VAL
1	B	262	VAL
1	B	276	LEU
1	B	313	LEU
1	B	332	GLU
1	B	343	ARG
1	B	354	VAL
1	B	370	SER
1	B	385	CYS
1	B	389	ILE
1	B	395	THR
1	B	413	ASP
1	B	436	LEU
1	B	453	ARG
1	B	463	LYS
1	B	482	LEU
1	B	514	LEU
1	B	521	GLU
1	B	536	LYS
1	B	546	VAL
1	B	566	TYR
1	B	589	LYS
1	B	597	ARG
1	B	602	GLU
1	B	614	SER
1	B	658	ARG
1	B	660	GLU
1	B	673	LEU
1	B	685	ASN
1	B	704	HIS
1	B	716	SER
1	B	764	SER
1	C	40	ARG
1	C	72	GLN
1	C	85	ASN
1	C	96	ASP
1	C	137	LEU
1	C	180	LEU
1	C	202	VAL
1	C	212	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	230	ASP
1	C	243	ASP
1	C	276	LEU
1	C	316	LEU
1	C	325	MET
1	C	378	GLU
1	C	385	CYS
1	C	392	LYS
1	C	453	ARG
1	C	463	LYS
1	C	464	GLU
1	C	472	CYS
1	C	482	LEU
1	C	492	ARG
1	C	502	LYS
1	C	504	LEU
1	C	514	LEU
1	C	589	LYS
1	C	594	ILE
1	C	597	ARG
1	C	615	LYS
1	C	627	TRP
1	C	658	ARG
1	C	665	VAL
1	C	673	LEU
1	C	711	VAL
1	C	731	GLN
1	C	761	GLN
1	D	40	ARG
1	D	57	LEU
1	D	71	LYS
1	D	73	GLU
1	D	76	ILE
1	D	137	LEU
1	D	147	ARG
1	D	164	LEU
1	D	184	ARG
1	D	202	VAL
1	D	211	TYR
1	D	262	VAL
1	D	276	LEU
1	D	280	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	285	ILE
1	D	297	ASP
1	D	316	LEU
1	D	339	CYS
1	D	343	ARG
1	D	354	VAL
1	D	360	SER
1	D	366	LEU
1	D	377	ASN
1	D	385	CYS
1	D	388	GLN
1	D	389	ILE
1	D	392	LYS
1	D	436	LEU
1	D	443	THR
1	D	448	GLU
1	D	450	ASN
1	D	453	ARG
1	D	482	LEU
1	D	504	LEU
1	D	514	LEU
1	D	536	LYS
1	D	592	HIS
1	D	597	ARG
1	D	604	GLU
1	D	615	LYS
1	D	627	TRP
1	D	658	ARG
1	D	688	VAL
1	D	728	VAL
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	123	GLN
1	A	169	ASN
1	A	196	ASN
1	A	227	GLN
1	A	344	GLN
1	A	592	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	75	ASN
1	B	92	ASN
1	B	169	ASN
1	B	196	ASN
1	B	344	GLN
1	B	388	GLN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	757	HIS
1	C	51	ASN
1	C	75	ASN
1	C	85	ASN
1	C	123	GLN
1	C	138	ASN
1	C	169	ASN
1	C	196	ASN
1	C	227	GLN
1	C	344	GLN
1	C	533	HIS
1	C	572	ASN
1	C	685	ASN
1	C	697	GLN
1	C	761	GLN
1	D	138	ASN
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	388	GLN
1	D	505	GLN
1	D	572	ASN
1	D	592	HIS

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)

8 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	I	1	1,3	14,14,15	0.64	0	17,19,21	1.27	2 (11%)
3	NAG	I	2	3	14,14,15	0.53	0	17,19,21	1.30	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.59	0	17,19,21	1.10	1 (5%)
3	NAG	J	2	3	14,14,15	0.52	0	17,19,21	0.94	0
3	NAG	K	1	1,3	14,14,15	0.63	0	17,19,21	0.99	1 (5%)
3	NAG	K	2	3	14,14,15	0.61	0	17,19,21	1.77	4 (23%)
3	NAG	L	1	1,3	14,14,15	0.52	0	17,19,21	1.16	2 (11%)
3	NAG	L	2	3	14,14,15	0.50	0	17,19,21	1.34	4 (23%)

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	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	NAG	C3-C4-C5	4.27	117.86	110.24
3	I	1	NAG	C1-O5-C5	3.31	116.67	112.19
3	I	2	NAG	C1-O5-C5	2.99	116.24	112.19
3	K	2	NAG	C8-C7-N2	2.77	120.79	116.10
3	L	2	NAG	C8-C7-N2	2.60	120.51	116.10
3	L	2	NAG	C2-N2-C7	2.49	126.45	122.90
3	L	1	NAG	C1-O5-C5	2.46	115.53	112.19
3	L	2	NAG	O7-C7-C8	-2.37	117.66	122.06
3	K	2	NAG	O5-C5-C4	2.23	116.25	110.83
3	K	2	NAG	O5-C1-C2	-2.20	107.81	111.29
3	I	2	NAG	C8-C7-N2	2.15	119.75	116.10
3	J	1	NAG	C3-C4-C5	2.15	114.08	110.24
3	K	1	NAG	C1-O5-C5	2.14	115.09	112.19
3	L	1	NAG	O5-C1-C2	-2.11	107.95	111.29
3	I	1	NAG	O5-C1-C2	-2.05	108.05	111.29
3	L	2	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

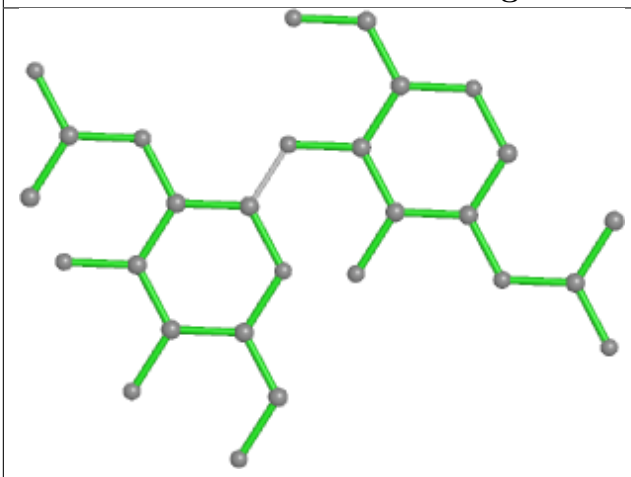
Mol	Chain	Res	Type	Atoms
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C8-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6

There are no ring outliers.

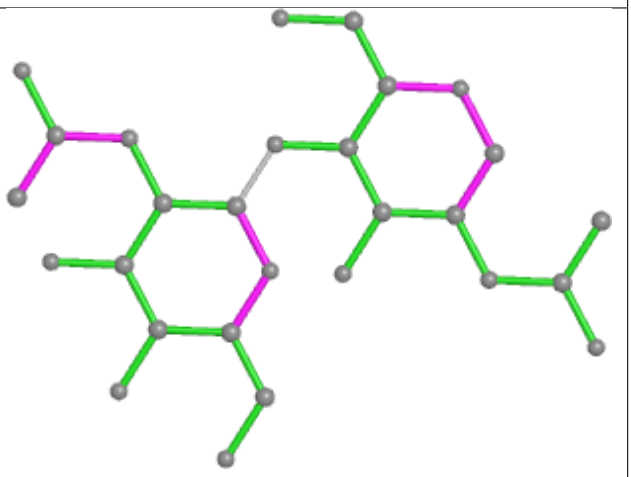
No monomer is involved in short contacts.

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

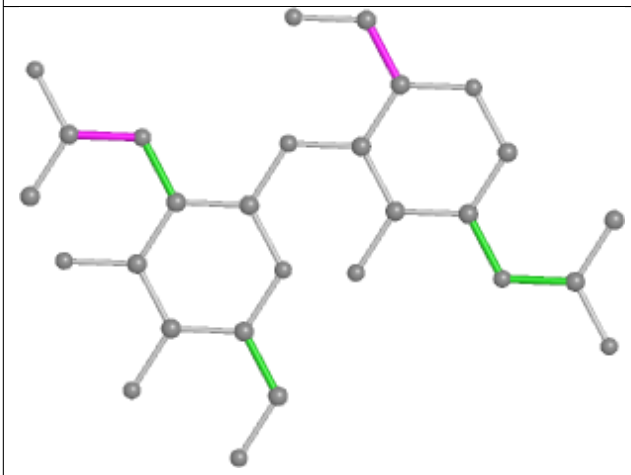
Oligosaccharide Chain I



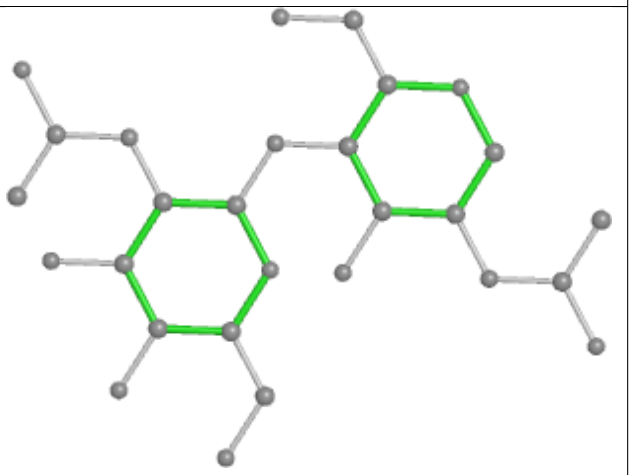
Bond lengths



Bond angles

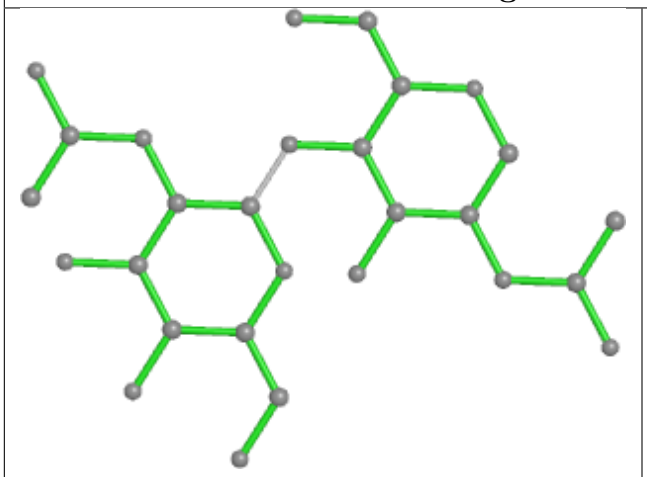


Torsions

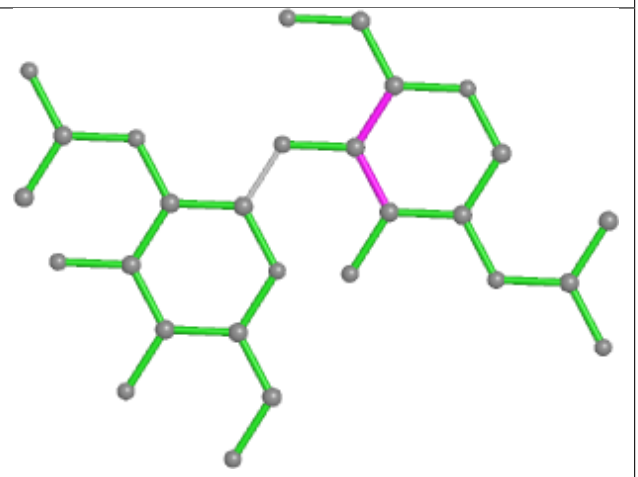


Rings

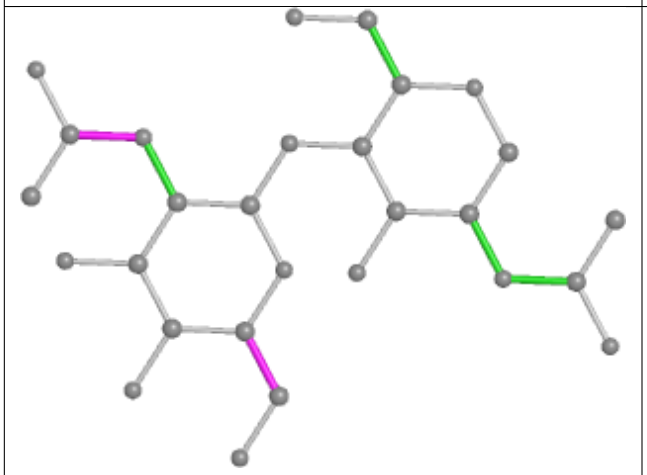
Oligosaccharide Chain J



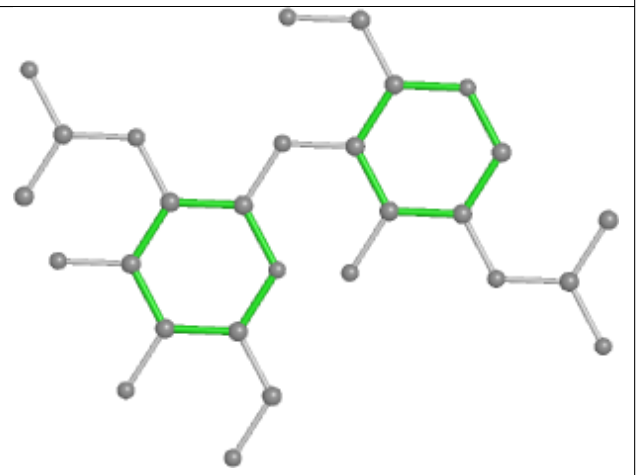
Bond lengths



Bond angles

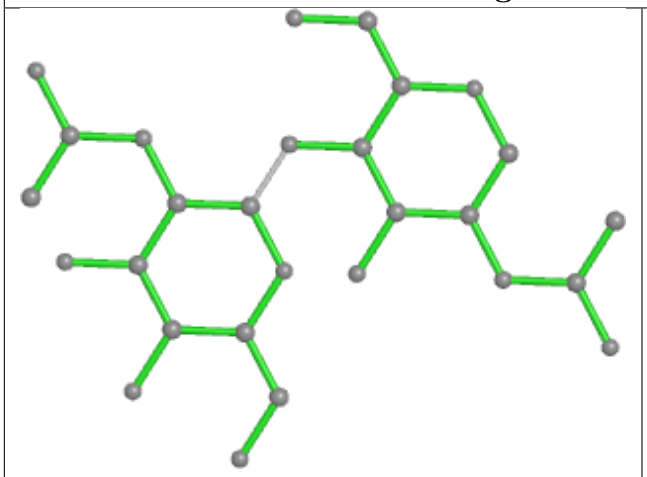


Torsions

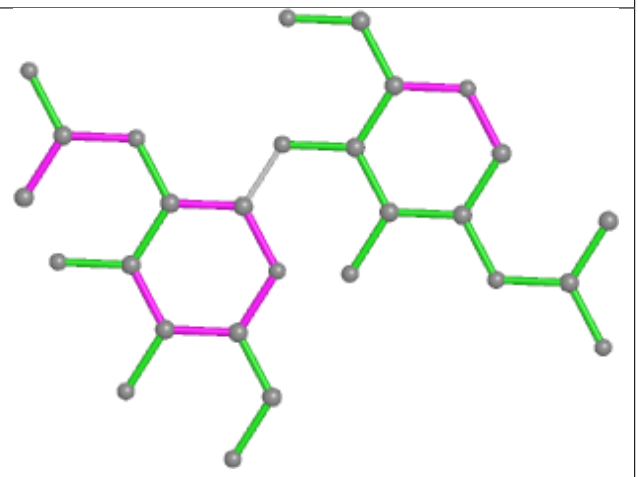


Rings

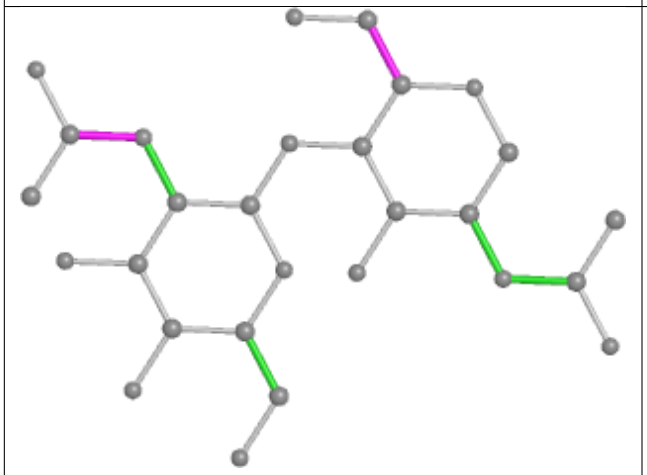
Oligosaccharide Chain K



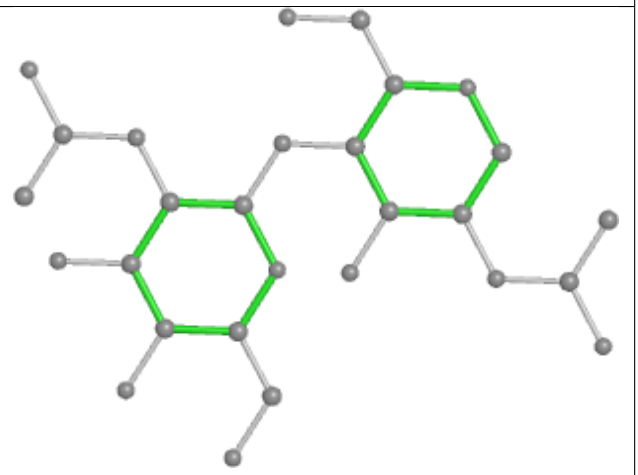
Bond lengths



Bond angles

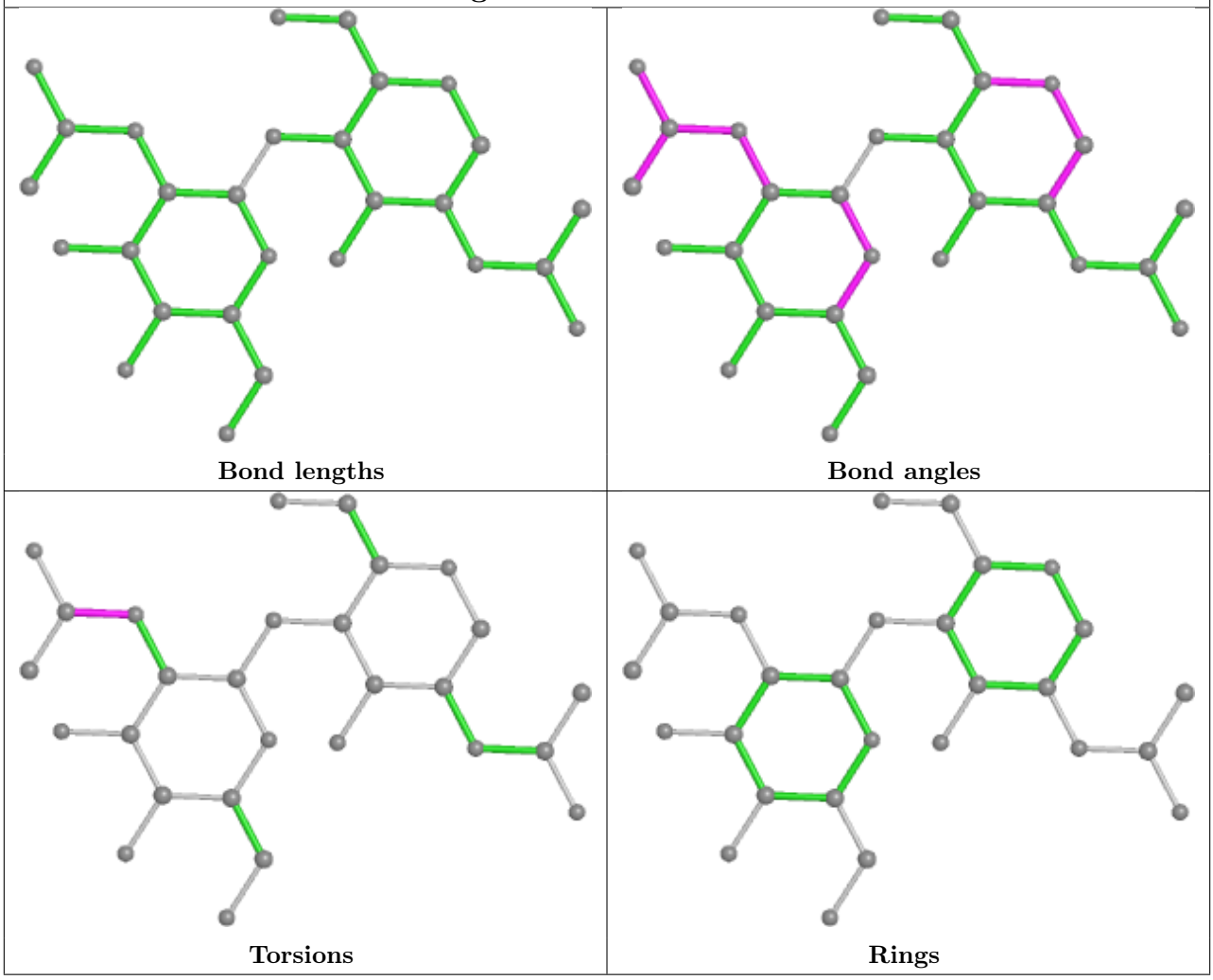


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

17 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	B	2191	1	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
4	NAG	A	2811	1	14,14,15	0.55	0	17,19,21	2.17	3 (17%)
4	NAG	A	2191	1	14,14,15	0.54	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1501	1	14,14,15	0.67	0	17,19,21	2.22	4 (23%)
4	NAG	D	2811	1	14,14,15	0.50	0	17,19,21	1.51	3 (17%)
4	NAG	B	851	1	14,14,15	0.59	0	17,19,21	1.94	2 (11%)
4	NAG	B	3211	1	14,14,15	0.49	0	17,19,21	1.58	1 (5%)
4	NAG	A	851	1	14,14,15	0.49	0	17,19,21	1.16	1 (5%)
4	NAG	A	3211	1	14,14,15	0.55	0	17,19,21	1.04	1 (5%)
4	NAG	B	2811	1	14,14,15	0.45	0	17,19,21	1.23	2 (11%)
4	NAG	B	1501	1	14,14,15	0.51	0	17,19,21	2.05	5 (29%)
4	NAG	C	3211	1	14,14,15	0.51	0	17,19,21	2.00	4 (23%)
4	NAG	A	6851	1	14,14,15	0.69	0	17,19,21	2.23	3 (17%)
4	NAG	C	2811	1	14,14,15	0.94	1 (7%)	17,19,21	1.15	2 (11%)
4	NAG	C	2191	1	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
4	NAG	C	5201	1	14,14,15	0.62	0	17,19,21	1.75	1 (5%)
4	NAG	D	2191	1	14,14,15	0.53	0	17,19,21	1.00	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	B	2191	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2811	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	3/6/23/26	0/1/1/1
4	NAG	D	2811	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	B	851	1	-	2/6/23/26	0/1/1/1
4	NAG	B	3211	1	-	0/6/23/26	0/1/1/1
4	NAG	A	851	1	-	3/6/23/26	0/1/1/1
4	NAG	A	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2811	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	1/6/23/26	0/1/1/1
4	NAG	C	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	A	6851	1	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	C	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2191	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	5201	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2191	1	-	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)
4	C	2811	NAG	O6-C6	2.50	1.53	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2811	NAG	C1-O5-C5	7.51	122.36	112.19
4	B	851	NAG	C1-O5-C5	6.09	120.45	112.19
4	A	6851	NAG	C1-O5-C5	6.01	120.34	112.19
4	C	5201	NAG	C1-O5-C5	5.98	120.30	112.19
4	C	3211	NAG	C1-O5-C5	5.77	120.01	112.19
4	A	1501	NAG	C1-O5-C5	5.66	119.85	112.19
4	B	3211	NAG	C1-O5-C5	5.19	119.23	112.19
4	A	6851	NAG	C2-N2-C7	5.10	130.17	122.90
4	B	1501	NAG	C2-N2-C7	4.87	129.83	122.90
4	A	1501	NAG	C4-C3-C2	-4.12	104.98	111.02
4	A	1501	NAG	C2-N2-C7	4.02	128.63	122.90
4	D	2811	NAG	C1-O5-C5	3.94	117.53	112.19
4	B	2811	NAG	C1-O5-C5	3.57	117.03	112.19
4	B	1501	NAG	C4-C3-C2	-3.47	105.93	111.02
4	B	1501	NAG	C1-O5-C5	3.16	116.47	112.19
4	C	3211	NAG	C4-C3-C2	3.13	115.61	111.02
4	B	1501	NAG	O5-C1-C2	-3.03	106.51	111.29
4	A	851	NAG	C1-O5-C5	2.90	116.13	112.19
4	B	1501	NAG	C1-C2-N2	2.83	115.32	110.49
4	D	2811	NAG	C3-C4-C5	2.75	115.14	110.24
4	A	1501	NAG	C1-C2-N2	2.68	115.07	110.49
4	B	851	NAG	C6-C5-C4	-2.65	106.79	113.00
4	C	2811	NAG	C1-O5-C5	2.64	115.77	112.19
4	A	3211	NAG	C1-O5-C5	2.61	115.73	112.19
4	A	2811	NAG	C4-C3-C2	-2.60	107.21	111.02
4	C	2191	NAG	C4-C3-C2	2.58	114.80	111.02
4	A	2191	NAG	C1-O5-C5	2.53	115.62	112.19
4	C	3211	NAG	C3-C4-C5	2.51	114.72	110.24
4	B	2191	NAG	C1-O5-C5	2.43	115.49	112.19
4	D	2811	NAG	C4-C3-C2	2.41	114.55	111.02
4	D	2191	NAG	C1-O5-C5	2.38	115.42	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3211	NAG	C2-N2-C7	2.38	126.29	122.90
4	A	2811	NAG	O5-C5-C6	2.20	110.65	107.20
4	A	6851	NAG	C4-C3-C2	-2.14	107.88	111.02
4	B	2811	NAG	O5-C5-C6	2.10	110.50	107.20
4	C	2811	NAG	O7-C7-C8	-2.10	118.16	122.06

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2811	NAG	C1
4	A	6851	NAG	C1
4	D	2811	NAG	C1

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	6851	NAG	C3-C2-N2-C7
4	B	851	NAG	C8-C7-N2-C2
4	B	851	NAG	O7-C7-N2-C2
4	B	2811	NAG	C8-C7-N2-C2
4	B	2811	NAG	O7-C7-N2-C2
4	C	2191	NAG	C8-C7-N2-C2
4	C	2191	NAG	O7-C7-N2-C2
4	C	5201	NAG	C8-C7-N2-C2
4	C	5201	NAG	O7-C7-N2-C2
4	D	2191	NAG	C8-C7-N2-C2
4	D	2191	NAG	O7-C7-N2-C2
4	A	2811	NAG	O5-C5-C6-O6
4	A	6851	NAG	C8-C7-N2-C2
4	A	6851	NAG	O7-C7-N2-C2
4	D	2811	NAG	O5-C5-C6-O6
4	B	2191	NAG	C8-C7-N2-C2
4	A	2811	NAG	C4-C5-C6-O6
4	A	3211	NAG	C4-C5-C6-O6
4	A	851	NAG	C8-C7-N2-C2
4	A	851	NAG	O7-C7-N2-C2
4	A	2811	NAG	C8-C7-N2-C2
4	B	2191	NAG	O7-C7-N2-C2
4	A	3211	NAG	O5-C5-C6-O6
4	C	2811	NAG	O5-C5-C6-O6
4	D	2811	NAG	C8-C7-N2-C2
4	D	2811	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	2811	NAG	C4-C5-C6-O6
4	A	2811	NAG	O7-C7-N2-C2
4	D	2811	NAG	O7-C7-N2-C2
4	C	3211	NAG	C8-C7-N2-C2
4	C	5201	NAG	C4-C5-C6-O6
4	A	851	NAG	O5-C5-C6-O6
4	A	1501	NAG	C8-C7-N2-C2
4	C	3211	NAG	O7-C7-N2-C2
4	A	1501	NAG	O7-C7-N2-C2
4	B	2811	NAG	C4-C5-C6-O6
4	A	1501	NAG	C3-C2-N2-C7
4	C	5201	NAG	O5-C5-C6-O6
4	B	1501	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	851	NAG	1	0
4	A	851	NAG	1	0
4	A	6851	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.