Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2023 – 04:11 am GMT

PDB ID	:	2C6F
Title	:	Structure of human somatic angiontensin-I converting enzyme N domain
Authors	:	Corradi, H.R.; Schwager, S.L.U.; Nichinda, A.; Sturrock, E.D.; Acharya, K.R.
Deposited on	:	2005-11-09
Resolution	:	3.01 Å(reported)

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

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

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

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

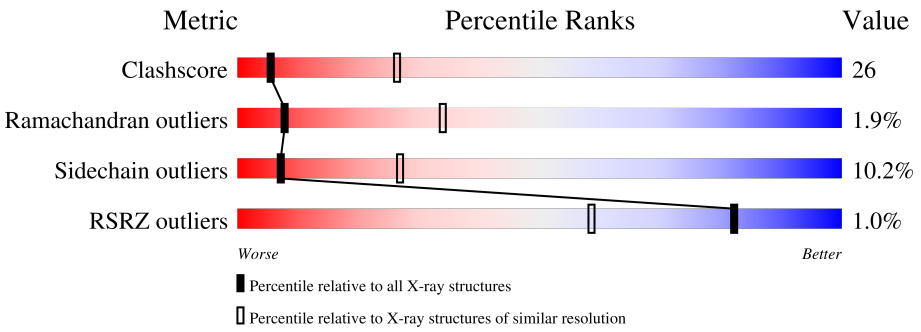
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 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	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	612	58% 36% 6%
1	B	612	% 57% 38% 5% •
2	C	2	50% 50%
2	D	2	50% 50%
2	E	2	50% 50%
2	F	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
2	NAG	E	2	-	-	-	X
3	NAG	A	697	-	-	-	X
6	ACT	A	800	-	-	-	X
7	GOL	A	2434	-	X	-	-
7	GOL	B	2433	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9970 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.

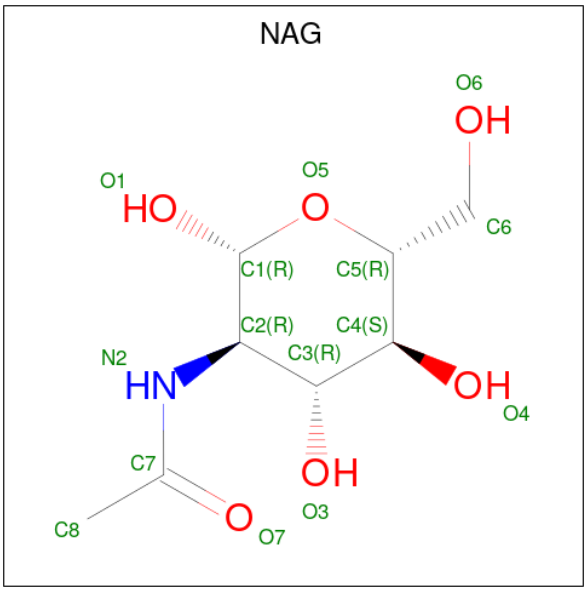
- Molecule 1 is a protein called ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	612	4884	3145	840	880	19	6	0	0
1	B	611	4852	3124	830	879	19	14	0	0

- Molecule 2 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			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

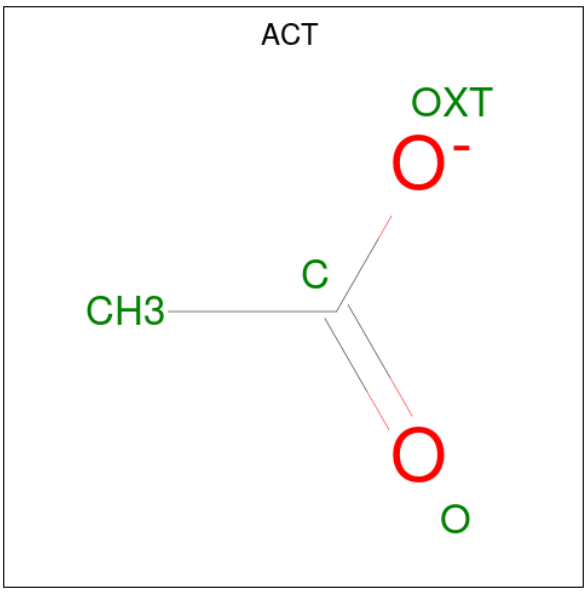
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
			Total	Zn		
4	B	1	1	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

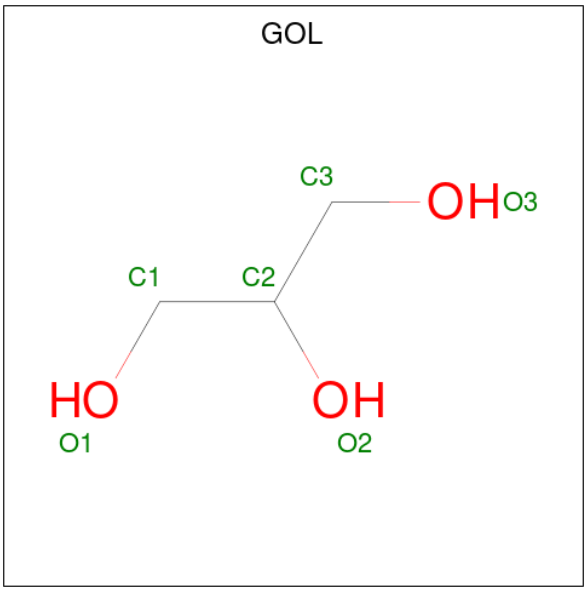
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
			Total	Cl		
5	B	1	1	1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	4	2	2		0	0
			Total	C	O			
6	A	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	B	1	6	3	3	0	0

- Molecule 8 is water.

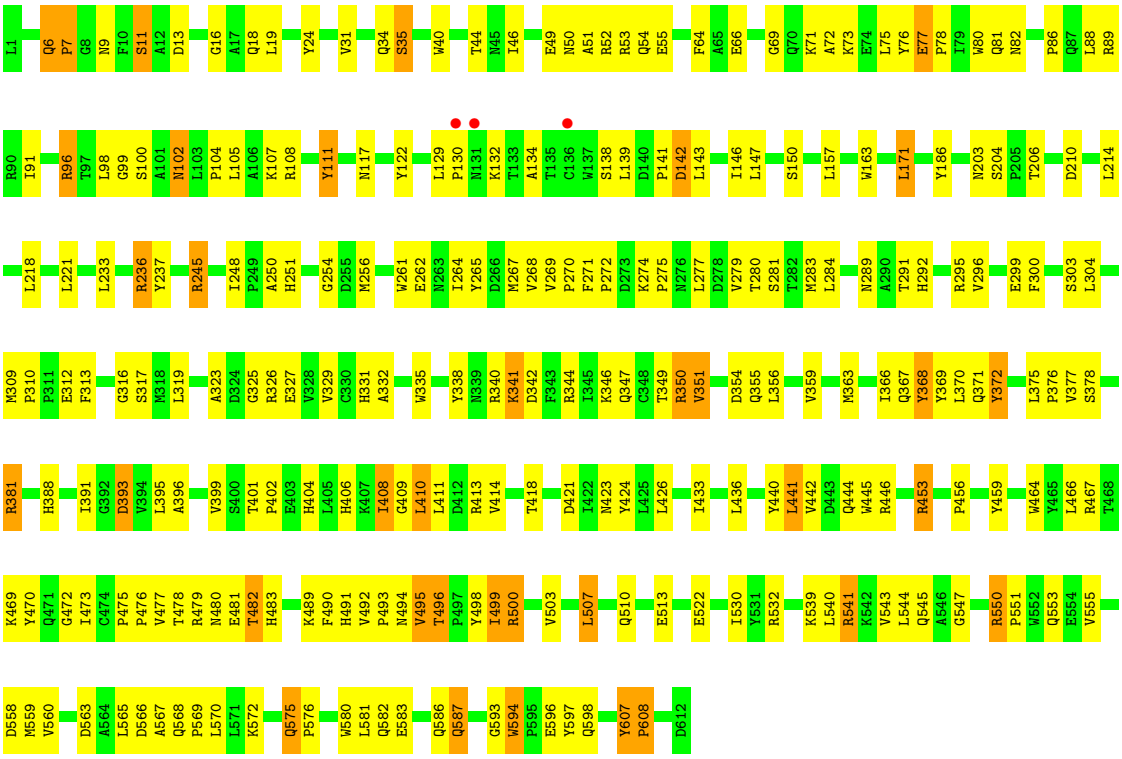
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	11	11	11	0	0
			Total	O		
8	B	13	13	13	0	0

3 Residue-property plots (i)

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

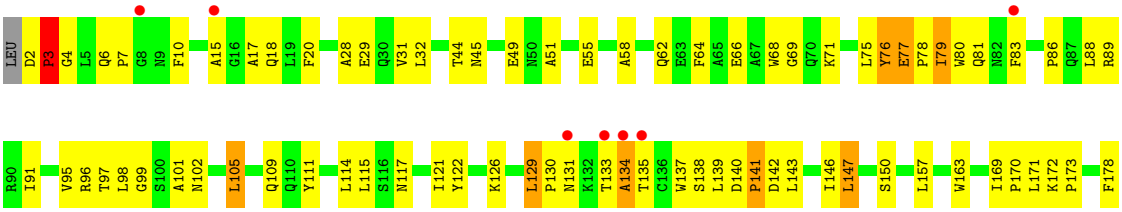
• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM

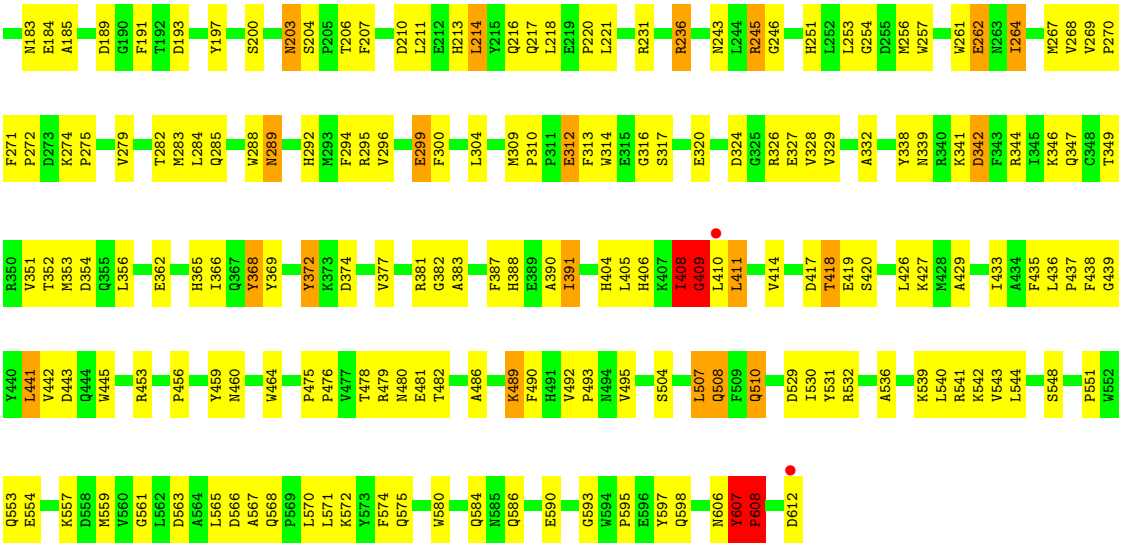
Chain A: 58% 36% 6%



• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM

Chain B: % 57% 38% 5%





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

Chain C:

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

Chain D:

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

Chain E:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.12Å 211.32Å 171.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 3.01 47.91 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.91-3.01) 96.8 (47.91-3.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.273 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9970	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NAG, ZN, GOL, ACT

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	0.51	1/5042 (0.0%)	0.74	3/6885 (0.0%)
1	B	0.49	0/5010	0.86	6/6845 (0.1%)
All	All	0.50	1/10052 (0.0%)	0.80	9/13730 (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
1	A	0	1
1	B	3	2
All	All	3	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	ASN	CB-CG	-5.47	1.38	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3	PRO	CA-N-CD	-22.64	79.80	111.50
1	B	608	PRO	CA-N-CD	-18.89	85.05	111.50
1	B	607	TYR	CB-CG-CD1	-9.99	115.01	121.00
1	B	607	TYR	CB-CG-CD2	7.49	125.49	121.00
1	B	409	GLY	N-CA-C	5.92	127.91	113.10
1	B	3	PRO	CA-CB-CG	-5.55	93.45	104.00
1	A	102	ASN	CB-CA-C	-5.48	99.43	110.40
1	A	142	ASP	CB-CG-OD2	5.22	123.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	GLY	C-N-CA	-5.12	108.89	121.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	79	ILE	CA
1	B	410	LEU	CA
1	B	530	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	607	TYR	Peptide
1	B	275	PRO	Peptide
1	B	409	GLY	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	4884	0	4582	252	0
1	B	4852	0	4514	243	0
2	C	28	0	25	1	0
2	D	28	0	25	6	0
2	E	28	0	25	3	0
2	F	28	0	25	2	0
3	A	42	0	36	4	0
3	B	28	0	23	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	A	8	0	6	0	0
6	B	4	0	3	0	0
7	A	6	0	6	1	0
7	B	6	0	6	1	0
8	A	11	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	13	0	0	0	0
All	All	9970	0	9276	499	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 26.

All (499) 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:B:3:PRO:HD3	1:B:6:GLN:NE2	1.36	1.40
1:B:282:THR:HG21	1:B:410:LEU:CB	1.60	1.31
1:A:279:VAL:HG21	1:A:410:LEU:CD1	1.60	1.29
1:B:282:THR:CG2	1:B:410:LEU:CB	2.18	1.20
1:A:279:VAL:CG1	1:A:410:LEU:HD13	1.73	1.17
1:B:80:TRP:HA	1:B:83:PHE:CD2	1.78	1.17
1:A:279:VAL:HG21	1:A:410:LEU:HD12	1.17	1.13
1:B:80:TRP:O	1:B:89:ARG:HG2	1.48	1.12
1:A:206:THR:HG23	1:A:210:ASP:OD2	1.51	1.10
1:B:3:PRO:CD	1:B:6:GLN:NE2	2.13	1.10
1:A:279:VAL:HG11	1:A:410:LEU:HD13	1.09	1.09
3:B:692:NAG:C8	3:B:692:NAG:H3	1.48	1.09
1:A:139:LEU:HD22	1:A:163:TRP:CZ2	1.89	1.08
3:B:692:NAG:C8	3:B:692:NAG:C3	2.30	1.08
1:A:6:GLN:HG3	1:A:7:PRO:HD2	1.35	1.07
1:B:80:TRP:HA	1:B:83:PHE:CE2	1.88	1.07
1:A:6:GLN:HG3	1:A:7:PRO:CD	1.85	1.06
1:A:279:VAL:HG11	1:A:410:LEU:CD1	1.85	1.04
1:B:3:PRO:CD	1:B:6:GLN:HE22	1.70	1.03
1:A:340:ARG:NH2	2:D:2:NAG:HN2	1.56	1.03
1:A:279:VAL:CG2	1:A:410:LEU:CD1	2.37	1.01
1:A:279:VAL:CG2	1:A:410:LEU:HD12	1.91	1.00
1:A:279:VAL:HG13	1:A:410:LEU:HB2	1.49	0.95
1:A:340:ARG:HH22	2:D:2:NAG:HN2	1.09	0.95
1:B:482:THR:HG21	2:E:1:NAG:H82	1.49	0.93
1:A:72:ALA:O	1:A:76:TYR:HB2	1.71	0.91
1:B:129:LEU:HD23	1:B:612:ASP:CB	2.00	0.91
1:B:10:PHE:O	1:B:75:LEU:HD21	1.72	0.90
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.52	0.90
1:A:139:LEU:HD22	1:A:163:TRP:CH2	2.08	0.88
1:A:46:ILE:HG13	1:A:327:GLU:O	1.72	0.88
1:A:279:VAL:HG21	1:A:410:LEU:HD13	1.53	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:CB	1:A:410:LEU:HD13	2.04	0.87
1:B:29:GLU:OE1	2:F:1:NAG:H5	1.74	0.87
1:B:80:TRP:CE2	1:B:81:GLN:HG3	2.10	0.86
1:A:157:LEU:HG	1:A:607:TYR:OH	1.76	0.85
1:A:279:VAL:HG13	1:A:410:LEU:CB	2.07	0.84
1:A:408:ILE:HG12	1:A:408:ILE:O	1.77	0.84
1:A:279:VAL:CG2	1:A:410:LEU:HD13	2.04	0.84
1:A:270:PRO:HD3	1:A:426:LEU:HD22	1.60	0.84
1:B:353:MET:HE1	1:B:427:LYS:HE3	1.60	0.84
1:B:3:PRO:HD3	1:B:6:GLN:HE22	0.76	0.83
1:A:566:ASP:OD2	1:A:568:GLN:HB2	1.79	0.83
1:A:441:LEU:HD23	1:A:442:VAL:N	1.94	0.82
1:B:464:TRP:CE3	1:B:475:PRO:HD3	2.16	0.81
1:B:282:THR:HG21	1:B:410:LEU:CA	2.10	0.80
1:A:80:TRP:O	1:A:81:GLN:HB2	1.79	0.80
1:B:289:ASN:HB3	1:B:292:HIS:H	1.45	0.80
1:B:236:ARG:HE	1:B:267:MET:HE2	1.47	0.80
1:B:77:GLU:H	1:B:78:PRO:HD2	1.46	0.79
1:A:500:ARG:HG2	5:B:703:CL:CL	2.19	0.79
1:B:91:ILE:O	1:B:95:VAL:HG23	1.81	0.79
1:B:406:HIS:HA	1:B:411:LEU:O	1.82	0.79
1:A:597:TYR:O	1:A:598:GLN:HB3	1.83	0.79
1:B:2:ASP:CB	1:B:3:PRO:HD2	2.13	0.79
3:A:692:NAG:C8	3:A:692:NAG:O3	2.31	0.79
1:B:507:LEU:HA	1:B:510:GLN:HG3	1.66	0.78
1:B:129:LEU:CD2	1:B:612:ASP:CB	2.61	0.78
1:A:480:ASN:OD1	1:A:482:THR:HG23	1.84	0.78
1:A:329:VAL:O	1:A:346:LYS:HE3	1.83	0.77
1:B:441:LEU:HD23	1:B:442:VAL:N	1.99	0.77
1:A:129:LEU:HD12	1:A:129:LEU:N	1.99	0.76
1:A:372:TYR:HB2	1:A:375:LEU:HD12	1.68	0.76
1:B:295:ARG:HG2	1:B:314:TRP:CH2	2.20	0.76
1:A:221:LEU:HD23	1:A:433:ILE:HD12	1.67	0.76
1:B:147:LEU:HD22	1:B:256:MET:HA	1.68	0.76
1:B:78:PRO:O	1:B:79:ILE:CB	2.32	0.75
1:A:441:LEU:O	1:A:444:GLN:HB2	1.87	0.74
1:B:80:TRP:CA	1:B:83:PHE:CE2	2.70	0.74
1:B:77:GLU:H	1:B:78:PRO:CD	2.01	0.74
1:B:530:ILE:HG23	1:B:530:ILE:O	1.86	0.74
1:A:96:ARG:HH21	1:A:96:ARG:HG3	1.54	0.73
1:A:369:TYR:HA	1:A:372:TYR:CE1	2.24	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PRO:HA	1:B:6:GLN:NE2	2.03	0.73
1:B:405:LEU:O	1:B:408:ILE:HG12	1.87	0.73
1:A:283:MET:HE1	1:A:356:LEU:HB2	1.70	0.72
1:B:129:LEU:O	1:B:131:ASN:N	2.22	0.72
1:A:279:VAL:CG1	1:A:410:LEU:CD1	2.54	0.72
1:A:69:GLY:HA3	1:A:98:LEU:HD21	1.70	0.72
1:B:540:LEU:O	1:B:543:VAL:HG22	1.89	0.72
1:B:332:ALA:HB2	1:B:347:GLN:HG3	1.71	0.72
1:A:279:VAL:CG1	1:A:410:LEU:CB	2.68	0.71
1:A:279:VAL:CG1	1:A:410:LEU:HB2	2.19	0.71
1:B:79:ILE:O	1:B:80:TRP:CD1	2.43	0.71
1:B:236:ARG:NE	1:B:267:MET:CE	2.53	0.71
1:B:129:LEU:HD12	1:B:129:LEU:N	2.05	0.71
1:A:279:VAL:HG12	1:A:283:MET:HG3	1.71	0.71
1:B:482:THR:CG2	2:E:1:NAG:H82	2.20	0.71
1:A:132:LYS:C	1:A:134:ALA:H	1.93	0.70
1:A:6:GLN:HG3	1:A:7:PRO:HD3	1.74	0.70
1:B:329:VAL:O	1:B:346:LYS:HE3	1.90	0.70
1:A:292:HIS:O	1:A:296:VAL:HG23	1.92	0.70
1:A:456:PRO:HA	1:A:459:TYR:CD2	2.26	0.69
1:B:282:THR:HG22	1:B:410:LEU:CB	2.19	0.69
1:A:489:LYS:HE3	1:A:491:HIS:HD2	1.56	0.69
1:B:284:LEU:HD23	1:B:351:VAL:HG11	1.73	0.69
1:B:129:LEU:C	1:B:131:ASN:H	1.96	0.69
1:B:464:TRP:CZ3	1:B:475:PRO:HD3	2.28	0.69
1:B:105:LEU:O	1:B:109:GLN:HG3	1.93	0.69
1:A:291:THR:HB	3:A:697:NAG:H2	1.73	0.69
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.73	0.68
1:B:489:LYS:O	1:B:493:PRO:HD2	1.93	0.68
1:A:147:LEU:HD22	1:A:256:MET:HA	1.75	0.68
1:A:279:VAL:HG11	1:A:410:LEU:CG	2.23	0.68
1:A:86:PRO:HA	1:A:89:ARG:NH1	2.09	0.68
1:B:279:VAL:HG12	1:B:279:VAL:O	1.91	0.68
1:A:489:LYS:O	1:A:493:PRO:HD2	1.94	0.67
1:B:129:LEU:HD21	1:B:137:TRP:CZ2	2.30	0.67
1:A:464:TRP:CE3	1:A:475:PRO:HD3	2.30	0.67
1:A:6:GLN:CG	1:A:7:PRO:HD2	2.19	0.67
1:B:203:ASN:N	1:B:203:ASN:HD22	1.93	0.66
1:B:264:ILE:O	1:B:264:ILE:HG23	1.94	0.66
1:B:171:LEU:HD21	1:B:493:PRO:HB3	1.77	0.66
1:B:58:ALA:O	1:B:62:GLN:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.77	0.66
1:A:206:THR:CG2	1:A:210:ASP:OD2	2.36	0.65
1:A:66:GLU:HA	1:A:98:LEU:HD22	1.78	0.65
1:B:29:GLU:HG2	1:B:338:TYR:O	1.97	0.65
1:B:353:MET:HE1	1:B:427:LYS:CE	2.27	0.65
1:A:440:TYR:O	1:A:444:GLN:HG2	1.97	0.65
1:A:395:LEU:O	1:A:399:VAL:HG23	1.98	0.64
1:B:316:GLY:HA3	1:B:344:ARG:HD3	1.79	0.64
1:B:221:LEU:HD12	1:B:433:ILE:HD13	1.80	0.64
1:B:264:ILE:O	1:B:264:ILE:CG2	2.46	0.64
1:A:340:ARG:NH2	2:D:2:NAG:N2	2.37	0.64
1:A:146:ILE:O	1:A:150:SER:HB3	1.98	0.64
1:A:73:LYS:HB2	1:A:77:GLU:HG3	1.78	0.64
1:B:236:ARG:NE	1:B:267:MET:HE2	2.13	0.64
1:B:441:LEU:HD23	1:B:441:LEU:C	2.17	0.64
1:B:183:ASN:HD21	1:B:193:ASP:HB2	1.64	0.63
1:A:332:ALA:HB2	1:A:347:GLN:HG3	1.80	0.63
1:B:607:TYR:CG	1:B:608:PRO:HD2	2.34	0.63
1:A:347:GLN:NE2	1:A:349:THR:OG1	2.31	0.63
1:A:31:VAL:HG21	1:A:64:PHE:CD1	2.33	0.63
1:A:541:ARG:O	1:A:541:ARG:HG3	1.99	0.63
1:A:251:HIS:CE1	1:A:476:PRO:HB3	2.34	0.62
1:B:203:ASN:HD22	1:B:203:ASN:H	1.45	0.62
1:A:340:ARG:NH1	2:D:2:NAG:H2	2.14	0.62
1:B:271:PHE:CD1	1:B:419:GLU:HB3	2.34	0.62
1:B:329:VAL:O	1:B:346:LYS:CE	2.48	0.62
1:B:3:PRO:CD	1:B:6:GLN:HE21	2.10	0.62
1:B:10:PHE:O	1:B:75:LEU:CD2	2.47	0.62
1:B:129:LEU:C	1:B:131:ASN:N	2.53	0.62
1:B:312:GLU:HG3	1:B:341:LYS:O	2.00	0.62
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.81	0.61
1:B:324:ASP:OD1	1:B:326:ARG:HG2	2.00	0.61
1:B:3:PRO:CA	1:B:6:GLN:NE2	2.64	0.61
1:A:96:ARG:HG3	1:A:96:ARG:NH2	2.14	0.61
1:B:279:VAL:O	1:B:279:VAL:CG1	2.48	0.61
1:A:270:PRO:HD3	1:A:426:LEU:CD2	2.30	0.61
1:B:404:HIS:HB2	1:B:529:ASP:OD2	2.01	0.61
1:B:279:VAL:HG13	1:B:282:THR:HB	1.83	0.60
1:A:73:LYS:CB	1:A:77:GLU:HG3	2.31	0.60
1:B:86:PRO:HA	1:B:89:ARG:HE	1.66	0.60
1:A:11:SER:C	1:A:13:ASP:H	2.05	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD22	1:A:256:MET:CA	2.32	0.59
1:A:377:VAL:HG13	1:A:378:SER:N	2.18	0.59
1:B:146:ILE:O	1:B:150:SER:HB3	2.02	0.59
1:B:316:GLY:C	1:B:344:ARG:HD3	2.22	0.59
1:A:513:GLU:OE2	1:A:572:LYS:HE3	2.02	0.59
1:B:441:LEU:CD2	1:B:442:VAL:N	2.64	0.59
1:B:530:ILE:O	1:B:530:ILE:CG2	2.51	0.59
1:B:142:ASP:O	1:B:146:ILE:HG13	2.02	0.59
1:A:300:PHE:HE2	1:A:304:LEU:HD11	1.68	0.59
1:B:98:LEU:HB2	1:B:102:ASN:ND2	2.18	0.59
1:B:504:SER:O	1:B:508:GLN:HB3	2.03	0.59
1:B:7:PRO:HB2	1:B:71:LYS:HG2	1.85	0.58
1:A:248:ILE:O	1:A:473:ILE:HA	2.03	0.58
1:B:77:GLU:N	1:B:78:PRO:CD	2.66	0.58
1:A:236:ARG:HG2	1:A:267:MET:CE	2.33	0.58
1:B:2:ASP:CB	1:B:3:PRO:CD	2.78	0.58
1:B:139:LEU:HD22	1:B:163:TRP:CZ2	2.39	0.58
1:B:580:TRP:O	1:B:584:GLN:HG2	2.04	0.58
1:A:147:LEU:HD22	1:A:256:MET:N	2.19	0.57
1:A:261:TRP:CD1	1:A:261:TRP:N	2.71	0.57
1:B:218:LEU:CD2	1:B:570:LEU:HD23	2.34	0.57
1:A:75:LEU:H	1:A:75:LEU:HD23	1.69	0.57
1:A:489:LYS:O	1:A:491:HIS:N	2.38	0.57
1:A:338:TYR:HD2	1:A:377:VAL:HG23	1.68	0.57
1:A:206:THR:HG23	1:A:210:ASP:CG	2.23	0.57
1:A:597:TYR:O	1:A:598:GLN:CB	2.53	0.57
1:A:142:ASP:O	1:A:146:ILE:HG13	2.05	0.57
1:B:541:ARG:O	1:B:541:ARG:HG2	2.04	0.57
1:A:51:ALA:O	1:A:55:GLU:HG3	2.04	0.57
1:B:97:THR:O	1:B:97:THR:HG22	2.04	0.56
1:B:80:TRP:CG	1:B:81:GLN:N	2.73	0.56
1:A:406:HIS:HD2	1:A:413:ARG:O	1.89	0.56
1:A:446:ARG:NH2	1:A:496:THR:O	2.35	0.56
1:A:404:HIS:O	1:A:408:ILE:HG23	2.05	0.56
1:A:75:LEU:HD23	1:A:75:LEU:N	2.21	0.56
1:A:129:LEU:HD12	1:A:129:LEU:H	1.71	0.55
1:B:283:MET:HE3	1:B:356:LEU:HD22	1.89	0.55
1:A:77:GLU:N	1:A:78:PRO:HD2	2.21	0.55
1:A:98:LEU:HB2	1:A:102:ASN:HD21	1.71	0.55
1:B:310:PRO:O	1:B:313:PHE:HB3	2.06	0.55
1:B:141:PRO:HG2	1:B:142:ASP:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:TRP:O	1:A:264:ILE:HG12	2.07	0.55
1:A:367:GLN:O	1:A:371:GLN:HG2	2.05	0.55
1:B:213:HIS:O	1:B:216:GLN:HB2	2.07	0.55
1:B:366:ILE:O	1:B:369:TYR:N	2.39	0.55
1:A:129:LEU:N	1:A:129:LEU:CD1	2.67	0.55
1:A:469:LYS:HE2	1:A:470:TYR:CZ	2.42	0.55
1:A:277:LEU:CD1	1:A:424:TYR:HA	2.37	0.54
1:B:270:PRO:O	1:B:272:PRO:HD3	2.08	0.54
1:B:279:VAL:HG21	1:B:405:LEU:HD13	1.89	0.54
1:B:270:PRO:HD3	1:B:426:LEU:HD22	1.89	0.54
1:A:91:ILE:HG23	1:A:378:SER:OG	2.06	0.54
1:A:104:PRO:HG2	1:A:107:LYS:HD2	1.88	0.54
1:B:316:GLY:CA	1:B:344:ARG:HD3	2.38	0.54
1:B:17:ALA:O	1:B:20:PHE:HB3	2.08	0.53
1:B:64:PHE:CE1	1:B:68:TRP:NE1	2.75	0.53
1:B:326:ARG:O	1:B:328:VAL:HG13	2.09	0.53
1:B:478:THR:O	1:B:479:ARG:HD2	2.08	0.53
1:A:492:VAL:N	1:A:493:PRO:HD2	2.23	0.53
1:B:607:TYR:C	1:B:608:PRO:O	2.43	0.53
1:B:251:HIS:CE1	1:B:476:PRO:HB3	2.43	0.53
1:A:147:LEU:O	1:A:254:GLY:HA2	2.09	0.53
1:B:99:GLY:O	1:B:102:ASN:ND2	2.36	0.53
1:B:147:LEU:O	1:B:254:GLY:HA2	2.08	0.53
1:A:54:GLN:HG3	1:A:55:GLU:N	2.24	0.53
1:A:326:ARG:HD2	3:A:692:NAG:HN2	1.72	0.52
1:A:607:TYR:CD1	1:A:608:PRO:HA	2.44	0.52
1:B:218:LEU:O	1:B:221:LEU:HB2	2.09	0.52
1:A:350:ARG:HD2	1:A:351:VAL:H	1.75	0.52
1:B:29:GLU:OE1	2:F:1:NAG:C5	2.54	0.52
1:B:29:GLU:CG	1:B:338:TYR:O	2.57	0.52
1:B:326:ARG:O	1:B:327:GLU:C	2.48	0.52
1:A:214:LEU:HD11	1:A:565:LEU:HB3	1.90	0.52
1:A:510:GLN:OE1	1:A:566:ASP:N	2.40	0.52
1:A:480:ASN:OD1	1:A:482:THR:CG2	2.57	0.52
1:B:426:LEU:O	1:B:429:ALA:HB3	2.10	0.52
1:A:98:LEU:HB2	1:A:102:ASN:ND2	2.24	0.52
1:A:441:LEU:HD23	1:A:441:LEU:C	2.29	0.52
1:A:69:GLY:HA3	1:A:98:LEU:CD2	2.38	0.52
1:B:292:HIS:O	1:B:296:VAL:HG23	2.09	0.52
1:A:147:LEU:CD2	1:A:256:MET:HA	2.41	0.51
1:B:408:ILE:CG1	1:B:409:GLY:N	2.70	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:HA	1:A:98:LEU:CD2	2.41	0.51
1:A:269:VAL:O	1:A:269:VAL:HG13	2.09	0.51
1:A:312:GLU:HG2	1:A:341:LYS:HE2	1.93	0.51
1:B:71:LYS:HE3	1:B:75:LEU:HD11	1.91	0.51
1:A:204:SER:OG	1:A:206:THR:HG22	2.11	0.51
1:A:495:VAL:HG12	1:A:495:VAL:O	2.10	0.51
1:B:294:PHE:HE1	1:B:349:THR:HG1	1.59	0.51
1:A:323:ALA:C	1:A:325:GLY:H	2.14	0.50
1:A:445:TRP:HB2	1:A:466:LEU:HD12	1.94	0.50
1:B:3:PRO:N	1:B:6:GLN:HE21	2.10	0.50
1:B:200:SER:O	1:B:203:ASN:ND2	2.44	0.50
1:A:583:GLU:O	1:A:587:GLN:HG3	2.12	0.50
1:B:510:GLN:OE1	1:B:566:ASP:N	2.44	0.49
1:B:563:ASP:OD1	1:B:563:ASP:O	2.30	0.49
1:A:40:TRP:CE2	1:A:44:THR:HG21	2.46	0.49
1:A:139:LEU:CD2	1:A:163:TRP:CZ2	2.79	0.49
1:A:478:THR:O	1:A:479:ARG:HD2	2.13	0.49
1:B:138:SER:O	1:B:143:LEU:HG	2.11	0.49
1:B:362:GLU:O	1:B:365:HIS:HB2	2.13	0.49
1:A:265:TYR:CZ	1:A:269:VAL:HG23	2.47	0.49
1:A:268:VAL:O	1:A:269:VAL:C	2.51	0.49
1:A:583:GLU:O	1:A:587:GLN:CG	2.61	0.49
1:A:218:LEU:HD13	1:A:436:LEU:HD13	1.95	0.49
1:B:2:ASP:O	1:B:3:PRO:HB2	2.12	0.49
1:B:129:LEU:N	1:B:129:LEU:CD1	2.76	0.49
1:B:332:ALA:CB	1:B:347:GLN:HG3	2.39	0.49
1:B:256:MET:HB3	1:B:257:TRP:CE3	2.48	0.48
1:A:499:ILE:HG13	1:A:499:ILE:O	2.14	0.48
1:B:3:PRO:CA	1:B:6:GLN:HE21	2.26	0.48
1:B:593:GLY:HA3	7:B:2433:GOL:O1	2.13	0.48
1:A:271:PHE:HB2	1:A:423:ASN:HD21	1.78	0.48
1:A:393:ASP:O	1:A:396:ALA:HB3	2.13	0.48
1:B:79:ILE:O	1:B:81:GLN:N	2.41	0.48
1:A:270:PRO:O	1:A:272:PRO:HD3	2.13	0.48
1:A:300:PHE:CE2	1:A:304:LEU:HD11	2.48	0.48
1:A:49:GLU:HG3	1:A:53:ARG:HE	1.79	0.48
1:A:99:GLY:HA2	1:A:186:TYR:CE2	2.48	0.48
1:B:169:ILE:N	1:B:170:PRO:HD2	2.29	0.48
1:A:399:VAL:HA	1:A:404:HIS:CD2	2.48	0.48
1:A:551:PRO:O	1:A:555:VAL:HG23	2.14	0.48
1:B:51:ALA:O	1:B:55:GLU:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD21	1:A:493:PRO:HB3	1.95	0.48
1:A:441:LEU:HD23	1:A:442:VAL:CA	2.43	0.48
1:A:507:LEU:HB3	1:A:565:LEU:CD2	2.44	0.48
1:B:295:ARG:HG2	1:B:314:TRP:HH2	1.72	0.48
1:B:482:THR:HG21	2:E:1:NAG:C8	2.34	0.48
1:A:139:LEU:HA	1:A:143:LEU:HB2	1.95	0.47
1:A:453:ARG:O	1:A:453:ARG:HG2	2.14	0.47
1:A:539:LYS:HE3	1:A:559:MET:O	2.13	0.47
1:B:44:THR:O	1:B:328:VAL:HG12	2.14	0.47
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.34	0.47
1:B:606:ASN:O	1:B:608:PRO:O	2.32	0.47
1:A:98:LEU:HD12	1:A:102:ASN:OD1	2.13	0.47
1:A:236:ARG:HG2	1:A:267:MET:HE3	1.96	0.47
1:B:80:TRP:CZ2	1:B:81:GLN:HG3	2.48	0.47
1:B:77:GLU:CG	1:B:77:GLU:O	2.62	0.47
1:B:141:PRO:O	1:B:142:ASP:C	2.51	0.47
1:A:355:GLN:O	1:A:359:VAL:HG23	2.15	0.47
1:A:482:THR:HG21	2:C:1:NAG:HN2	1.80	0.47
1:B:243:ASN:OD1	1:B:245:ARG:N	2.41	0.47
1:B:299:GLU:HG2	1:B:300:PHE:N	2.30	0.47
1:A:274:LYS:CB	1:A:275:PRO:HD2	2.35	0.47
1:B:98:LEU:HB2	1:B:102:ASN:HD21	1.78	0.47
1:B:218:LEU:HD22	1:B:570:LEU:HD23	1.95	0.47
1:A:122:TYR:CD1	1:A:493:PRO:HG3	2.49	0.47
1:A:277:LEU:HD11	1:A:424:TYR:HB2	1.97	0.47
1:B:236:ARG:HE	1:B:267:MET:CE	2.11	0.47
1:A:490:PHE:O	1:A:493:PRO:HG2	2.15	0.47
1:A:597:TYR:CD1	1:A:597:TYR:C	2.88	0.47
1:B:551:PRO:HB2	1:B:554:GLU:HG3	1.96	0.47
1:A:34:GLN:HG3	1:A:35:SER:H	1.80	0.46
1:A:284:LEU:HD23	1:A:351:VAL:HG11	1.97	0.46
1:A:489:LYS:O	1:A:490:PHE:C	2.53	0.46
1:B:262:GLU:OE1	1:B:262:GLU:N	2.48	0.46
1:B:270:PRO:HD3	1:B:426:LEU:CD2	2.44	0.46
1:B:329:VAL:HB	1:B:346:LYS:HE3	1.97	0.46
1:B:418:THR:HG22	1:B:419:GLU:N	2.29	0.46
1:B:495:VAL:HG12	1:B:495:VAL:O	2.14	0.46
1:A:129:LEU:H	1:A:129:LEU:CD1	2.27	0.46
1:B:486:ALA:O	1:B:492:VAL:HG21	2.16	0.46
1:A:77:GLU:N	1:A:78:PRO:CD	2.78	0.46
1:A:456:PRO:HA	1:A:459:TYR:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:O	1:B:134:ALA:C	2.53	0.46
1:B:597:TYR:CD1	1:B:597:TYR:C	2.89	0.46
1:B:217:GLN:O	1:B:220:PRO:HD2	2.15	0.46
1:A:80:TRP:CE2	1:A:81:GLN:HG3	2.50	0.46
1:A:507:LEU:O	1:A:507:LEU:HG	2.16	0.46
1:B:75:LEU:HD23	1:B:76:TYR:CZ	2.51	0.46
1:B:492:VAL:HB	1:B:493:PRO:CD	2.46	0.46
1:A:80:TRP:O	1:A:81:GLN:CB	2.57	0.46
1:A:279:VAL:HG11	1:A:410:LEU:HD22	1.98	0.46
1:B:408:ILE:HG12	1:B:409:GLY:N	2.30	0.46
1:B:437:PRO:O	1:B:441:LEU:HB3	2.15	0.46
1:B:529:ASP:OD1	1:B:531:TYR:HB2	2.16	0.46
1:A:143:LEU:O	1:A:147:LEU:HD12	2.15	0.46
1:A:338:TYR:HD2	1:A:377:VAL:CG2	2.29	0.46
1:A:481:GLU:HA	1:A:481:GLU:OE2	2.16	0.46
1:A:418:THR:O	1:A:421:ASP:N	2.49	0.46
1:B:140:ASP:OD1	1:B:140:ASP:C	2.53	0.46
1:A:510:GLN:HE21	1:A:560:VAL:HG11	1.81	0.46
1:A:340:ARG:CZ	2:D:2:NAG:HN2	2.21	0.46
1:B:147:LEU:HD22	1:B:256:MET:CA	2.44	0.46
1:B:607:TYR:CD2	1:B:608:PRO:HD2	2.50	0.46
1:A:204:SER:C	1:A:206:THR:H	2.18	0.45
1:B:44:THR:O	1:B:44:THR:HG22	2.15	0.45
1:B:45:ASN:OD1	1:B:326:ARG:HB2	2.17	0.45
1:B:435:PHE:CE2	1:B:439:GLY:HA3	2.51	0.45
1:B:141:PRO:CG	1:B:142:ASP:N	2.79	0.45
1:B:369:TYR:HD2	1:B:372:TYR:HH	1.64	0.45
1:B:507:LEU:O	1:B:507:LEU:HG	2.16	0.45
1:B:129:LEU:HD12	1:B:129:LEU:H	1.78	0.45
1:B:536:ALA:O	1:B:539:LYS:N	2.50	0.45
1:B:309:MET:HB3	1:B:313:PHE:CD2	2.52	0.45
1:B:406:HIS:O	1:B:408:ILE:O	2.34	0.45
1:B:98:LEU:HB3	1:B:101:ALA:HB3	1.99	0.45
1:B:191:PHE:CZ	1:B:197:TYR:HD1	2.35	0.45
1:B:438:PHE:O	1:B:442:VAL:HG23	2.17	0.45
1:B:570:LEU:CD1	1:B:574:PHE:HE1	2.30	0.45
1:B:607:TYR:CD2	1:B:608:PRO:CD	3.00	0.45
1:A:369:TYR:HA	1:A:372:TYR:HE1	1.79	0.45
1:A:469:LYS:HE2	1:A:470:TYR:CE1	2.51	0.45
1:A:570:LEU:O	1:A:570:LEU:HD12	2.17	0.45
1:B:32:LEU:CD1	1:B:377:VAL:HG11	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LYS:HE2	1:B:559:MET:O	2.16	0.45
1:B:568:GLN:HA	1:B:571:LEU:HD12	1.98	0.45
2:D:1:NAG:H61	2:D:2:NAG:C7	2.47	0.45
1:B:71:LYS:HE3	1:B:75:LEU:CD1	2.47	0.45
1:B:289:ASN:HB2	1:B:292:HIS:HB2	1.99	0.45
1:A:31:VAL:O	1:A:34:GLN:HG3	2.17	0.45
1:A:289:ASN:HB3	1:A:292:HIS:H	1.82	0.45
1:A:377:VAL:CG1	1:A:378:SER:N	2.80	0.45
1:B:3:PRO:O	1:B:4:GLY:C	2.52	0.45
1:B:77:GLU:N	1:B:78:PRO:HD2	2.23	0.44
1:A:279:VAL:O	1:A:281:SER:N	2.50	0.44
1:A:575:GLN:HB3	1:A:576:PRO:HD3	1.99	0.44
1:B:111:TYR:CE2	1:B:115:LEU:HD11	2.53	0.44
1:B:218:LEU:HD21	1:B:570:LEU:HD23	1.99	0.44
1:A:480:ASN:OD1	1:A:483:HIS:CE1	2.71	0.44
1:B:417:ASP:HB3	1:B:420:SER:OG	2.16	0.44
1:B:86:PRO:HB3	1:B:89:ARG:HH21	1.81	0.44
1:A:18:GLN:HG2	1:A:88:LEU:HD22	2.00	0.44
1:A:300:PHE:CD2	1:A:395:LEU:HD23	2.53	0.44
1:B:172:LYS:N	1:B:173:PRO:HD2	2.32	0.44
1:A:77:GLU:H	1:A:78:PRO:HD2	1.82	0.44
1:B:80:TRP:NE1	1:B:81:GLN:HG3	2.32	0.44
1:B:117:ASN:O	1:B:121:ILE:HG13	2.18	0.44
1:A:218:LEU:O	1:A:221:LEU:HB2	2.18	0.44
1:A:279:VAL:HG11	1:A:410:LEU:CD2	2.47	0.44
1:A:283:MET:CE	1:A:356:LEU:HD22	2.47	0.44
1:A:44:THR:O	1:A:326:ARG:NH2	2.47	0.44
1:A:221:LEU:HD23	1:A:433:ILE:CD1	2.42	0.44
1:B:69:GLY:HA3	1:B:98:LEU:CD2	2.47	0.44
1:B:171:LEU:HD21	1:B:493:PRO:CB	2.47	0.44
1:B:183:ASN:HD21	1:B:193:ASP:CB	2.30	0.44
1:B:288:TRP:CH2	1:B:296:VAL:HG21	2.51	0.44
1:B:383:ALA:HB3	1:B:387:PHE:CG	2.53	0.44
1:A:233:LEU:HD22	1:A:237:TYR:HE1	1.83	0.43
1:A:269:VAL:O	1:A:269:VAL:CG1	2.65	0.43
1:A:593:GLY:HA3	7:A:2434:GOL:O1	2.18	0.43
1:B:75:LEU:HD23	1:B:76:TYR:OH	2.17	0.43
1:A:24:TYR:CE1	1:A:64:PHE:HE2	2.35	0.43
1:A:494:ASN:N	1:A:494:ASN:HD22	2.15	0.43
1:B:15:ALA:HA	1:B:18:GLN:HB2	2.00	0.43
1:B:207:PHE:CZ	1:B:211:LEU:HD11	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:LEU:HB3	1:B:565:LEU:CD2	2.49	0.43
1:A:71:LYS:O	1:A:75:LEU:HD23	2.17	0.43
1:A:441:LEU:CD1	1:A:467:ARG:HA	2.48	0.43
1:B:122:TYR:CE1	1:B:163:TRP:HZ2	2.36	0.43
1:B:352:THR:HG22	1:B:353:MET:N	2.32	0.43
1:A:464:TRP:CZ3	1:A:475:PRO:HD3	2.52	0.43
1:B:489:LYS:O	1:B:490:PHE:C	2.56	0.43
1:A:580:TRP:CZ3	1:A:581:LEU:HD23	2.54	0.43
1:B:245:ARG:O	1:B:595:PRO:HD2	2.19	0.43
1:B:317:SER:HA	1:B:344:ARG:HB3	2.01	0.43
1:B:442:VAL:O	1:B:445:TRP:HB3	2.19	0.43
1:A:366:ILE:O	1:A:370:LEU:HG	2.18	0.43
1:A:503:VAL:HG13	1:A:565:LEU:HD11	2.00	0.43
1:B:83:PHE:CD2	1:B:88:LEU:HD12	2.53	0.43
1:A:478:THR:HG22	1:A:479:ARG:N	2.34	0.43
1:A:498:TYR:C	1:A:500:ARG:H	2.22	0.43
1:A:245:ARG:O	1:A:596:GLU:HB2	2.18	0.43
1:A:510:GLN:HG2	1:A:569:PRO:HG3	2.00	0.43
1:B:567:ALA:O	1:B:568:GLN:C	2.57	0.43
1:A:472:GLY:CA	1:A:594:TRP:CE2	3.02	0.42
1:A:594:TRP:CE3	1:A:594:TRP:N	2.87	0.42
1:A:141:PRO:O	1:A:142:ASP:C	2.57	0.42
1:A:381:ARG:O	1:A:547:GLY:HA2	2.20	0.42
1:A:132:LYS:C	1:A:134:ALA:N	2.63	0.42
1:A:368:TYR:CE2	1:A:544:LEU:HA	2.54	0.42
1:B:115:LEU:HD21	1:B:178:PHE:CE1	2.54	0.42
1:B:140:ASP:HA	1:B:141:PRO:HA	1.86	0.42
1:B:304:LEU:HD21	1:B:530:ILE:O	2.19	0.42
1:A:31:VAL:HG21	1:A:64:PHE:HD1	1.79	0.42
1:A:316:GLY:C	1:A:344:ARG:HD3	2.39	0.42
1:A:366:ILE:HA	1:A:369:TYR:CD1	2.54	0.42
1:A:472:GLY:HA2	1:A:594:TRP:CE2	2.53	0.42
1:A:490:PHE:C	1:A:490:PHE:CD2	2.92	0.42
1:B:390:ALA:O	1:B:391:ILE:C	2.57	0.42
1:B:405:LEU:O	1:B:408:ILE:CG1	2.63	0.42
1:B:460:ASN:N	1:B:481:GLU:OE2	2.34	0.42
1:A:143:LEU:HD13	1:A:163:TRP:HB2	2.01	0.42
1:A:607:TYR:HA	1:A:608:PRO:HA	1.76	0.42
1:B:570:LEU:CD1	1:B:574:PHE:CE1	3.03	0.42
1:A:335:TRP:CD1	1:A:335:TRP:N	2.87	0.42
1:A:510:GLN:HE21	1:A:510:GLN:HB3	1.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:HB2	1:B:89:ARG:HG3	2.02	0.42
1:B:436:LEU:N	1:B:437:PRO:HD2	2.35	0.42
1:A:210:ASP:O	1:A:214:LEU:HB2	2.19	0.42
1:B:362:GLU:OE1	1:B:362:GLU:HA	2.19	0.42
1:A:108:ARG:O	1:A:111:TYR:HB3	2.20	0.41
1:A:312:GLU:OE1	1:A:312:GLU:N	2.46	0.41
1:B:283:MET:HE3	1:B:356:LEU:CD2	2.49	0.41
1:A:309:MET:HA	1:A:310:PRO:HD3	1.93	0.41
1:A:567:ALA:O	1:A:570:LEU:HB3	2.20	0.41
1:B:406:HIS:CA	1:B:411:LEU:O	2.61	0.41
1:B:531:TYR:O	1:B:532:ARG:HB2	2.20	0.41
1:B:541:ARG:O	1:B:541:ARG:CG	2.66	0.41
1:A:303:SER:HB2	1:A:532:ARG:HG2	2.03	0.41
1:A:498:TYR:O	1:A:500:ARG:N	2.54	0.41
1:B:279:VAL:CG2	1:B:405:LEU:HD13	2.49	0.41
1:B:382:GLY:O	1:B:383:ALA:C	2.58	0.41
1:A:157:LEU:HD23	1:A:607:TYR:CZ	2.56	0.41
1:A:326:ARG:HD2	3:A:692:NAG:N2	2.36	0.41
1:B:114:LEU:HD23	1:B:114:LEU:HA	1.93	0.41
1:B:339:ASN:OD1	1:B:342:ASP:N	2.50	0.41
1:A:317:SER:HB3	1:A:319:LEU:HD21	2.01	0.41
1:A:350:ARG:HD2	1:A:351:VAL:HG23	2.01	0.41
1:B:268:VAL:O	1:B:269:VAL:C	2.57	0.41
1:B:557:LYS:O	1:B:561:GLY:HA2	2.19	0.41
1:A:331:HIS:CB	1:A:490:PHE:CE1	3.04	0.41
1:A:104:PRO:CG	1:A:107:LYS:HD2	2.51	0.41
1:A:375:LEU:O	1:A:376:PRO:C	2.58	0.41
1:A:441:LEU:HD23	1:A:442:VAL:HA	2.03	0.41
1:A:11:SER:C	1:A:13:ASP:N	2.73	0.41
1:A:138:SER:O	1:A:139:LEU:C	2.59	0.41
1:A:401:THR:HA	1:A:402:PRO:HD3	1.97	0.41
1:B:79:ILE:O	1:B:80:TRP:CG	2.74	0.41
1:B:147:LEU:HD13	1:B:256:MET:CE	2.51	0.41
1:B:210:ASP:O	1:B:214:LEU:HB2	2.21	0.41
1:B:243:ASN:OD1	1:B:246:GLY:N	2.54	0.41
1:A:309:MET:HB3	1:A:313:PHE:CD2	2.56	0.41
1:A:351:VAL:O	1:A:351:VAL:HG12	2.21	0.41
1:A:550:ARG:HG2	1:A:550:ARG:HH11	1.85	0.41
1:A:586:GLN:O	1:A:587:GLN:C	2.58	0.41
1:B:261:TRP:CD1	1:B:261:TRP:N	2.88	0.41
1:B:368:TYR:CE2	1:B:544:LEU:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:CD2	1:A:607:TYR:CZ	3.03	0.40
1:A:279:VAL:HG13	1:A:410:LEU:HB3	1.98	0.40
1:A:500:ARG:H	1:A:500:ARG:HG3	1.54	0.40
1:A:550:ARG:HG2	1:A:550:ARG:NH1	2.36	0.40
1:B:28:ALA:HA	1:B:31:VAL:HG12	2.03	0.40
1:B:441:LEU:C	1:B:441:LEU:CD2	2.89	0.40
1:A:6:GLN:CG	1:A:7:PRO:CD	2.77	0.40
1:A:16:GLY:O	1:A:19:LEU:HB2	2.21	0.40
1:A:279:VAL:HG12	1:A:279:VAL:O	2.22	0.40
1:B:253:LEU:HG	1:B:261:TRP:CE2	2.56	0.40
1:A:6:GLN:HE21	1:A:6:GLN:HB2	1.60	0.40
1:A:50:ASN:HA	1:A:53:ARG:HD2	2.02	0.40
1:B:31:VAL:HG11	1:B:64:PHE:CD2	2.56	0.40
1:B:204:SER:C	1:B:206:THR:H	2.23	0.40
1:B:381:ARG:HB2	1:B:548:SER:HB2	2.02	0.40
1:B:456:PRO:HA	1:B:459:TYR:CD2	2.57	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	610/612 (100%)	537 (88%)	60 (10%)	13 (2%)	7 31
1	B	609/612 (100%)	526 (86%)	73 (12%)	10 (2%)	9 38
All	All	1219/1224 (100%)	1063 (87%)	133 (11%)	23 (2%)	8 34

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	608	PRO
1	B	3	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	608	PRO
1	A	7	PRO
1	A	250	ALA
1	A	280	THR
1	A	545	GLN
1	B	130	PRO
1	B	134	ALA
1	B	135	THR
1	B	391	ILE
1	A	351	VAL
1	A	111	TYR
1	A	414	VAL
1	B	77	GLU
1	A	391	ILE
1	A	495	VAL
1	B	185	ALA
1	B	408	ILE
1	A	130	PRO
1	B	79	ILE
1	A	499	ILE
1	A	530	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	496/526 (94%)	448 (90%)	48 (10%)	8 29
1	B	489/526 (93%)	437 (89%)	52 (11%)	6 25
All	All	985/1052 (94%)	885 (90%)	100 (10%)	7 27

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	11	SER
1	A	35	SER
1	A	52	ARG
1	A	77	GLU
1	A	82	ASN
1	A	96	ARG
1	A	100	SER
1	A	105	LEU
1	A	171	LEU
1	A	203	ASN
1	A	236	ARG
1	A	245	ARG
1	A	262	GLU
1	A	295	ARG
1	A	299	GLU
1	A	341	LYS
1	A	342	ASP
1	A	350	ARG
1	A	354	ASP
1	A	363	MET
1	A	368	TYR
1	A	372	TYR
1	A	381	ARG
1	A	388	HIS
1	A	393	ASP
1	A	408	ILE
1	A	410	LEU
1	A	411	LEU
1	A	441	LEU
1	A	453	ARG
1	A	482	THR
1	A	496	THR
1	A	500	ARG
1	A	507	LEU
1	A	522	GLU
1	A	540	LEU
1	A	541	ARG
1	A	543	VAL
1	A	550	ARG
1	A	553	GLN
1	A	558	ASP
1	A	563	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	575	GLN
1	A	582	GLN
1	A	587	GLN
1	A	594	TRP
1	B	3	PRO
1	B	49	GLU
1	B	66	GLU
1	B	76	TYR
1	B	96	ARG
1	B	105	LEU
1	B	126	LYS
1	B	129	LEU
1	B	141	PRO
1	B	147	LEU
1	B	184	GLU
1	B	189	ASP
1	B	203	ASN
1	B	214	LEU
1	B	231	ARG
1	B	236	ARG
1	B	245	ARG
1	B	262	GLU
1	B	264	ILE
1	B	274	LYS
1	B	285	GLN
1	B	289	ASN
1	B	299	GLU
1	B	312	GLU
1	B	320	GLU
1	B	342	ASP
1	B	354	ASP
1	B	368	TYR
1	B	372	TYR
1	B	374	ASP
1	B	388	HIS
1	B	408	ILE
1	B	411	LEU
1	B	414	VAL
1	B	418	THR
1	B	441	LEU
1	B	443	ASP
1	B	453	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	480	ASN
1	B	489	LYS
1	B	507	LEU
1	B	508	GLN
1	B	510	GLN
1	B	542	LYS
1	B	553	GLN
1	B	572	LYS
1	B	575	GLN
1	B	586	GLN
1	B	590	GLU
1	B	598	GLN
1	B	607	TYR
1	B	608	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	50	ASN
1	A	81	GLN
1	A	347	GLN
1	A	406	HIS
1	A	491	HIS
1	A	494	ASN
1	A	545	GLN
1	A	575	GLN
1	B	6	GLN
1	B	18	GLN
1	B	50	ASN
1	B	183	ASN
1	B	203	ASN
1	B	416	ASN
1	B	545	GLN
1	B	575	GLN
1	B	579	GLN
1	B	582	GLN
1	B	587	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	0.65	0
2	NAG	D	1	2,1	14,14,15	0.58	0	17,19,21	0.72	1 (5%)
2	NAG	D	2	2	14,14,15	0.50	0	17,19,21	0.65	0
2	NAG	E	1	2,1	14,14,15	0.57	0	17,19,21	0.72	1 (5%)
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	0.65	0
2	NAG	F	1	2,1	14,14,15	2.35	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	F	2	2	14,14,15	2.34	1 (7%)	17,19,21	1.04	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C8-C7	-8.75	1.32	1.50
2	F	2	NAG	C8-C7	-8.70	1.32	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C1-C2-N2	-3.21	105.01	110.49
2	F	2	NAG	C1-C2-N2	-3.19	105.04	110.49
2	C	1	NAG	C2-N2-C7	-2.04	120.00	122.90
2	D	1	NAG	C2-N2-C7	-2.01	120.04	122.90
2	E	1	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

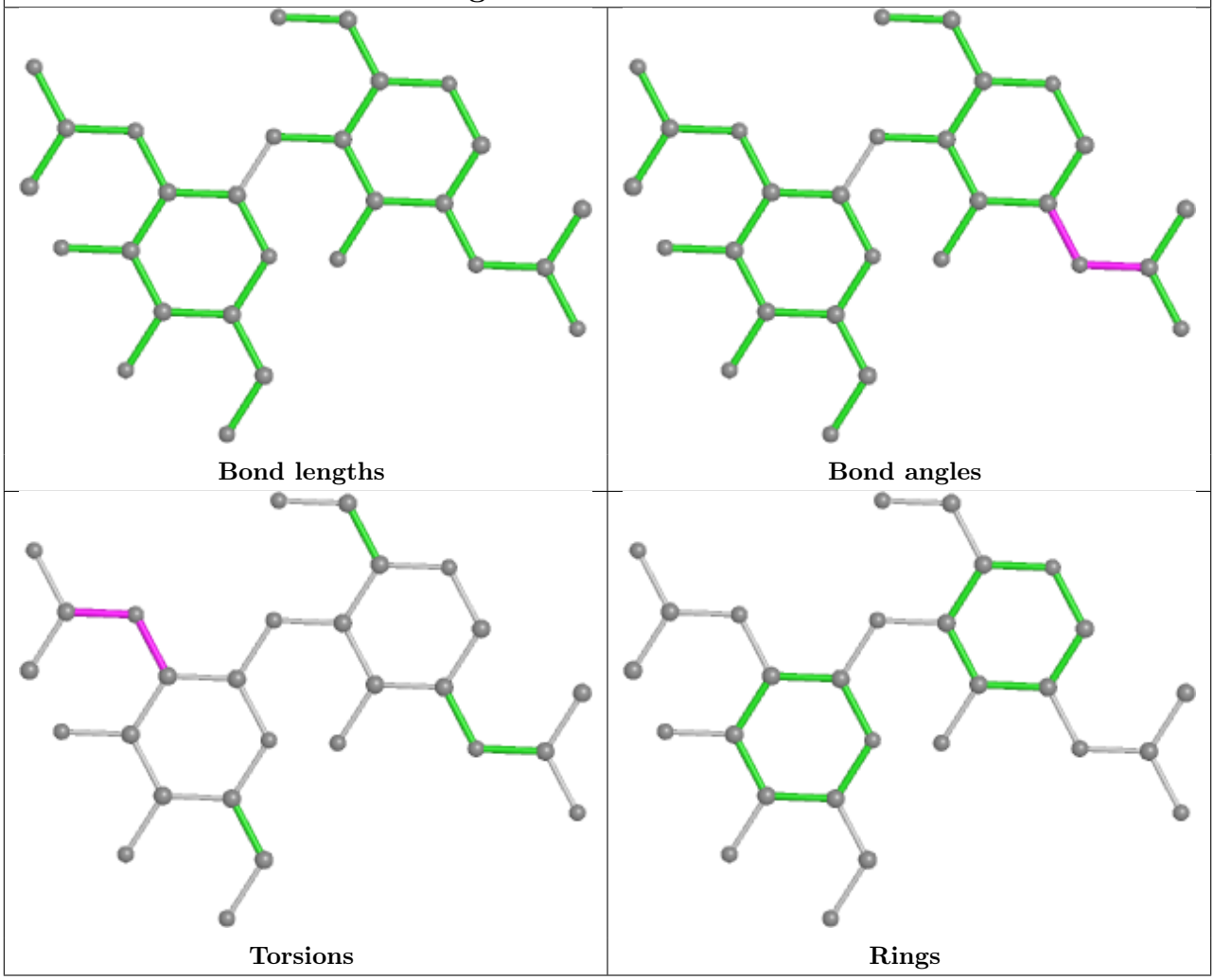
Continued on next page...

Continued from previous page...

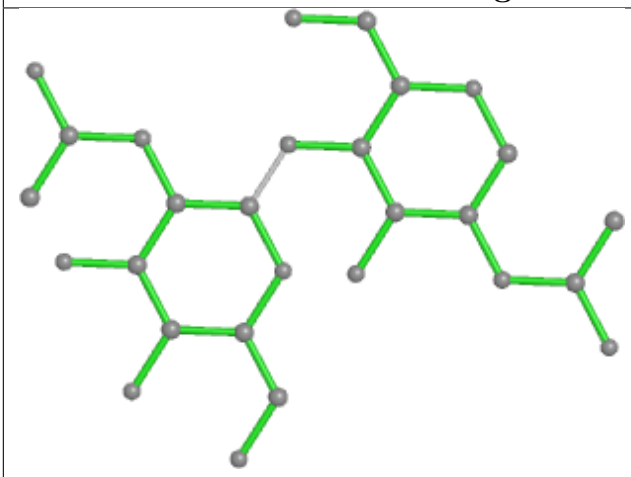
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	2	0
2	D	2	NAG	6	0
2	E	1	NAG	3	0
2	D	1	NAG	1	0

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

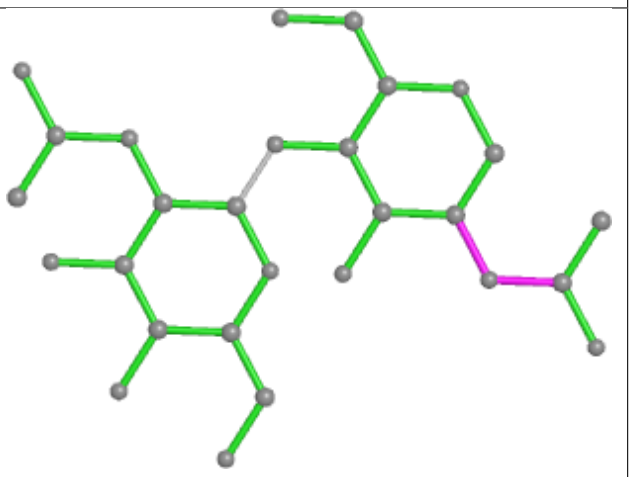
Oligosaccharide Chain C



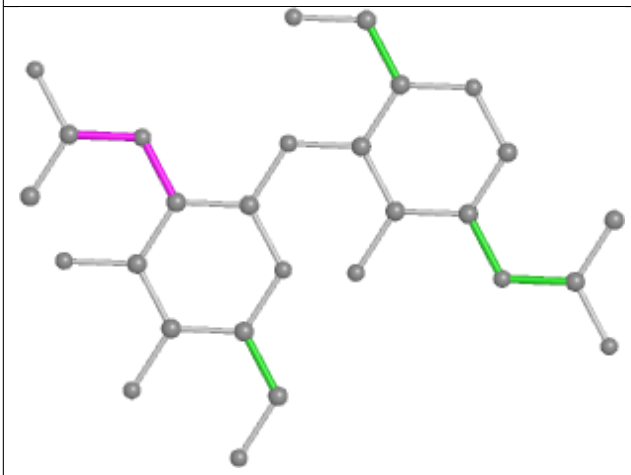
Oligosaccharide Chain D



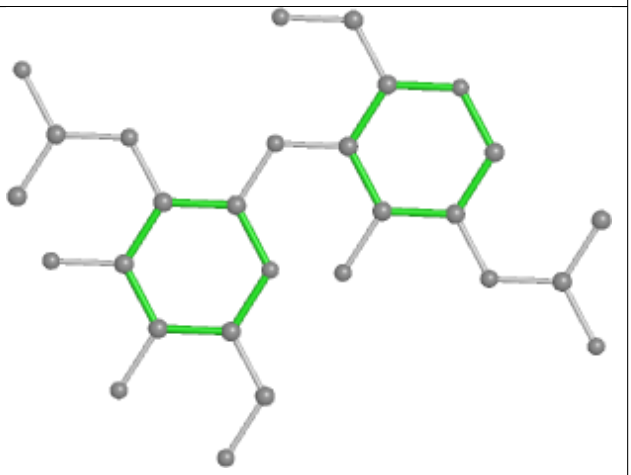
Bond lengths



Bond angles

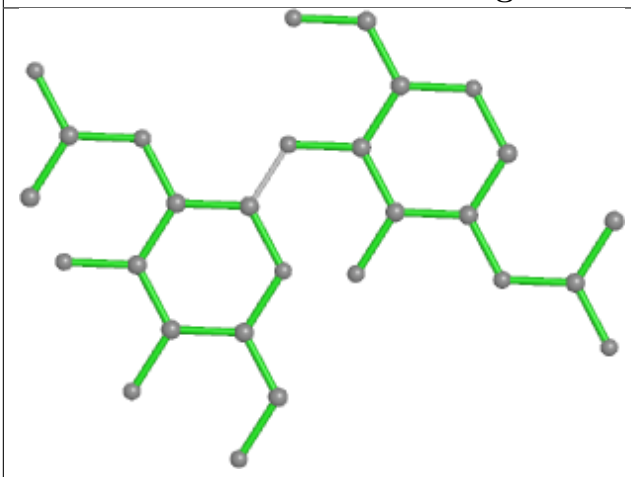


Torsions

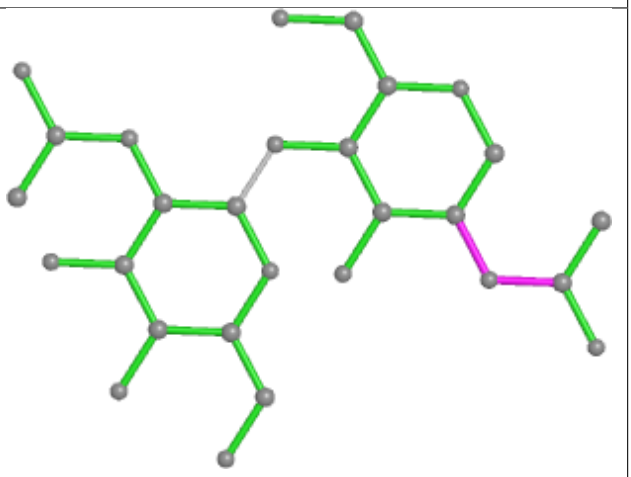


Rings

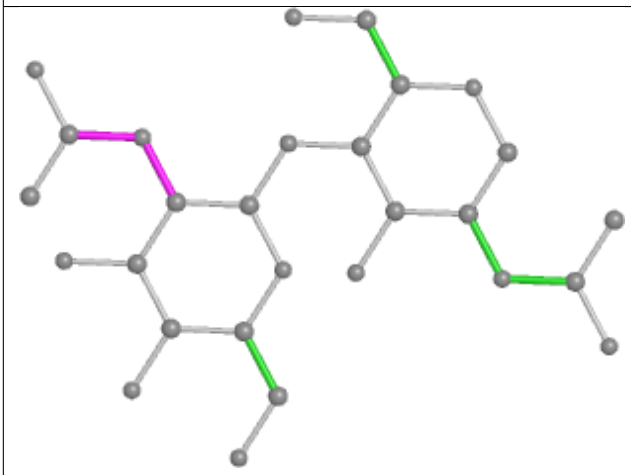
Oligosaccharide Chain E



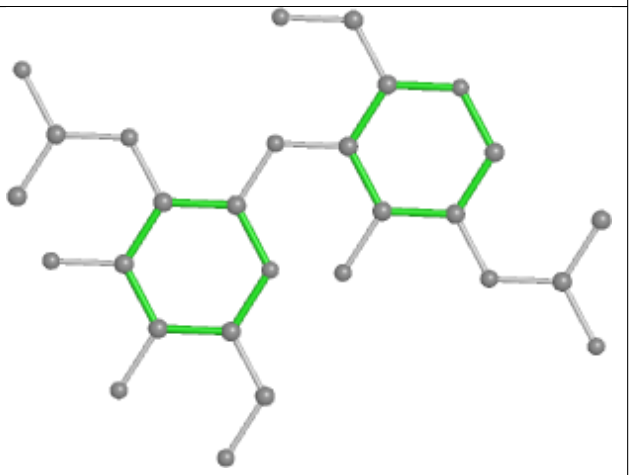
Bond lengths



Bond angles

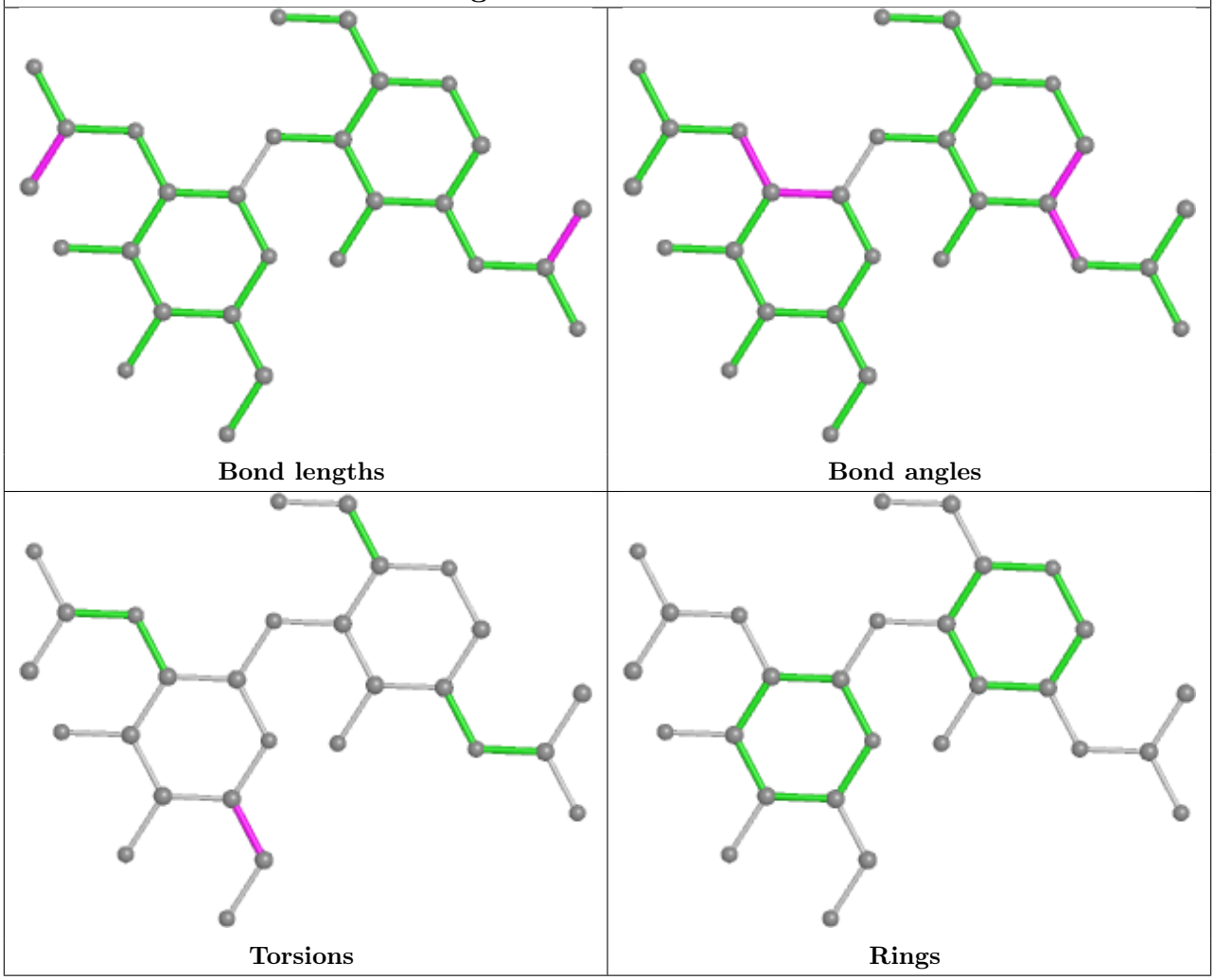


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	697	1	14,14,15	0.58	0	17,19,21	0.72	1 (5%)
7	GOL	A	2434	-	5,5,5	3.24	3 (60%)	5,5,5	1.91	3 (60%)
3	NAG	B	692	1	14,14,15	3.78	2 (14%)	17,19,21	1.59	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	695	1	14,14,15	0.57	0	17,19,21	0.72	1 (5%)
6	ACT	B	801	-	3,3,3	1.29	0	3,3,3	1.63	1 (33%)
6	ACT	A	800	-	3,3,3	1.17	0	3,3,3	1.53	1 (33%)
6	ACT	A	801	-	3,3,3	1.28	0	3,3,3	1.60	1 (33%)
3	NAG	A	695	1	14,14,15	0.58	0	17,19,21	0.71	1 (5%)
3	NAG	A	692	1	14,14,15	3.97	3 (21%)	17,19,21	1.90	4 (23%)
7	GOL	B	2433	-	5,5,5	3.26	3 (60%)	5,5,5	2.08	4 (80%)

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	A	697	1	-	0/6/23/26	0/1/1/1
7	GOL	A	2434	-	-	1/4/4/4	-
3	NAG	B	692	1	-	5/6/23/26	0/1/1/1
3	NAG	B	695	1	-	0/6/23/26	0/1/1/1
3	NAG	A	695	1	-	0/6/23/26	0/1/1/1
3	NAG	A	692	1	-	6/6/23/26	0/1/1/1
7	GOL	B	2433	-	-	1/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	692	NAG	C8-C7	-13.55	1.22	1.50
3	B	692	NAG	C8-C7	-13.50	1.22	1.50
7	B	2433	GOL	C3-C2	-6.09	1.26	1.51
7	A	2434	GOL	C3-C2	-6.03	1.26	1.51
3	A	692	NAG	O5-C5	4.37	1.52	1.43
3	A	692	NAG	O7-C7	4.09	1.32	1.23
3	B	692	NAG	O7-C7	4.06	1.32	1.23
7	B	2433	GOL	O2-C2	2.73	1.51	1.43
7	A	2434	GOL	O2-C2	2.56	1.51	1.43
7	A	2434	GOL	C1-C2	2.51	1.62	1.51
7	B	2433	GOL	C1-C2	2.28	1.61	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	692	NAG	C1-O5-C5	-4.41	106.22	112.19
3	A	692	NAG	C8-C7-N2	4.06	122.98	116.10
3	B	692	NAG	C8-C7-N2	4.05	122.96	116.10
3	B	692	NAG	C1-C2-N2	-3.22	104.99	110.49
3	A	692	NAG	C1-C2-N2	-3.19	105.03	110.49
3	A	692	NAG	O7-C7-N2	-2.97	116.49	121.95
3	B	692	NAG	O7-C7-N2	-2.94	116.55	121.95
7	B	2433	GOL	O2-C2-C3	-2.58	97.75	109.12
7	A	2434	GOL	O2-C2-C3	-2.36	98.73	109.12
7	B	2433	GOL	O2-C2-C1	-2.35	98.79	109.12
6	B	801	ACT	O-C-CH3	-2.25	113.56	122.33
7	B	2433	GOL	O3-C3-C2	-2.23	99.51	110.20
6	A	801	ACT	O-C-CH3	-2.22	113.68	122.33
7	A	2434	GOL	O2-C2-C1	-2.19	99.46	109.12
6	A	800	ACT	O-C-CH3	-2.13	114.05	122.33
7	B	2433	GOL	C3-C2-C1	2.11	119.90	111.70
3	A	697	NAG	C2-N2-C7	-2.02	120.02	122.90
3	B	695	NAG	C2-N2-C7	-2.02	120.03	122.90
7	A	2434	GOL	O3-C3-C2	-2.01	100.57	110.20
3	A	695	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	692	NAG	C3-C2-N2-C7
3	A	692	NAG	O5-C5-C6-O6
3	A	692	NAG	C1-C2-N2-C7
3	A	692	NAG	C4-C5-C6-O6
3	A	692	NAG	C8-C7-N2-C2
3	A	692	NAG	O7-C7-N2-C2
3	B	692	NAG	C8-C7-N2-C2
3	B	692	NAG	O7-C7-N2-C2
3	B	692	NAG	O5-C5-C6-O6
3	B	692	NAG	C4-C5-C6-O6
7	A	2434	GOL	O2-C2-C3-O3
7	B	2433	GOL	O2-C2-C3-O3
3	A	692	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	697	NAG	1	0
7	A	2434	GOL	1	0
3	B	692	NAG	2	0
3	A	692	NAG	3	0
7	B	2433	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	612/612 (100%)	-0.40	3 (0%)	91	75	12, 36, 58, 82	3 (0%)
1	B	611/612 (99%)	-0.28	9 (1%)	73	46	12, 38, 68, 84	6 (0%)
All	All	1223/1224 (99%)	-0.34	12 (0%)	82	58	12, 37, 64, 84	9 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	ASN	3.2
1	B	612	ASP	3.1
1	B	134	ALA	3.1
1	B	135	THR	2.8
1	B	410	LEU	2.7
1	B	131	ASN	2.5
1	B	133	THR	2.5
1	A	136	CYS	2.3
1	B	8	GLY	2.2
1	B	83	PHE	2.1
1	A	130	PRO	2.1
1	B	15	ALA	2.0

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

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

6.3 Carbohydrates (i)

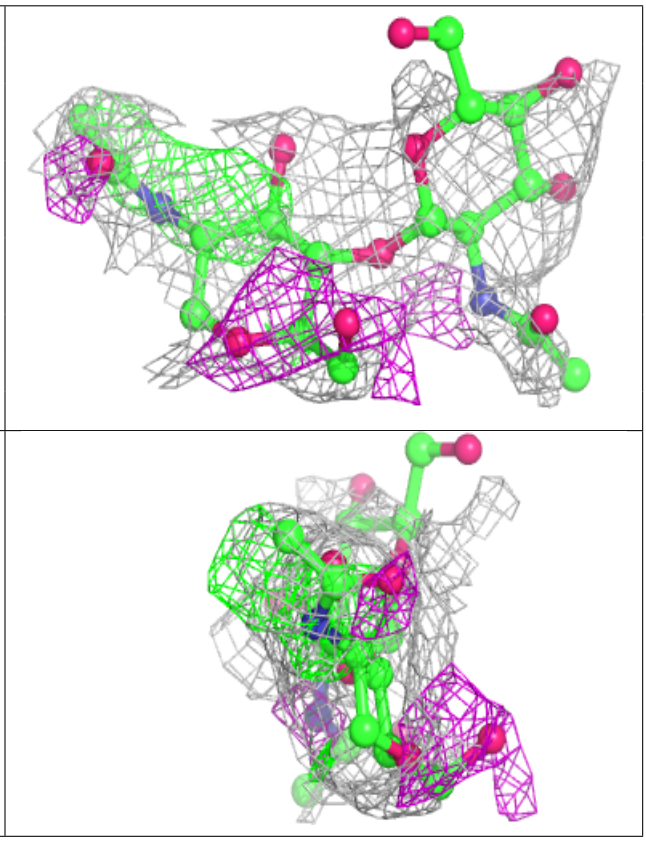
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	2	14/15	0.62	0.42	86,90,91,91	0
2	NAG	D	2	14/15	0.70	0.29	69,72,73,75	0
2	NAG	C	2	14/15	0.72	0.37	95,96,97,97	0
2	NAG	C	1	14/15	0.74	0.34	56,60,68,72	0
2	NAG	F	2	14/15	0.78	0.34	79,80,81,81	0
2	NAG	E	1	14/15	0.80	0.33	55,57,62,69	0
2	NAG	F	1	14/15	0.86	0.24	61,65,67,68	0
2	NAG	D	1	14/15	0.90	0.23	56,58,60,60	0

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

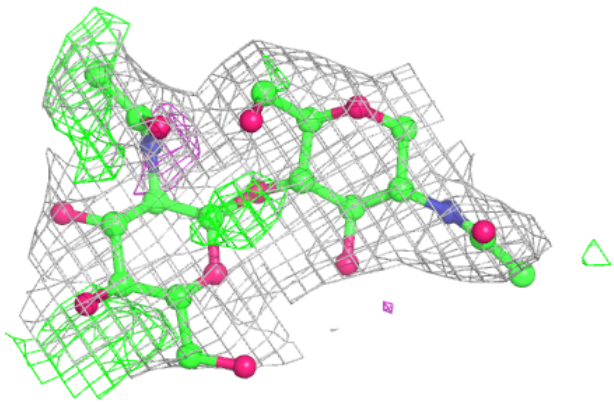
Electron density around Chain C:

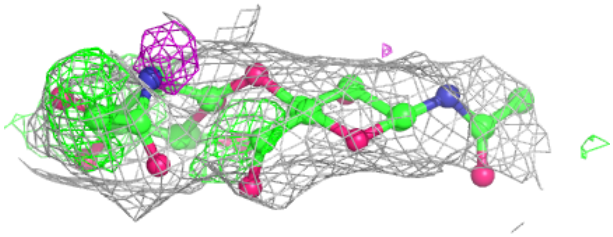
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

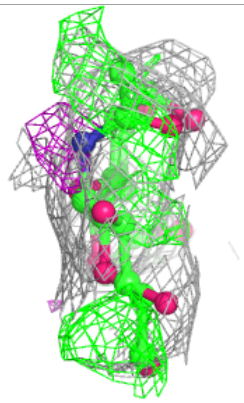


Electron density around Chain D:

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

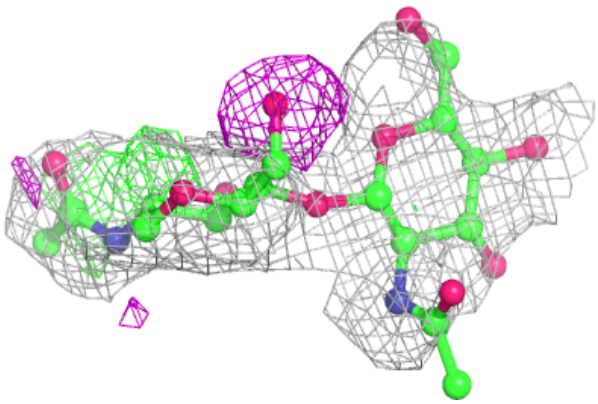


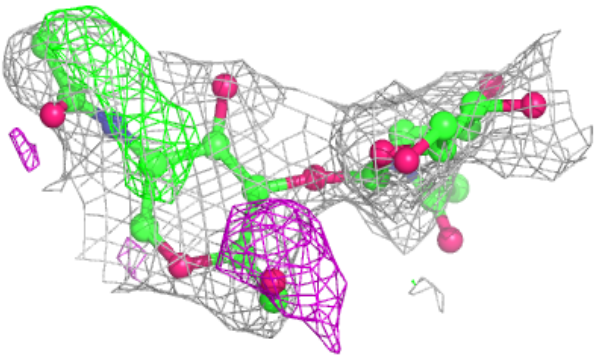


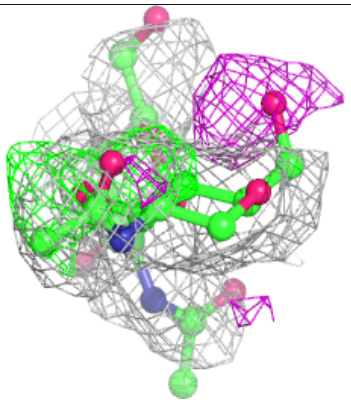


Electron density around Chain E:

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

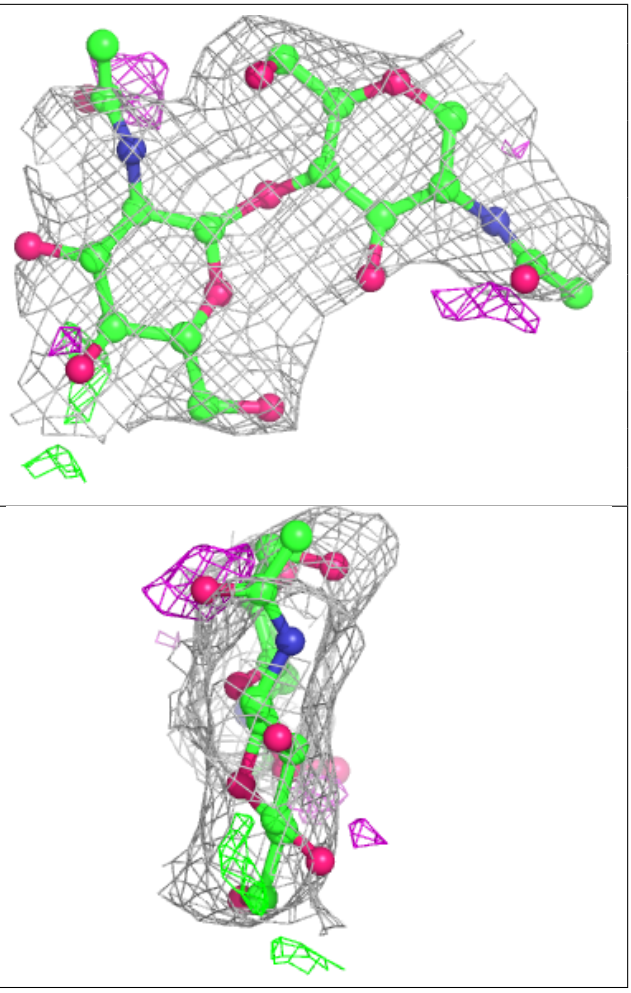






Electron density around Chain F:

$2mF_o$-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
3	NAG	A	697	14/15	0.51	0.87	116,117,118,119	0
3	NAG	B	692	14/15	0.70	0.35	83,86,86,87	0
3	NAG	A	692	14/15	0.72	0.34	66,68,70,71	0
6	ACT	A	800	4/4	0.76	0.46	49,51,52,53	0
3	NAG	B	695	14/15	0.84	0.36	76,78,80,83	0
6	ACT	B	801	4/4	0.85	0.41	52,52,53,53	0
3	NAG	A	695	14/15	0.86	0.32	75,76,79,79	0
6	ACT	A	801	4/4	0.91	0.39	32,33,34,35	0
7	GOL	A	2434	6/6	0.91	0.26	29,31,32,33	0
7	GOL	B	2433	6/6	0.93	0.25	31,34,35,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	B	703	1/1	0.95	0.13	29,29,29,29	0
5	CL	A	702	1/1	0.95	0.12	37,37,37,37	0
4	ZN	B	701	1/1	0.99	0.17	29,29,29,29	0
4	ZN	A	701	1/1	1.00	0.12	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.