Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 01:58 AM EDT

PDB ID	:	3NW8
Title	:	Glycoprotein B from Herpes simplex virus type 1, Y179S mutant, high-pH
Authors	:	Stampfer, S.D.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Heldwein, E.E.
Deposited on	:	2010-07-09
Resolution	:	2.76 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:

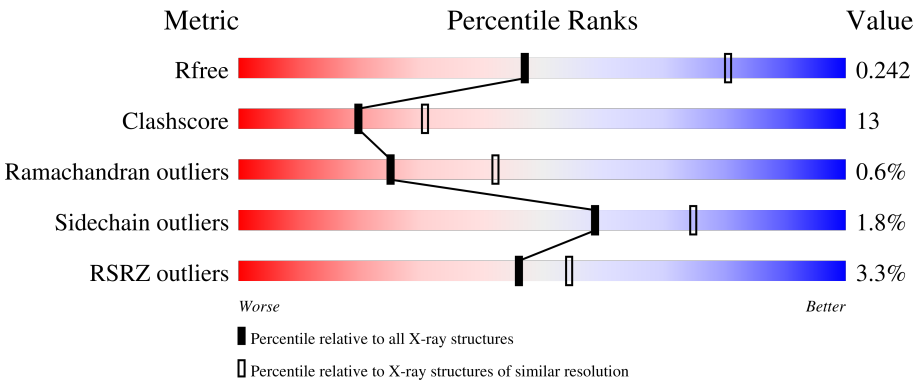
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	703	3%, 62%, 23%, •, 14%
1	B	703	3%, 63%, 22%, •, 14%
1	C	703	3%, 59%, 27%, 14%
1	D	703	2%, 64%, 21%, •, 13%
2	E	2	50%, 50%

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Mol	Chain	Length	Quality of chain
2	F	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
3	NAG	B	1674	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19958 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	606	4857	3062	852	921	22	0	0	0
1	A	607	4863	3062	856	923	22	0	0	0
1	C	605	4853	3059	856	916	22	0	0	0
1	D	609	4881	3077	861	921	22	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	expression tag	UNP P06437
B	29	PRO	-	expression tag	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	179	SER	TYR	engineered mutation	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	expression tag	UNP P06437
A	29	PRO	-	expression tag	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	179	SER	TYR	engineered mutation	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
C	28	ASP	-	expression tag	UNP P06437
C	29	PRO	-	expression tag	UNP P06437
C	58	ALA	PRO	SEE REMARK 999	UNP P06437
C	179	SER	TYR	engineered mutation	UNP P06437
C	313	SER	THR	SEE REMARK 999	UNP P06437
C	443	LEU	GLN	SEE REMARK 999	UNP P06437
D	28	ASP	-	expression tag	UNP P06437
D	29	PRO	-	expression tag	UNP P06437
D	58	ALA	PRO	SEE REMARK 999	UNP P06437

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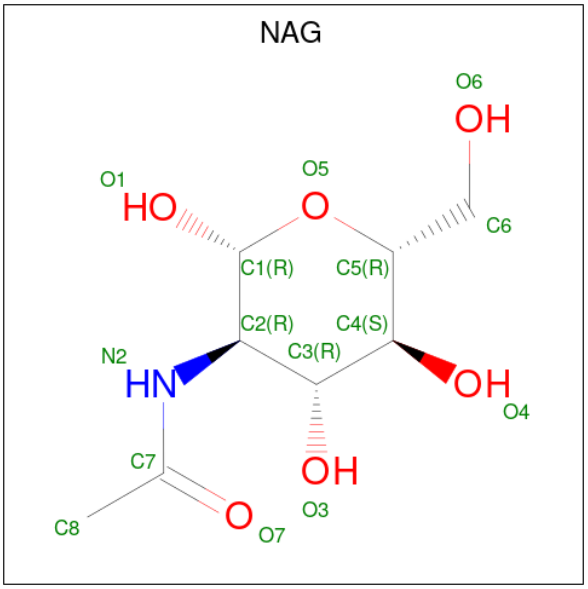
Chain	Residue	Modelled	Actual	Comment	Reference
D	179	SER	TYR	engineered mutation	UNP P06437
D	313	SER	THR	SEE REMARK 999	UNP P06437
D	443	LEU	GLN	SEE REMARK 999	UNP P06437

- 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	E	2	28	16	2	10	0	0	0
			Total	C	N	O			
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	B	1	14	8	1	5	0	0
			Total	C	N	O		
3	B	1	14	8	1	5	0	0

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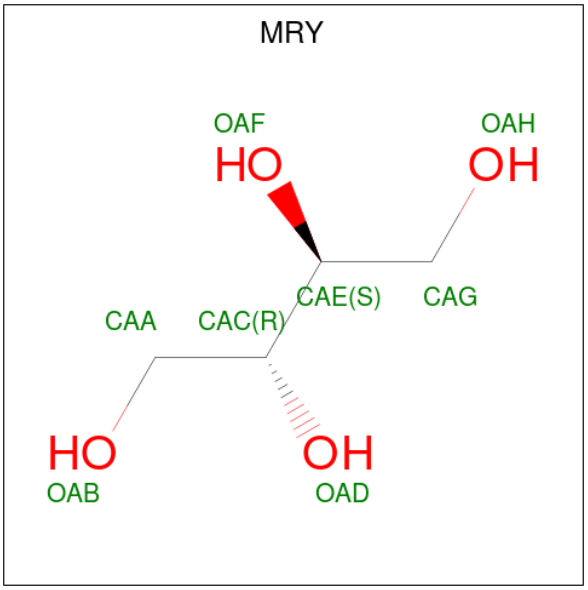
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0

- Molecule 4 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: $C_4H_{10}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	B	1	8	4	4		0	0
4	B	1	8	4	4		0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0
4	C	1	Total C O 8 4 4	0	0
4	C	1	Total C O 8 4 4	0	0
4	C	1	Total C O 8 4 4	0	0
4	D	1	Total C O 8 4 4	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0
5	C	2	Total Na 2 2	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	61	Total O 61 61	0	0
7	A	53	Total O 53 53	0	0
7	C	44	Total O 44 44	0	0

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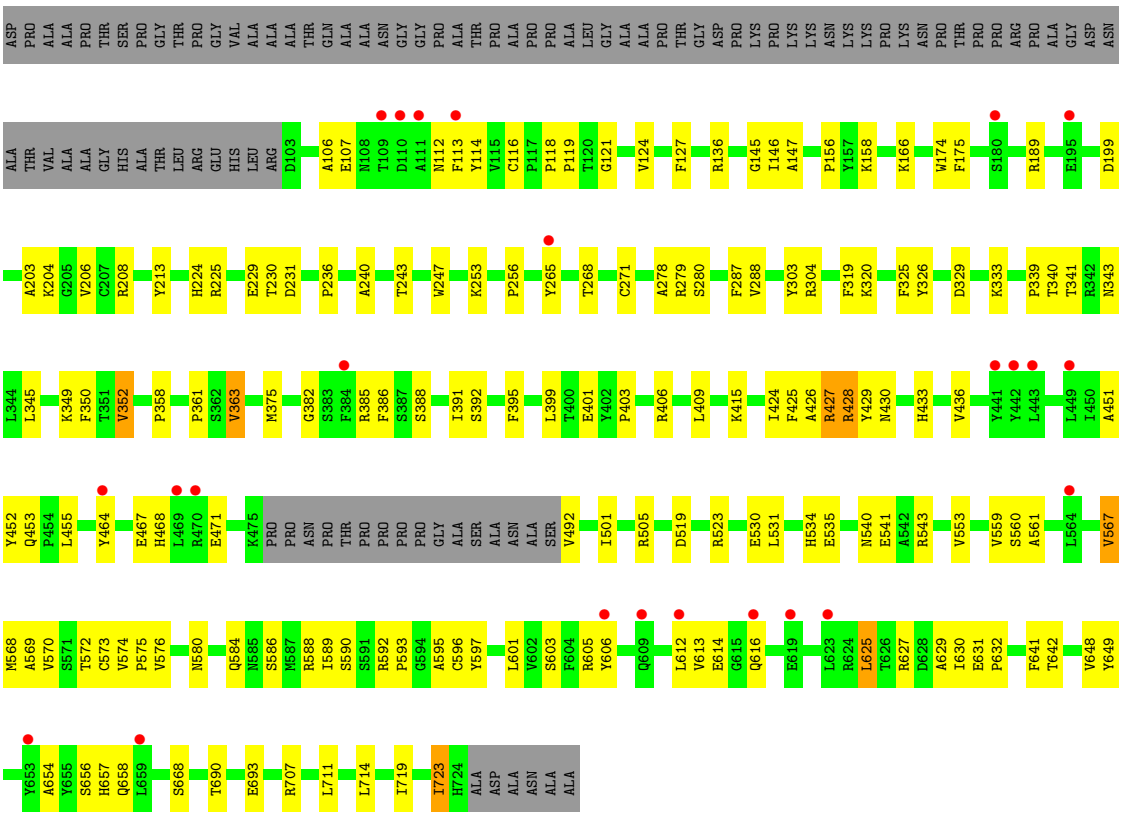
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	D	51	51	51	0	0

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.

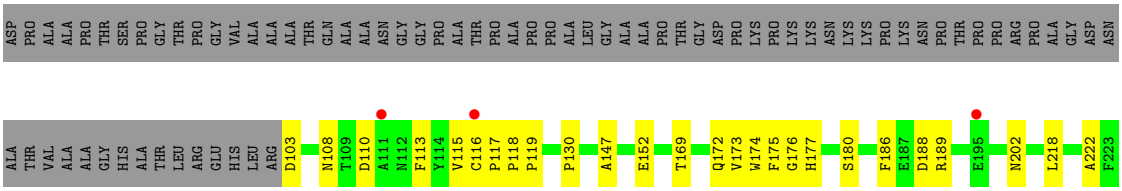
• Molecule 1: Envelope glycoprotein B

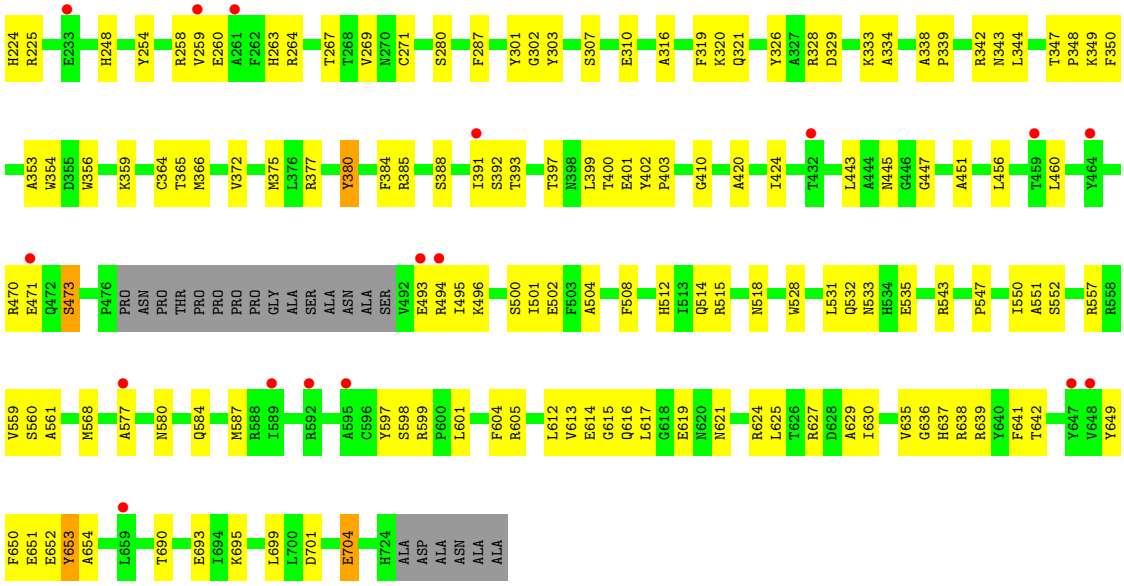
Chain B:



• Molecule 1: Envelope glycoprotein B

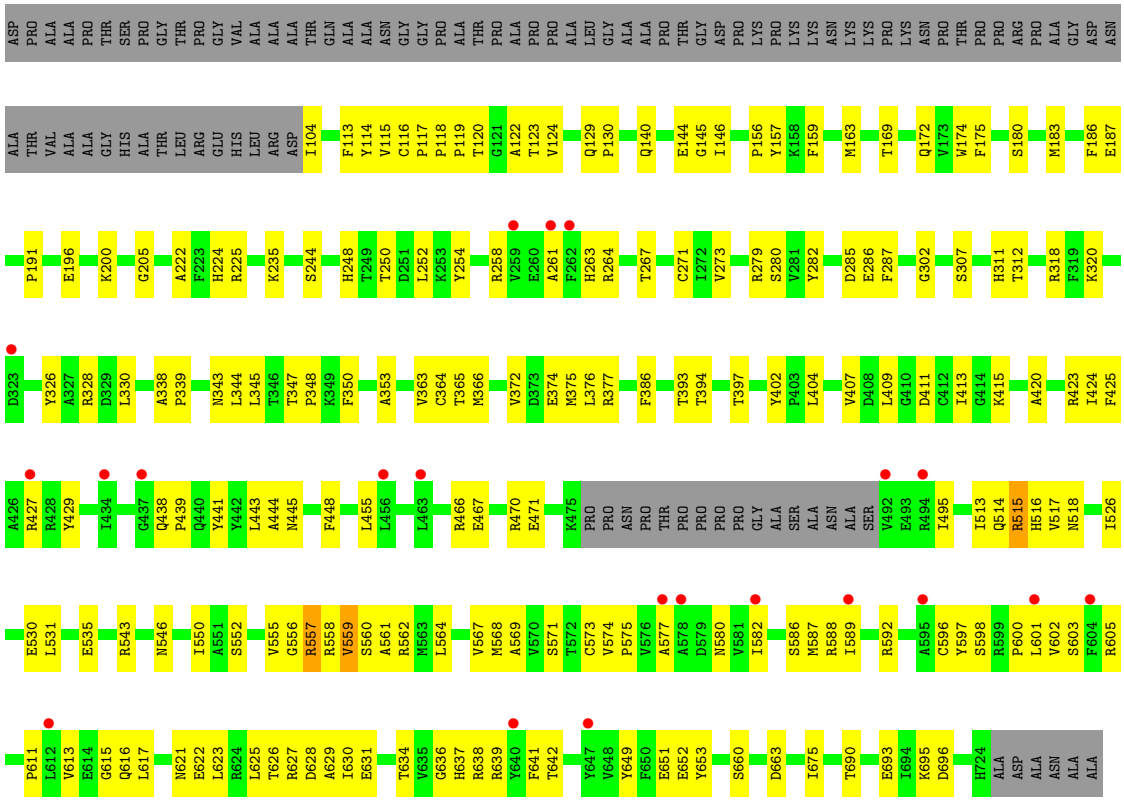
Chain A:





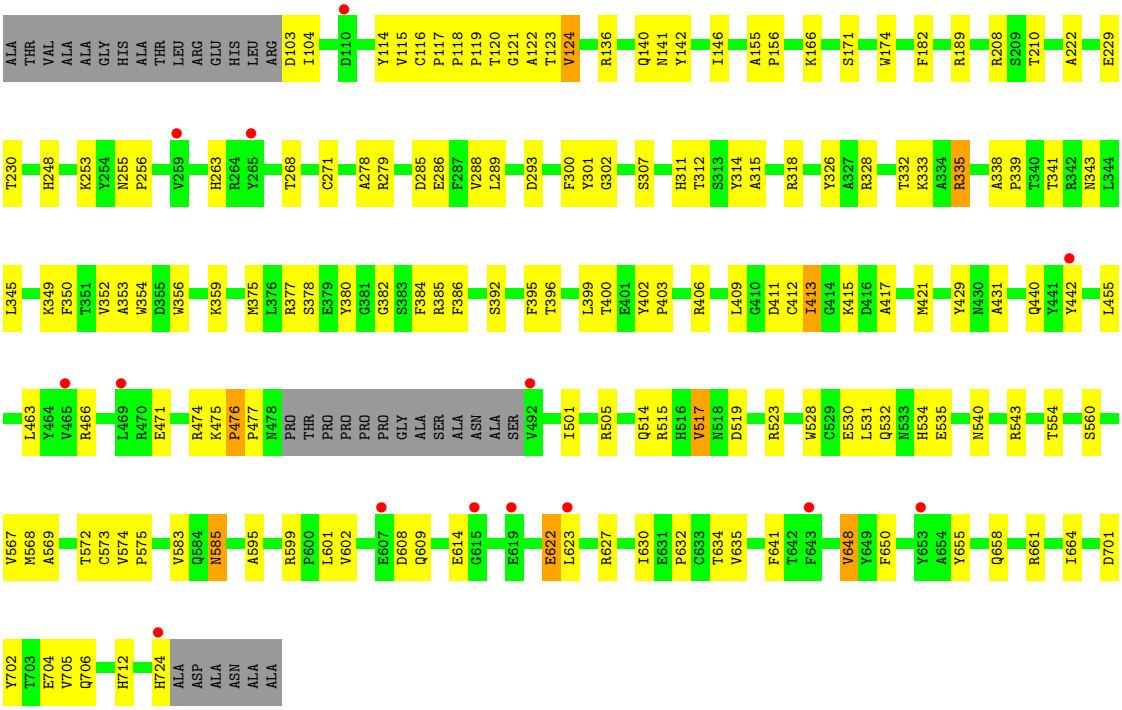
- Molecule 1: Envelope glycoprotein B

Chain C:



- Molecule 1: Envelope glycoprotein B

Chain D:

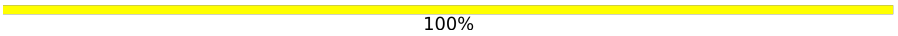


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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	P 3	Depositor
Cell constants a, b, c, α, β, γ	117.98Å 117.98Å 321.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.69 – 2.76 48.69 – 2.76	Depositor EDS
% Data completeness (in resolution range)	84.4 (48.69-2.76) 84.4 (48.69-2.76)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.202 , 0.242 0.198 , 0.242	Depositor DCC
R_{free} test set	5794 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 25.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.477 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19958	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4278e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NA, NAG, CL, MRY

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	0.23	0/4981	0.40	0/6771
1	B	0.23	0/4976	0.40	0/6764
1	C	0.23	0/4972	0.40	0/6757
1	D	0.23	0/5001	0.41	0/6800
All	All	0.23	0/19930	0.40	0/27092

There are no bond length outliers.

There are no bond angle outliers.

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	4863	0	4644	118	0
1	B	4857	0	4637	124	0
1	C	4853	0	4637	130	0
1	D	4881	0	4668	116	0
2	E	28	0	25	2	0
2	F	28	0	25	1	0
3	A	56	0	52	1	0
3	B	42	0	39	0	0
3	C	28	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	26	0	0
4	A	32	0	40	1	0
4	B	16	0	20	3	0
4	C	24	0	30	2	0
4	D	8	0	10	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
7	A	53	0	0	0	0
7	B	61	0	0	3	0
7	C	44	0	0	1	0
7	D	51	0	0	0	0
All	All	19958	0	18879	490	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 13.

All (490) 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:C:116:CYS:HB3	1:C:560:SER:HB3	1.37	1.03
1:A:116:CYS:HB3	1:A:560:SER:HB3	1.53	0.89
1:C:119:PRO:HD2	1:C:562:ARG:HG3	1.54	0.89
1:D:400:THR:HB	1:D:476:PRO:HG3	1.57	0.87
1:C:466:ARG:HH11	1:C:470:ARG:HH22	1.20	0.86
1:B:614:GLU:HB3	1:B:627:ARG:HH21	1.39	0.86
1:C:634:THR:H	1:C:653:TYR:HE1	1.26	0.83
1:B:136:ARG:HD2	1:B:523:ARG:HG2	1.64	0.80
1:B:428:ARG:HG3	1:B:428:ARG:HH11	1.47	0.79
1:C:637:HIS:HB3	1:C:652:GLU:HA	1.65	0.78
1:B:382:GLY:HA2	1:B:399:LEU:HD11	1.66	0.78
1:C:602:VAL:HG11	1:C:623:LEU:HD22	1.66	0.78
1:A:326:TYR:CZ	1:A:339:PRO:HG3	2.20	0.77
1:D:540:ASN:O	1:D:543:ARG:HG2	1.87	0.75
1:D:567:VAL:HG12	1:D:568:MET:H	1.50	0.75
1:B:428:ARG:HG3	1:B:428:ARG:NH1	2.02	0.74
1:B:603:SER:HB3	1:B:612:LEU:HD21	1.71	0.73
1:C:601:LEU:HD22	1:C:627:ARG:HG2	1.72	0.72
1:B:428:ARG:HH11	1:B:428:ARG:CG	2.04	0.69
1:B:625:LEU:HD12	1:B:625:LEU:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HD2	1:A:254:TYR:CD1	2.27	0.69
1:A:599:ARG:NH2	1:A:619:GLU:HG2	2.07	0.69
1:D:595:ALA:HA	1:D:632:PRO:HA	1.74	0.69
1:C:559:VAL:HG23	1:C:571:SER:O	1.93	0.68
1:B:253:LYS:HA	1:B:268:THR:HG21	1.75	0.68
1:A:347:THR:HG23	1:A:348:PRO:HD2	1.75	0.68
1:A:302:GLY:H	1:A:307:SER:HB3	1.58	0.67
1:B:553:VAL:HG23	7:B:766:HOH:O	1.94	0.67
1:C:466:ARG:NH1	1:C:470:ARG:HH22	1.92	0.67
1:B:224:HIS:CD2	1:B:225:ARG:HD3	2.30	0.66
1:D:567:VAL:HG12	1:D:568:MET:N	2.10	0.66
1:B:240:ALA:HB3	1:B:243:THR:HG21	1.78	0.66
1:D:156:PRO:HG2	1:D:279:ARG:NH2	2.11	0.65
1:A:649:TYR:CE2	1:A:651:GLU:HB2	2.32	0.65
1:D:531:LEU:O	1:D:535:GLU:HG2	1.97	0.65
1:B:601:LEU:HD22	1:B:627:ARG:HH11	1.62	0.65
1:C:119:PRO:HG2	1:C:561:ALA:HA	1.79	0.65
1:C:597:TYR:CZ	1:C:601:LEU:HD21	2.32	0.65
1:B:540:ASN:O	1:B:543:ARG:HG2	1.95	0.64
1:B:519:ASP:O	1:B:523:ARG:HG3	1.97	0.64
1:A:175:PHE:HD2	1:A:180:SER:HG	1.44	0.64
1:C:129:GLN:HB3	1:C:130:PRO:HD2	1.78	0.64
1:A:248:HIS:HA	1:A:271:CYS:O	1.98	0.63
1:C:605:ARG:HB3	1:C:611:PRO:O	1.98	0.63
1:C:397:THR:HG22	1:C:444:ALA:HA	1.79	0.63
1:C:411:ASP:HB3	1:C:415:LYS:HE3	1.80	0.63
1:C:649:TYR:HE2	1:C:651:GLU:HB2	1.65	0.62
1:A:470:ARG:O	1:A:473:SER:HB3	1.99	0.62
1:D:124:VAL:HG13	1:D:567:VAL:HG11	1.81	0.62
1:C:444:ALA:HB3	1:C:448:PHE:HB2	1.81	0.61
1:B:543:ARG:HB2	1:B:568:MET:HE1	1.81	0.61
1:C:120:THR:HG23	1:C:122:ALA:H	1.65	0.61
1:B:107:GLU:H	1:B:658:GLN:HE22	1.47	0.61
1:D:174:TRP:HD1	1:D:263:HIS:CE1	2.19	0.61
1:B:174:TRP:HD1	1:B:175:PHE:N	1.98	0.60
1:D:116:CYS:HB3	1:D:560:SER:HB3	1.84	0.60
1:A:384:PHE:CD2	1:A:399:LEU:HA	2.36	0.60
1:B:256:PRO:HG3	1:B:265:TYR:C	2.22	0.60
1:A:222:ALA:HB1	1:A:267:THR:HG21	1.82	0.60
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.83	0.60
1:C:115:VAL:HG22	1:C:623:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:SER:HA	1:C:557:ARG:O	2.03	0.59
1:A:173:VAL:O	1:A:263:HIS:HA	2.03	0.59
1:C:438:GLN:HB3	1:C:439:PRO:HD2	1.84	0.59
1:C:225:ARG:HA	1:C:254:TYR:CD2	2.38	0.59
1:D:411:ASP:O	1:D:415:LYS:HG2	2.03	0.59
1:B:429:TYR:CE2	1:B:455:LEU:HD13	2.38	0.59
1:C:557:ARG:O	1:C:559:VAL:HG12	2.02	0.59
1:D:440:GLN:NE2	1:D:471:GLU:HB3	2.17	0.59
1:C:636:GLY:O	1:C:638:ARG:HG3	2.02	0.58
1:C:183:MET:HG3	1:C:263:HIS:ND1	2.19	0.58
1:D:543:ARG:HB2	1:D:568:MET:HE1	1.85	0.58
1:D:289:LEU:HD11	1:D:352:VAL:HG11	1.86	0.58
1:D:189:ARG:HB3	1:D:349:LYS:HE2	1.85	0.58
1:A:147:ALA:HA	1:A:451:ALA:O	2.03	0.58
1:D:314:TYR:CE1	1:D:345:LEU:HD21	2.39	0.58
1:D:648:VAL:HG23	1:D:658:GLN:HG2	1.84	0.58
1:B:543:ARG:HB2	1:B:568:MET:CE	2.33	0.58
1:D:382:GLY:HA2	1:D:399:LEU:HD11	1.86	0.58
1:B:350:PHE:CE1	1:B:352:VAL:HG13	2.39	0.57
1:C:615:GLY:HA2	1:C:625:LEU:O	2.05	0.57
1:D:380:TYR:CD2	1:D:385:ARG:HD2	2.39	0.57
1:B:145:GLY:HA3	1:B:452:TYR:CZ	2.40	0.57
1:A:119:PRO:HG2	1:A:561:ALA:HA	1.85	0.57
1:B:559:VAL:HG12	1:B:572:THR:HA	1.86	0.57
1:C:280:SER:HB2	1:C:287:PHE:HB3	1.85	0.57
1:B:601:LEU:HD22	1:B:627:ARG:NH1	2.19	0.57
1:C:326:TYR:CZ	1:C:339:PRO:HG3	2.40	0.57
1:D:530:GLU:O	1:D:534:HIS:HB2	2.05	0.57
1:C:191:PRO:HA	1:C:350:PHE:HA	1.86	0.56
1:C:690:THR:HB	1:C:693:GLU:HG3	1.87	0.56
1:A:115:VAL:O	1:A:117:PRO:HD3	2.05	0.56
1:D:343:ASN:O	1:D:353:ALA:HA	2.04	0.56
1:A:202:ASN:O	1:A:328:ARG:HB3	2.06	0.56
1:C:222:ALA:HB1	1:C:267:THR:HG21	1.86	0.56
1:B:385:ARG:HA	1:B:395:PHE:O	2.06	0.56
1:B:567:VAL:CG1	1:B:568:MET:N	2.69	0.56
1:B:403:PRO:HG2	1:B:406:ARG:NH2	2.20	0.56
1:C:445:ASN:OD1	2:E:1:NAG:H82	2.05	0.56
1:A:598:SER:H	1:A:630:ILE:HA	1.71	0.56
1:A:615:GLY:HA3	1:A:624:ARG:O	2.06	0.56
1:C:580:ASN:ND2	1:C:605:ARG:HE	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:PHE:HB2	1:B:395:PHE:HB2	1.87	0.56
1:C:600:PRO:O	1:C:616:GLN:HB2	2.05	0.56
1:B:116:CYS:HB3	1:B:560:SER:HB3	1.88	0.55
1:A:393:THR:HG23	1:A:504:ALA:HB1	1.87	0.55
1:A:599:ARG:HH21	1:A:619:GLU:HG2	1.69	0.55
1:C:183:MET:HG3	1:C:263:HIS:CE1	2.41	0.55
1:A:174:TRP:CZ3	1:A:176:GLY:HA3	2.42	0.55
1:A:445:ASN:OD1	3:A:1398:NAG:H82	2.06	0.55
1:D:142:TYR:CD2	1:D:378:SER:HB3	2.42	0.55
1:D:543:ARG:HB2	1:D:568:MET:CE	2.36	0.55
1:B:204:LYS:HB2	1:B:206:VAL:HG22	1.89	0.55
1:C:420:ALA:HA	1:C:423:ARG:NH2	2.21	0.55
1:B:146:ILE:HG13	1:B:455:LEU:HD11	1.89	0.55
1:B:467:GLU:O	1:B:471:GLU:HG2	2.06	0.55
1:D:124:VAL:HG13	1:D:567:VAL:CG1	2.36	0.55
1:C:515:ARG:HE	1:C:515:ARG:C	2.11	0.55
1:D:332:THR:O	1:D:333:LYS:HB2	2.07	0.54
1:D:702:TYR:O	1:D:706:GLN:HG2	2.06	0.54
1:B:166:LYS:HG2	1:B:271:CYS:HA	1.88	0.54
1:D:622:GLU:HG3	1:D:623:LEU:N	2.22	0.54
1:A:551:ALA:HB2	1:A:568:MET:SD	2.47	0.54
1:C:443:LEU:O	2:E:1:NAG:H81	2.08	0.54
1:D:375:MET:HG2	1:D:386:PHE:HD2	1.73	0.54
1:B:208:ARG:HD3	1:B:229:GLU:OE2	2.08	0.54
1:B:345:LEU:HB3	1:B:352:VAL:HG23	1.89	0.54
1:B:501:ILE:O	1:B:505:ARG:HG3	2.08	0.54
1:C:587:MET:HE2	1:C:653:TYR:CD2	2.43	0.54
1:D:583:VAL:HG22	1:D:602:VAL:HG12	1.89	0.54
1:B:189:ARG:NH1	4:B:2000:MRY:HAG2	2.23	0.53
1:C:596:CYS:O	1:C:630:ILE:HG23	2.08	0.53
1:D:103:ASP:HB3	1:D:104:ILE:HD12	1.90	0.53
1:A:690:THR:OG1	1:A:693:GLU:HG3	2.08	0.53
1:A:152:GLU:HA	1:A:366:MET:HE2	1.91	0.53
1:A:584:GLN:HB2	1:A:601:LEU:HB2	1.89	0.53
1:D:328:ARG:HA	1:D:335:ARG:HG2	1.91	0.53
1:B:649:TYR:O	1:B:656:SER:HB3	2.08	0.53
1:D:120:THR:HG23	1:D:122:ALA:H	1.74	0.53
1:A:695:LYS:HD3	1:A:695:LYS:C	2.29	0.53
1:C:318:ARG:O	1:C:345:LEU:HD12	2.09	0.53
1:C:598:SER:HB3	1:C:631:GLU:HB3	1.91	0.53
1:D:475:LYS:C	1:D:477:PRO:HD3	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:TYR:CZ	1:C:558:ARG:HG3	2.44	0.52
1:B:350:PHE:HE1	1:B:352:VAL:HG13	1.73	0.52
1:A:637:HIS:O	1:A:651:GLU:HA	2.09	0.52
1:D:121:GLY:HA2	1:D:569:ALA:HB1	1.92	0.52
1:D:314:TYR:HB3	1:D:318:ARG:HD2	1.92	0.52
1:B:567:VAL:HG13	1:B:568:MET:N	2.24	0.52
1:B:107:GLU:H	1:B:658:GLN:NE2	2.08	0.52
1:B:614:GLU:HB3	1:B:627:ARG:NH2	2.18	0.52
3:C:1430:NAG:H2	7:C:760:HOH:O	2.09	0.52
1:A:601:LEU:HD22	1:A:627:ARG:HD3	1.92	0.52
1:C:115:VAL:O	1:C:117:PRO:HD3	2.10	0.52
1:D:650:PHE:CZ	1:D:655:TYR:HB2	2.45	0.52
1:C:364:CYS:HA	1:C:409:LEU:O	2.10	0.51
1:C:365:THR:O	1:C:366:MET:HE2	2.10	0.51
1:C:114:TYR:CE1	1:C:558:ARG:HG3	2.45	0.51
1:D:156:PRO:HG2	1:D:279:ARG:HH21	1.74	0.51
1:B:424:ILE:HG12	1:B:427:ARG:NH2	2.26	0.51
1:A:512:HIS:HA	4:A:2002:MRY:HAG2	1.92	0.51
1:C:145:GLY:HA2	1:C:455:LEU:HD12	1.93	0.51
1:D:514:GLN:O	1:D:517:VAL:HG13	2.10	0.51
1:D:104:ILE:HD12	1:D:104:ILE:N	2.25	0.51
1:B:719:ILE:HD12	1:B:719:ILE:N	2.25	0.51
1:A:637:HIS:HB3	1:A:652:GLU:HA	1.93	0.51
1:C:156:PRO:HG2	1:C:279:ARG:NH2	2.25	0.51
1:D:278:ALA:HA	1:D:288:VAL:O	2.10	0.51
1:D:585:ASN:CB	1:D:655:TYR:HB3	2.40	0.51
1:A:319:PHE:O	1:A:320:LYS:HD2	2.11	0.51
1:A:638:ARG:HG2	1:A:649:TYR:OH	2.11	0.51
1:C:649:TYR:CE2	1:C:651:GLU:HB2	2.45	0.51
1:B:189:ARG:NH1	4:B:2000:MRY:HAA1	2.26	0.51
1:B:464:TYR:HE1	1:B:468:HIS:HD1	1.59	0.51
1:D:253:LYS:HA	1:D:268:THR:HG21	1.93	0.51
1:A:637:HIS:CD2	1:A:653:TYR:CZ	2.99	0.50
1:C:556:GLY:O	1:C:557:ARG:HB3	2.11	0.50
1:A:347:THR:HG22	1:A:349:LYS:H	1.75	0.50
1:C:695:LYS:HD3	1:C:696:ASP:N	2.26	0.50
1:D:208:ARG:HD3	1:D:229:GLU:OE1	2.10	0.50
1:B:589:ILE:HG13	1:B:596:CYS:HA	1.92	0.50
1:A:597:TYR:CE1	1:A:601:LEU:HD11	2.46	0.50
1:B:392:SER:HB2	1:B:505:ARG:HH21	1.75	0.50
1:B:501:ILE:O	1:B:501:ILE:HG13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ARG:HD3	1:A:612:LEU:HG	1.94	0.50
1:D:463:LEU:HG	1:D:466:ARG:HB3	1.93	0.50
1:A:224:HIS:HB2	1:A:269:VAL:HB	1.93	0.50
1:A:597:TYR:HA	1:A:630:ILE:HG13	1.94	0.50
1:C:589:ILE:HG21	1:C:592:ARG:HG2	1.93	0.50
1:D:174:TRP:CD1	1:D:263:HIS:CE1	2.98	0.50
1:B:325:PHE:HB3	1:B:340:THR:O	2.12	0.50
1:A:577:ALA:HB3	1:A:580:ASN:HD22	1.76	0.50
1:C:169:THR:HA	1:C:186:PHE:O	2.12	0.50
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.11	0.50
1:C:372:VAL:HG11	1:C:375:MET:HE2	1.94	0.50
1:B:436:VAL:HG12	1:B:471:GLU:HG3	1.94	0.49
1:C:377:ARG:HD2	1:C:386:PHE:CE2	2.47	0.49
1:D:567:VAL:CG1	1:D:568:MET:H	2.24	0.49
1:B:278:ALA:HA	1:B:288:VAL:O	2.12	0.49
1:B:319:PHE:O	1:B:320:LYS:HD2	2.11	0.49
1:C:144:GLU:HA	1:C:376:LEU:HD23	1.94	0.49
1:A:420:ALA:O	1:A:424:ILE:HG13	2.12	0.49
1:C:517:VAL:HG23	1:C:518:ASN:N	2.26	0.49
1:C:129:GLN:HB3	1:C:130:PRO:CD	2.43	0.49
1:C:225:ARG:HD2	1:C:254:TYR:CD1	2.47	0.49
1:D:701:ASP:OD1	1:D:704:GLU:HG3	2.13	0.49
1:B:580:ASN:HB3	1:B:605:ARG:HB2	1.95	0.49
1:A:218:LEU:HD23	1:A:218:LEU:C	2.33	0.49
1:C:326:TYR:OH	1:C:339:PRO:HG3	2.12	0.49
1:C:467:GLU:O	1:C:471:GLU:HG2	2.13	0.49
1:C:637:HIS:HB3	1:C:652:GLU:CA	2.41	0.49
1:B:597:TYR:CD1	1:B:601:LEU:HD21	2.48	0.49
1:D:440:GLN:HE22	1:D:471:GLU:HB3	1.77	0.49
1:B:415:LYS:H	1:B:415:LYS:HD2	1.77	0.49
1:A:543:ARG:HB3	1:A:550:ILE:HG21	1.95	0.49
1:C:196:GLU:O	1:C:200:LYS:HB2	2.13	0.49
1:C:411:ASP:HB3	1:C:415:LYS:CE	2.42	0.49
1:B:145:GLY:HA2	1:B:455:LEU:HD12	1.95	0.48
1:D:403:PRO:HB2	1:D:406:ARG:HB2	1.95	0.48
1:B:424:ILE:HA	1:B:427:ARG:HH21	1.78	0.48
1:A:188:ASP:OD1	1:A:189:ARG:N	2.46	0.48
1:C:172:GLN:HA	1:C:264:ARG:O	2.14	0.48
1:D:114:TYR:HB3	1:D:573:CYS:HB3	1.96	0.48
1:B:119:PRO:HG2	1:B:561:ALA:HA	1.95	0.48
1:C:639:ARG:HB3	1:C:641:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:HD2	1:C:386:PHE:CZ	2.48	0.48
1:C:626:THR:HG22	1:C:628:ASP:OD1	2.13	0.48
1:B:189:ARG:HB3	1:B:349:LYS:HD3	1.96	0.48
1:B:326:TYR:OH	1:B:339:PRO:HG3	2.14	0.48
1:B:707:ARG:O	1:B:707:ARG:HD3	2.14	0.48
1:C:597:TYR:CE2	1:C:601:LEU:HD21	2.49	0.48
1:A:365:THR:HB	1:A:494:ARG:HD2	1.96	0.47
1:B:606:TYR:HE2	1:B:613:VAL:HG21	1.78	0.47
1:C:598:SER:HA	1:C:631:GLU:OE1	2.14	0.47
1:D:311:HIS:CG	1:D:312:THR:N	2.81	0.47
1:A:447:GLY:HA3	1:A:496:LYS:O	2.14	0.47
1:D:114:TYR:HA	1:D:574:VAL:O	2.14	0.47
1:B:114:TYR:HA	1:B:574:VAL:O	2.14	0.47
1:A:443:LEU:HD13	1:A:495:ILE:HD13	1.96	0.47
1:A:584:GLN:HE21	1:A:627:ARG:HH22	1.60	0.47
1:A:552:SER:HA	1:A:557:ARG:O	2.14	0.47
1:C:113:PHE:CD2	1:C:621:ASN:HB3	2.49	0.47
1:D:285:ASP:HB2	1:D:311:HIS:HB3	1.96	0.47
1:B:711:LEU:HD23	1:B:714:LEU:HD12	1.97	0.47
1:C:124:VAL:HG12	1:C:569:ALA:HA	1.95	0.47
1:C:302:GLY:N	1:C:307:SER:HB3	2.29	0.47
1:A:639:ARG:HB3	1:A:641:PHE:CE1	2.50	0.47
1:C:175:PHE:HD2	1:C:180:SER:HG	1.62	0.47
1:C:393:THR:HG22	1:C:394:THR:N	2.29	0.47
1:D:630:ILE:O	1:D:630:ILE:HD12	2.15	0.47
1:B:174:TRP:CD1	1:B:175:PHE:N	2.81	0.47
1:A:364:CYS:SG	1:A:410:GLY:HA2	2.54	0.47
1:A:528:TRP:O	1:A:532:GLN:HG2	2.15	0.47
1:B:114:TYR:HB3	1:B:573:CYS:HB3	1.97	0.47
1:B:388:SER:OG	1:B:391:ILE:HG12	2.14	0.47
1:B:588:ARG:HG2	1:B:596:CYS:SG	2.55	0.47
1:A:301:TYR:CD1	1:A:310:GLU:HB2	2.50	0.47
1:A:613:VAL:HG12	1:A:614:GLU:N	2.30	0.47
1:A:501:ILE:O	1:A:501:ILE:HG13	2.16	0.46
1:C:425:PHE:C	1:C:427:ARG:H	2.17	0.46
1:B:113:PHE:HB2	1:B:576:VAL:HB	1.97	0.46
1:B:363:VAL:HG11	1:B:409:LEU:HD13	1.97	0.46
1:B:158:LYS:HE2	1:B:279:ARG:NH1	2.30	0.46
1:B:304:ARG:HD2	1:B:341:THR:HG21	1.98	0.46
1:D:229:GLU:HG2	1:D:230:THR:N	2.30	0.46
1:A:147:ALA:HB2	1:A:375:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:HIS:CD2	1:C:225:ARG:HG3	2.50	0.46
1:D:474:ARG:HD2	1:D:474:ARG:N	2.30	0.46
1:D:701:ASP:O	1:D:705:VAL:HG23	2.16	0.46
1:B:127:PHE:HD1	1:B:540:ASN:OD1	1.98	0.46
1:A:301:TYR:HD1	1:A:310:GLU:HB2	1.79	0.46
1:B:156:PRO:HG2	1:B:279:ARG:NH2	2.31	0.46
1:B:236:PRO:HA	1:B:247:TRP:CD1	2.51	0.46
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.98	0.46
1:D:412:CYS:SG	1:D:413:ILE:N	2.88	0.46
1:D:474:ARG:HD2	1:D:474:ARG:H	1.81	0.46
1:D:300:PHE:CD2	1:D:359:LYS:HA	2.51	0.46
1:D:403:PRO:HG2	1:D:406:ARG:NH2	2.30	0.46
1:D:476:PRO:N	1:D:477:PRO:HD3	2.31	0.46
1:C:513:ILE:O	1:C:516:HIS:HB3	2.16	0.46
1:B:723:ILE:HD12	1:B:723:ILE:N	2.31	0.45
1:D:104:ILE:HD12	1:D:104:ILE:H	1.81	0.45
1:C:695:LYS:HD3	1:C:695:LYS:C	2.36	0.45
1:B:118:PRO:HA	1:B:119:PRO:HD3	1.80	0.45
1:D:442:TYR:OH	1:D:474:ARG:HG2	2.16	0.45
1:D:634:THR:HG22	1:D:635:VAL:N	2.31	0.45
1:A:342:ARG:HD2	1:A:354:TRP:O	2.17	0.45
1:C:402:TYR:HE2	1:C:407:VAL:HG23	1.81	0.45
1:C:577:ALA:HB3	1:C:580:ASN:OD1	2.16	0.45
1:C:617:LEU:HD21	1:C:642:THR:O	2.17	0.45
1:D:601:LEU:HD13	1:D:627:ARG:NH1	2.32	0.45
1:C:564:LEU:HG	1:C:569:ALA:HB2	1.98	0.45
1:C:597:TYR:HD2	1:C:629:ALA:O	2.00	0.45
1:D:338:ALA:HA	1:D:339:PRO:HD3	1.83	0.45
1:A:392:SER:HA	1:A:508:PHE:CE2	2.52	0.45
1:D:104:ILE:HD11	1:D:585:ASN:OD1	2.16	0.45
1:B:589:ILE:HG22	1:B:592:ARG:H	1.82	0.45
1:B:723:ILE:HD12	1:B:723:ILE:H	1.82	0.45
1:D:171:SER:HB2	1:D:182:PHE:HE1	1.81	0.45
1:B:106:ALA:HA	1:B:658:GLN:OE1	2.18	0.44
1:C:543:ARG:HB2	1:C:568:MET:CE	2.46	0.44
1:D:118:PRO:HA	1:D:119:PRO:HD3	1.86	0.44
1:B:530:GLU:O	1:B:534:HIS:HB2	2.17	0.44
1:A:130:PRO:HB3	1:A:533:ASN:HB3	1.98	0.44
1:A:280:SER:HB2	1:A:287:PHE:CB	2.47	0.44
1:C:404:LEU:HD11	1:C:441:TYR:CG	2.51	0.44
4:C:2001:MRY:OAH	4:C:2001:MRY:HAA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ARG:HD2	1:A:384:PHE:CE1	2.52	0.44
1:C:116:CYS:HB2	1:C:622:GLU:OE2	2.17	0.44
1:C:363:VAL:HA	4:C:2000:MRY:OAF	2.17	0.44
1:C:637:HIS:CD2	1:C:653:TYR:CZ	3.05	0.44
1:C:660:SER:O	1:C:663:ASP:HB2	2.17	0.44
1:B:174:TRP:HD1	1:B:175:PHE:H	1.64	0.44
1:B:329:ASP:O	1:B:333:LYS:HA	2.17	0.44
1:B:648:VAL:HG13	1:B:648:VAL:O	2.17	0.44
1:A:175:PHE:O	1:A:260:GLU:HA	2.17	0.44
1:A:338:ALA:HA	1:A:339:PRO:HD3	1.80	0.44
1:B:589:ILE:HD12	1:B:595:ALA:O	2.18	0.44
1:A:343:ASN:ND2	1:A:356:TRP:HB2	2.32	0.44
1:A:531:LEU:O	1:A:535:GLU:HG2	2.18	0.44
1:A:604:PHE:O	1:A:613:VAL:N	2.50	0.44
1:D:641:PHE:HB2	1:D:648:VAL:HG12	1.99	0.44
1:B:429:TYR:HD2	1:B:433:HIS:HB2	1.83	0.44
1:A:108:ASN:C	1:A:110:ASP:H	2.21	0.44
1:D:300:PHE:CG	1:D:359:LYS:HB2	2.53	0.44
1:D:567:VAL:CG1	1:D:568:MET:N	2.80	0.44
1:D:124:VAL:CG1	1:D:567:VAL:HG11	2.47	0.44
1:D:189:ARG:HH22	1:D:293:ASP:CG	2.21	0.44
1:D:343:ASN:HB2	1:D:354:TRP:O	2.18	0.44
1:D:574:VAL:HA	1:D:575:PRO:HD3	1.84	0.44
1:A:175:PHE:CG	1:A:258:ARG:HG3	2.53	0.44
1:A:500:SER:OG	1:A:502:GLU:HG2	2.17	0.44
1:D:501:ILE:HG13	1:D:501:ILE:O	2.17	0.44
1:A:365:THR:O	1:A:366:MET:HE2	2.18	0.44
1:A:701:ASP:OD1	1:A:704:GLU:HB2	2.18	0.44
1:B:584:GLN:HB2	1:B:601:LEU:HB2	2.00	0.43
1:C:174:TRP:CH2	1:C:261:ALA:HA	2.53	0.43
1:C:328:ARG:HH22	1:C:330:LEU:HD23	1.83	0.43
1:D:392:SER:HB2	1:D:505:ARG:HH21	1.82	0.43
1:B:630:ILE:HG22	1:B:631:GLU:N	2.33	0.43
1:A:366:MET:CE	1:A:495:ILE:HB	2.48	0.43
1:A:617:LEU:HD21	1:A:642:THR:O	2.17	0.43
1:D:384:PHE:O	1:D:396:THR:HA	2.17	0.43
1:B:113:PHE:O	1:B:575:PRO:HA	2.18	0.43
1:B:428:ARG:HB3	1:B:429:TYR:CD1	2.53	0.43
1:B:641:PHE:O	1:B:648:VAL:HG12	2.18	0.43
1:A:303:TYR:HB2	1:A:321:GLN:OE1	2.18	0.43
1:C:163:MET:O	1:C:273:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:HD3	1:A:515:ARG:C	2.39	0.43
1:A:584:GLN:CG	1:A:601:LEU:HB2	2.48	0.43
1:D:301:TYR:CD2	1:D:302:GLY:N	2.86	0.43
1:B:147:ALA:HA	1:B:451:ALA:O	2.19	0.43
1:A:597:TYR:CD2	1:A:601:LEU:HD21	2.54	0.43
1:C:119:PRO:HG2	1:C:561:ALA:CA	2.46	0.43
1:D:142:TYR:HD2	1:D:378:SER:HB3	1.83	0.43
1:D:146:ILE:HG13	1:D:455:LEU:HD11	2.00	0.43
1:D:341:THR:HG22	1:D:356:TRP:HB3	2.00	0.43
1:C:104:ILE:N	1:C:582:ILE:HG23	2.34	0.43
1:C:157:TYR:CE2	1:C:159:PHE:CD2	3.06	0.43
1:C:531:LEU:O	1:C:535:GLU:HG2	2.19	0.43
1:C:603:SER:HA	1:C:613:VAL:O	2.19	0.43
1:B:668:SER:HA	7:B:776:HOH:O	2.19	0.43
1:A:302:GLY:N	1:A:307:SER:HB3	2.30	0.43
1:A:347:THR:CG2	1:A:348:PRO:HD2	2.46	0.43
1:A:347:THR:N	1:A:350:PHE:O	2.52	0.43
1:D:155:ALA:HA	1:D:156:PRO:HD3	1.89	0.43
1:D:377:ARG:HD3	1:D:384:PHE:CZ	2.54	0.43
1:D:601:LEU:HD22	1:D:627:ARG:HD3	2.00	0.43
1:A:613:VAL:HG12	1:A:614:GLU:H	1.83	0.43
1:C:343:ASN:O	1:C:353:ALA:HA	2.19	0.43
1:B:199:ASP:O	1:B:203:ALA:HB3	2.19	0.43
1:A:343:ASN:O	1:A:353:ALA:HA	2.19	0.43
1:C:118:PRO:HA	1:C:119:PRO:HD3	1.78	0.43
1:D:528:TRP:CE2	1:D:532:GLN:NE2	2.86	0.43
1:B:531:LEU:O	1:B:535:GLU:HG2	2.18	0.42
1:B:595:ALA:HA	1:B:632:PRO:HA	2.01	0.42
1:C:374:GLU:HG2	1:C:429:TYR:OH	2.19	0.42
1:B:453:GLN:O	1:B:455:LEU:HG	2.19	0.42
1:B:561:ALA:HB2	1:B:570:VAL:HG12	2.01	0.42
1:B:572:THR:HG22	1:B:573:CYS:N	2.34	0.42
1:A:344:LEU:HG	1:A:353:ALA:HB2	2.01	0.42
1:B:121:GLY:HA2	1:B:569:ALA:HB1	2.00	0.42
1:A:557:ARG:HG3	1:A:559:VAL:HG13	2.02	0.42
1:C:248:HIS:HA	1:C:271:CYS:O	2.18	0.42
1:C:311:HIS:CG	1:C:312:THR:N	2.87	0.42
1:D:115:VAL:O	1:D:117:PRO:HD3	2.18	0.42
1:B:656:SER:O	1:B:657:HIS:HB3	2.19	0.42
1:A:400:THR:HG22	1:A:401:GLU:N	2.34	0.42
1:C:285:ASP:O	1:C:286:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ILE:HD12	1:C:550:ILE:N	2.34	0.42
1:D:429:TYR:C	1:D:431:ALA:H	2.22	0.42
1:A:587:MET:HB2	1:A:653:TYR:HB3	2.02	0.42
1:C:637:HIS:O	1:C:651:GLU:HA	2.19	0.42
1:B:319:PHE:HE1	1:B:343:ASN:HB3	1.84	0.42
1:B:406:ARG:O	1:B:492:VAL:HA	2.19	0.42
1:A:493:GLU:HG2	1:A:494:ARG:N	2.34	0.42
1:A:615:GLY:HA2	1:A:625:LEU:O	2.19	0.42
1:C:366:MET:SD	1:C:495:ILE:HB	2.60	0.42
1:C:574:VAL:HA	1:C:575:PRO:HD3	1.87	0.42
1:A:113:PHE:CD2	1:A:621:ASN:HB3	2.55	0.42
1:A:391:ILE:O	1:A:391:ILE:HG22	2.20	0.42
1:C:587:MET:O	1:C:596:CYS:HB3	2.20	0.42
1:B:230:THR:HG22	1:B:231:ASP:N	2.35	0.42
1:B:603:SER:OG	1:B:614:GLU:HG2	2.20	0.42
1:A:514:GLN:HG2	1:A:518:ASN:ND2	2.34	0.42
1:C:586:SER:OG	1:C:588:ARG:HG2	2.20	0.42
1:D:146:ILE:HD11	1:D:429:TYR:HD1	1.85	0.42
1:D:174:TRP:HD1	1:D:263:HIS:NE2	2.17	0.42
1:D:326:TYR:OH	1:D:339:PRO:HG3	2.19	0.42
1:D:417:ALA:O	1:D:421:MET:HG3	2.20	0.42
1:D:572:THR:HG22	1:D:573:CYS:O	2.19	0.42
1:D:585:ASN:HA	1:D:655:TYR:HB3	2.00	0.42
1:C:282:TYR:HE1	1:C:409:LEU:HD12	1.83	0.42
1:C:514:GLN:HG2	1:C:518:ASN:ND2	2.35	0.42
1:C:546:ASN:O	1:C:550:ILE:HD13	2.19	0.42
1:C:587:MET:HE3	1:C:597:TYR:O	2.19	0.42
1:B:213:TYR:N	1:B:213:TYR:CD2	2.87	0.41
1:A:557:ARG:O	1:A:559:VAL:HG13	2.20	0.41
1:C:175:PHE:CE2	1:C:258:ARG:HA	2.55	0.41
1:C:205:GLY:CA	1:C:328:ARG:NH2	2.83	0.41
1:C:555:VAL:HG12	1:C:555:VAL:O	2.19	0.41
1:D:378:SER:OG	1:D:385:ARG:HB2	2.20	0.41
1:B:303:TYR:HB3	1:A:316:ALA:HB1	2.01	0.41
1:C:347:THR:HB	1:C:348:PRO:HD2	2.02	0.41
1:C:365:THR:HG23	1:C:409:LEU:HB2	2.02	0.41
1:B:541:GLU:HG2	7:B:767:HOH:O	2.20	0.41
1:A:225:ARG:HA	1:A:254:TYR:CD2	2.55	0.41
1:D:341:THR:CG2	1:D:356:TRP:HB3	2.51	0.41
1:B:253:LYS:HD3	1:B:268:THR:HG21	2.01	0.41
1:A:380:TYR:HB3	1:A:385:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:HB2	1:B:361:PRO:HD2	2.02	0.41
1:B:586:SER:HA	1:B:654:ALA:HA	2.01	0.41
1:B:625:LEU:HD12	1:B:625:LEU:N	2.28	0.41
1:A:471:GLU:C	1:A:473:SER:H	2.23	0.41
1:D:210:THR:HA	1:D:222:ALA:O	2.19	0.41
1:D:302:GLY:N	1:D:307:SER:HB3	2.36	0.41
1:D:614:GLU:HG3	1:D:627:ARG:NH2	2.36	0.41
1:A:597:TYR:CE2	1:A:601:LEU:HD21	2.56	0.41
1:C:124:VAL:HB	1:C:567:VAL:CG1	2.50	0.41
1:C:146:ILE:HD13	1:C:424:ILE:HG22	2.02	0.41
1:D:255:ASN:HB3	1:D:256:PRO:HD2	2.01	0.41
1:D:664:ILE:N	1:D:664:ILE:HD12	2.36	0.41
1:B:425:PHE:HA	1:B:429:TYR:HB2	2.02	0.41
1:B:719:ILE:HD12	1:B:719:ILE:H	1.85	0.41
1:A:605:ARG:HD3	1:A:612:LEU:CD1	2.50	0.41
1:D:285:ASP:O	1:D:286:GLU:HB3	2.21	0.41
1:D:515:ARG:O	1:D:519:ASP:HB2	2.20	0.41
1:A:616:GLN:CD	1:A:629:ALA:HB3	2.41	0.41
1:D:140:GLN:HG2	1:D:380:TYR:OH	2.20	0.41
2:F:1:NAG:H62	2:F:2:NAG:HN2	1.85	0.41
1:B:375:MET:SD	1:B:386:PHE:HB3	2.61	0.41
1:B:425:PHE:O	1:B:430:ASN:N	2.54	0.41
1:B:590:SER:O	1:B:593:PRO:HD3	2.21	0.41
1:B:616:GLN:NE2	1:B:629:ALA:HB3	2.35	0.41
1:A:375:MET:HE2	1:A:388:SER:HB2	2.03	0.41
1:C:124:VAL:HB	1:C:567:VAL:HG12	2.03	0.41
1:C:191:PRO:HB3	1:C:350:PHE:O	2.20	0.41
1:C:526:ILE:O	1:C:530:GLU:HG3	2.21	0.41
1:C:559:VAL:HA	1:C:573:CYS:SG	2.61	0.41
1:D:350:PHE:CD1	1:D:352:VAL:HG13	2.56	0.41
1:D:385:ARG:HA	1:D:395:PHE:O	2.21	0.41
1:A:543:ARG:O	1:A:547:PRO:HG3	2.21	0.41
1:A:635:VAL:HG12	1:A:636:GLY:N	2.35	0.41
1:A:652:GLU:O	1:A:654:ALA:N	2.54	0.41
1:C:250:THR:HG22	1:C:252:LEU:H	1.86	0.41
1:C:320:LYS:HB2	1:C:344:LEU:HB2	2.03	0.41
1:D:375:MET:SD	1:D:386:PHE:HB3	2.61	0.41
1:D:519:ASP:O	1:D:523:ARG:HG3	2.21	0.41
1:B:189:ARG:HH12	4:B:2000:MRY:HAA1	1.86	0.40
1:A:169:THR:HA	1:A:186:PHE:O	2.21	0.40
1:C:338:ALA:HA	1:C:339:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PRO:HA	1:A:119:PRO:HD3	1.83	0.40
1:A:152:GLU:HA	1:A:366:MET:CE	2.50	0.40
1:A:328:ARG:HA	1:A:334:ALA:O	2.21	0.40
1:A:599:ARG:HB2	1:A:616:GLN:NE2	2.36	0.40
1:C:616:GLN:HB2	1:C:616:GLN:HE21	1.75	0.40
1:D:116:CYS:HB2	1:D:622:GLU:OE2	2.22	0.40
1:B:428:ARG:HD2	1:B:429:TYR:CE1	2.57	0.40
1:A:175:PHE:CZ	1:A:258:ARG:HA	2.56	0.40
1:A:329:ASP:O	1:A:333:LYS:HA	2.21	0.40
1:A:402:TYR:HA	1:A:403:PRO:HD3	1.87	0.40
1:D:166:LYS:HG2	1:D:271:CYS:HA	2.03	0.40
1:A:172:GLN:HA	1:A:264:ARG:O	2.21	0.40
1:A:310:GLU:OE2	1:A:359:LYS:HD2	2.21	0.40
1:A:372:VAL:HG11	1:A:375:MET:HE2	2.04	0.40
1:D:136:ARG:HD2	1:D:523:ARG:HG2	2.03	0.40
1:D:359:LYS:HE2	1:D:409:LEU:HD21	2.03	0.40
1:D:402:TYR:HA	1:D:403:PRO:HD3	1.85	0.40
1:D:585:ASN:CA	1:D:655:TYR:HB3	2.52	0.40
1:A:456:LEU:HD11	1:A:460:LEU:O	2.22	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	603/703 (86%)	556 (92%)	43 (7%)	4 (1%)	22	39
1	B	602/703 (86%)	543 (90%)	56 (9%)	3 (0%)	29	47
1	C	601/703 (86%)	551 (92%)	47 (8%)	3 (0%)	29	47
1	D	605/703 (86%)	545 (90%)	56 (9%)	4 (1%)	22	39
All	All	2411/2812 (86%)	2195 (91%)	202 (8%)	14 (1%)	25	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	476	PRO
1	B	401	GLU
1	A	653	TYR
1	A	699	LEU
1	B	642	THR
1	A	259	VAL
1	D	315	ALA
1	D	712	HIS
1	A	177	HIS
1	C	557	ARG
1	B	426	ALA
1	C	244	SER
1	C	413	ILE
1	D	413	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	520/593 (88%)	514 (99%)	6 (1%)	71	82
1	B	520/593 (88%)	511 (98%)	9 (2%)	60	76
1	C	518/593 (87%)	511 (99%)	7 (1%)	67	79
1	D	522/593 (88%)	507 (97%)	15 (3%)	42	62
All	All	2080/2372 (88%)	2043 (98%)	37 (2%)	59	75

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	112	ASN
1	B	124	VAL
1	B	352	VAL
1	B	363	VAL
1	B	427	ARG
1	B	428	ARG

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Mol	Chain	Res	Type
1	B	567	VAL
1	B	625	LEU
1	B	723	ILE
1	A	103	ASP
1	A	380	TYR
1	A	397	THR
1	A	473	SER
1	A	650	PHE
1	A	704	GLU
1	C	123	THR
1	C	140	GLN
1	C	187	GLU
1	C	235	LYS
1	C	515	ARG
1	C	559	VAL
1	C	675	ILE
1	D	123	THR
1	D	124	VAL
1	D	141	ASN
1	D	248	HIS
1	D	335	ARG
1	D	517	VAL
1	D	554	THR
1	D	585	ASN
1	D	599	ARG
1	D	608	ASP
1	D	609	GLN
1	D	622	GLU
1	D	648	VAL
1	D	661	ARG
1	D	724	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	321	GLN
1	C	580	ASN

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)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.60	0	17,19,21	1.00	1 (5%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.93	0
2	NAG	F	1	2,1	14,14,15	0.58	0	17,19,21	0.71	0
2	NAG	F	2	2	14,14,15	0.47	0	17,19,21	0.89	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

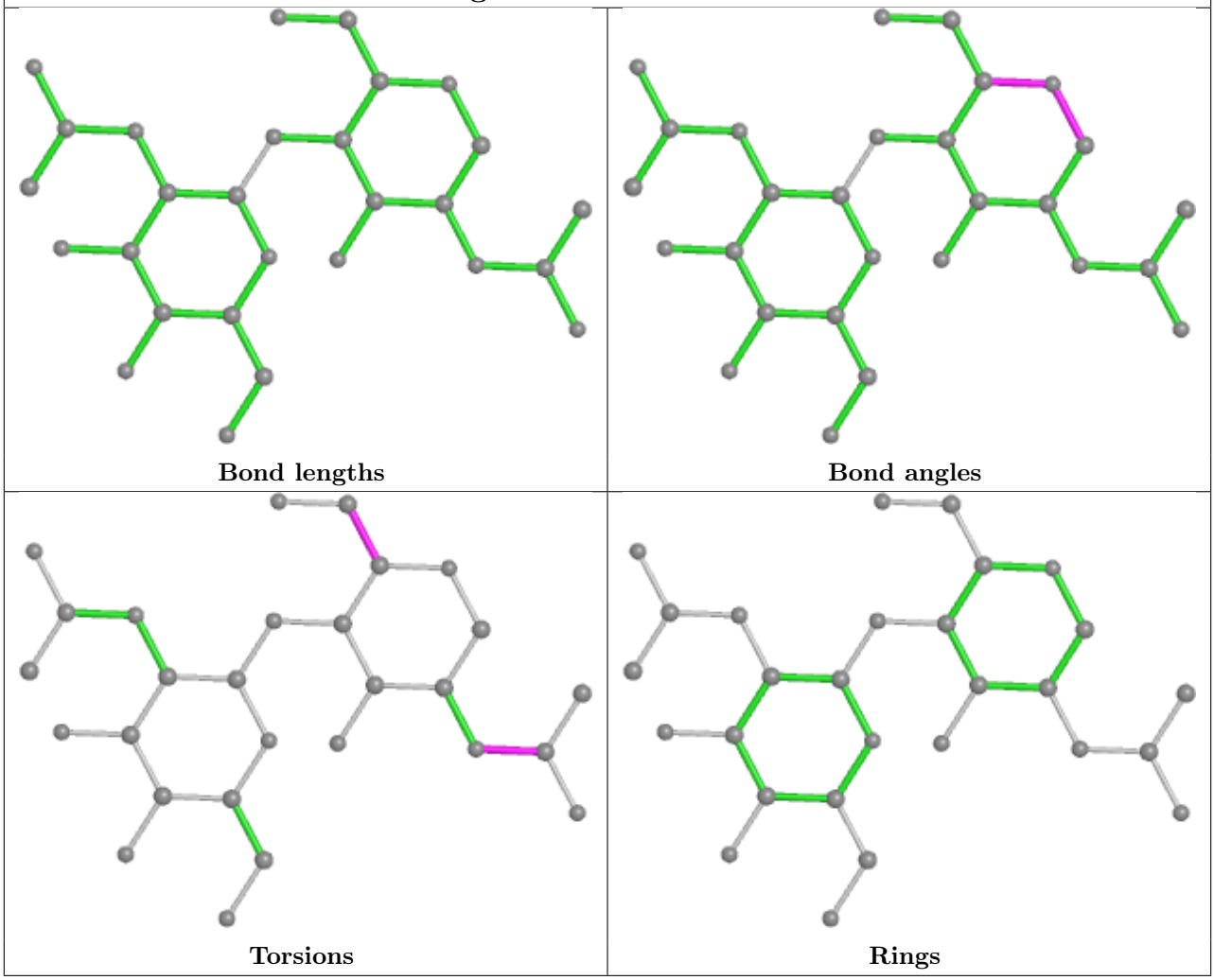
There are no ring outliers.

3 monomers are involved in 3 short contacts:

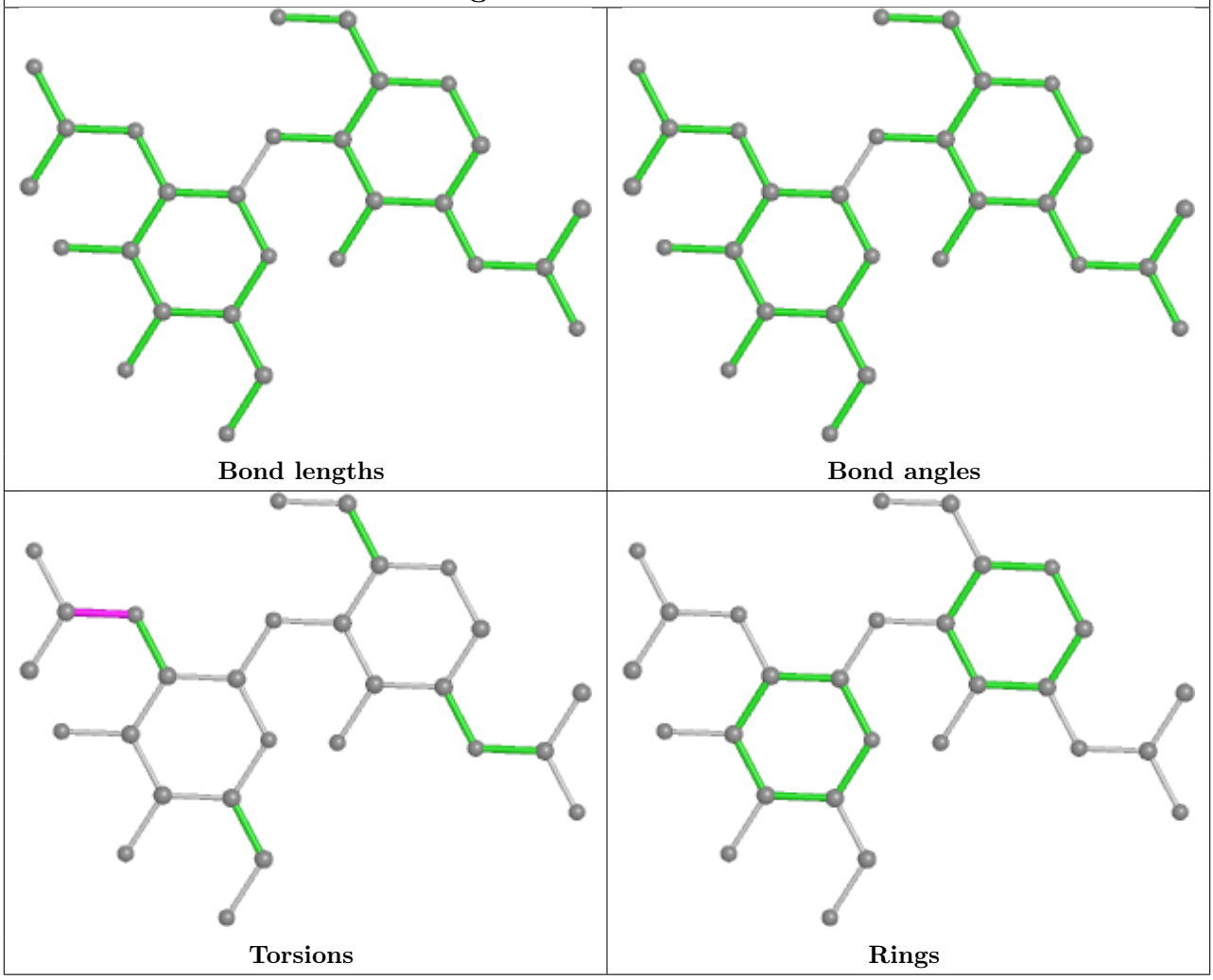
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	E	1	NAG	2	0
2	F	2	NAG	1	0

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 E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
4	MRY	B	2000	-	7,7,7	0.27	0	8,8,8	0.60	0
3	NAG	C	1674	1	14,14,15	0.55	0	17,19,21	0.63	0
3	NAG	D	1141	1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1398	1	14,14,15	0.51	0	17,19,21	0.77	1 (5%)
3	NAG	B	1141	1	14,14,15	0.58	0	17,19,21	0.78	0
3	NAG	D	1430	1	14,14,15	0.49	0	17,19,21	1.17	1 (5%)
4	MRY	A	2002	-	7,7,7	0.32	0	8,8,8	0.65	0
3	NAG	B	1674	1	14,14,15	0.54	0	17,19,21	0.75	1 (5%)
3	NAG	C	1430	1	14,14,15	0.45	0	17,19,21	1.26	1 (5%)
3	NAG	A	1398	1	14,14,15	0.47	0	17,19,21	0.82	0
3	NAG	A	1141	1	14,14,15	0.53	0	17,19,21	0.68	0
3	NAG	A	1674	1	14,14,15	0.54	0	17,19,21	0.61	0
4	MRY	A	2001	-	7,7,7	0.27	0	8,8,8	0.68	0
4	MRY	C	2000	-	7,7,7	0.30	0	8,8,8	0.60	0
4	MRY	C	2002	-	7,7,7	0.28	0	8,8,8	0.62	0
4	MRY	A	731	-	7,7,7	0.31	0	8,8,8	0.69	0
4	MRY	A	2000	-	7,7,7	0.39	0	8,8,8	0.65	0
3	NAG	A	1430	-	14,14,15	0.57	0	17,19,21	0.91	0
4	MRY	D	2000	-	7,7,7	0.30	0	8,8,8	0.56	0
4	MRY	C	2001	-	7,7,7	0.53	0	8,8,8	0.35	0
4	MRY	B	2001	-	7,7,7	0.35	0	8,8,8	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRY	B	2000	-	-	0/8/8/8	-
3	NAG	C	1674	1	-	1/6/23/26	0/1/1/1
3	NAG	D	1141	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1398	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1141	1	-	3/6/23/26	0/1/1/1
3	NAG	D	1430	1	-	4/6/23/26	0/1/1/1
4	MRY	A	2002	-	-	0/8/8/8	-
3	NAG	B	1674	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	1430	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1398	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1141	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1674	1	-	2/6/23/26	0/1/1/1
4	MRY	A	2001	-	-	0/8/8/8	-
4	MRY	C	2000	-	-	0/8/8/8	-
4	MRY	C	2002	-	-	0/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRY	A	731	-	-	0/8/8/8	-
4	MRY	A	2000	-	-	0/8/8/8	-
3	NAG	A	1430	-	-	3/6/23/26	0/1/1/1
4	MRY	D	2000	-	-	0/8/8/8	-
4	MRY	C	2001	-	-	0/8/8/8	-
4	MRY	B	2001	-	-	0/8/8/8	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1430	NAG	C1-O5-C5	4.09	117.73	112.19
3	D	1430	NAG	C1-O5-C5	2.70	115.85	112.19
3	D	1141	NAG	O5-C5-C6	2.36	110.90	107.20
3	B	1398	NAG	C1-O5-C5	2.09	115.02	112.19
3	B	1674	NAG	O5-C5-C6	2.06	110.44	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1674	NAG	C1

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1674	NAG	C8-C7-N2-C2
3	A	1398	NAG	C8-C7-N2-C2
3	A	1674	NAG	C8-C7-N2-C2
3	D	1141	NAG	O5-C5-C6-O6
3	D	1430	NAG	O5-C5-C6-O6
3	B	1141	NAG	O5-C5-C6-O6
3	D	1430	NAG	C4-C5-C6-O6
3	A	1674	NAG	O7-C7-N2-C2
3	D	1430	NAG	C8-C7-N2-C2
3	D	1430	NAG	O7-C7-N2-C2
3	B	1674	NAG	O7-C7-N2-C2
3	A	1398	NAG	O7-C7-N2-C2
3	B	1141	NAG	C4-C5-C6-O6
3	D	1141	NAG	C4-C5-C6-O6
3	C	1430	NAG	O5-C5-C6-O6
3	A	1430	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1430	NAG	C1-C2-N2-C7
3	C	1674	NAG	O5-C5-C6-O6
3	B	1398	NAG	C8-C7-N2-C2
3	B	1141	NAG	C1-C2-N2-C7
3	B	1398	NAG	O7-C7-N2-C2
3	D	1141	NAG	C1-C2-N2-C7
3	A	1430	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2000	MRY	3	0
4	A	2002	MRY	1	0
3	C	1430	NAG	1	0
3	A	1398	NAG	1	0
4	C	2000	MRY	1	0
4	C	2001	MRY	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	607/703 (86%)	0.28	20 (3%)	46	54	20, 49, 110, 233	0
1	B	606/703 (86%)	0.33	24 (3%)	38	45	21, 55, 118, 212	0
1	C	605/703 (86%)	0.31	21 (3%)	44	52	21, 52, 114, 207	0
1	D	609/703 (86%)	0.26	14 (2%)	60	69	18, 51, 107, 175	0
All	All	2427/2812 (86%)	0.30	79 (3%)	46	54	18, 52, 113, 233	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ARG	6.3
1	C	589	ILE	6.1
1	A	116	CYS	5.9
1	B	623	LEU	5.9
1	A	471	GLU	5.2
1	C	259	VAL	5.0
1	D	265	TYR	4.9
1	D	469	LEU	4.8
1	B	609	GLN	4.7
1	B	442	TYR	4.5
1	A	261	ALA	4.4
1	B	470	ARG	4.3
1	A	259	VAL	4.2
1	B	449	LEU	4.1
1	C	595	ALA	4.0
1	B	109	THR	3.9
1	C	323	ASP	3.9
1	B	110	ASP	3.9
1	B	469	LEU	3.9
1	B	265	TYR	3.9
1	C	262	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	647	TYR	3.9
1	A	595	ALA	3.8
1	A	589	ILE	3.7
1	B	619	GLU	3.5
1	B	616	GLN	3.5
1	A	493	GLU	3.4
1	D	623	LEU	3.4
1	D	615	GLY	3.2
1	A	577	ALA	3.1
1	C	261	ALA	3.1
1	B	111	ALA	3.1
1	C	582	ILE	3.1
1	B	443	LEU	3.0
1	B	606	TYR	3.0
1	C	494	ARG	3.0
1	D	653	TYR	2.9
1	D	643	PHE	2.9
1	D	442	TYR	2.9
1	C	434	ILE	2.8
1	C	578	ALA	2.8
1	B	612	LEU	2.8
1	C	577	ALA	2.6
1	C	604	PHE	2.6
1	C	492	VAL	2.6
1	D	110	ASP	2.5
1	A	464	TYR	2.4
1	C	437	GLY	2.4
1	B	653	TYR	2.4
1	C	601	LEU	2.4
1	A	459	THR	2.4
1	B	441	TYR	2.3
1	B	180	SER	2.3
1	C	463	LEU	2.3
1	A	195	GLU	2.3
1	B	195	GLU	2.3
1	D	607	GLU	2.3
1	B	659	LEU	2.3
1	C	612	LEU	2.3
1	A	111	ALA	2.3
1	A	648	VAL	2.3
1	C	427	ARG	2.2
1	A	432	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	659	LEU	2.1
1	B	113	PHE	2.1
1	D	259	VAL	2.1
1	D	465	VAL	2.1
1	A	233	GLU	2.1
1	B	564	LEU	2.1
1	C	456	LEU	2.1
1	B	384	PHE	2.1
1	D	619	GLU	2.1
1	D	492	VAL	2.0
1	C	640	TYR	2.0
1	A	592	ARG	2.0
1	D	724	HIS	2.0
1	A	391	ILE	2.0
1	B	464	TYR	2.0
1	A	647	TYR	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)

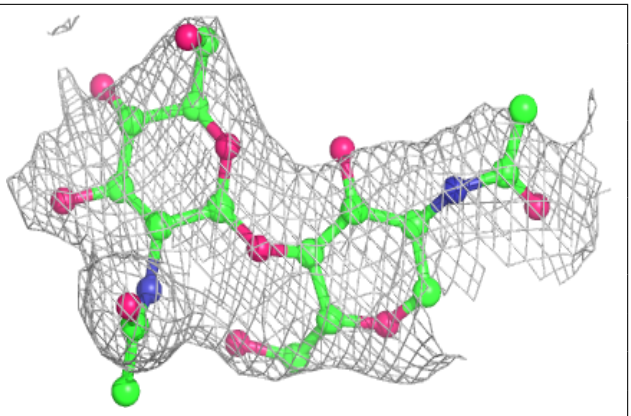
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

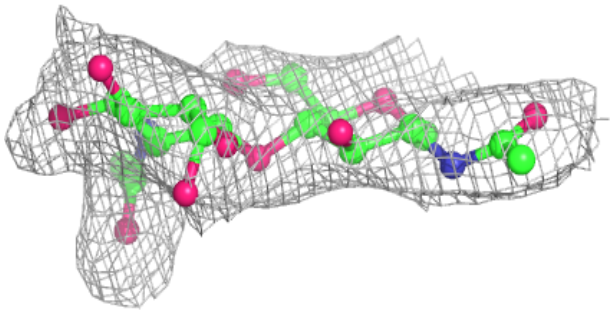
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	2	14/15	0.82	0.25	123,123,123,123	0
2	NAG	E	2	14/15	0.87	0.21	105,105,105,105	0
2	NAG	E	1	14/15	0.91	0.22	100,100,100,100	0
2	NAG	F	1	14/15	0.94	0.21	101,101,101,101	0

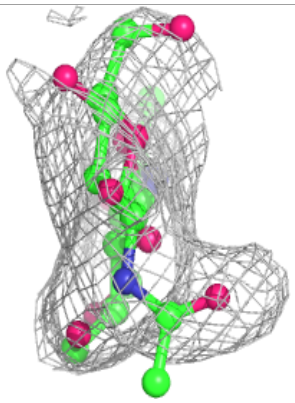
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

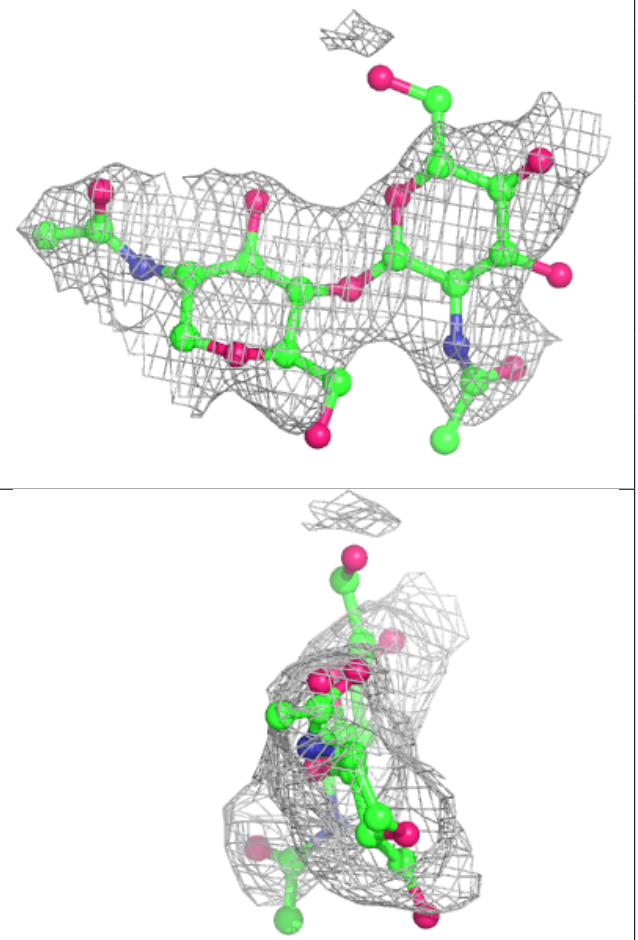






Electron density around Chain F:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	1141	14/15	0.75	0.36	147,147,147,147	0
3	NAG	B	1141	14/15	0.78	0.23	134,134,134,134	0
3	NAG	A	1430	14/15	0.79	0.24	96,96,96,96	0
3	NAG	D	1141	14/15	0.81	0.22	63,131,131,131	0
4	MRY	C	2001	8/8	0.82	0.32	72,72,72,72	0
3	NAG	B	1674	14/15	0.84	0.34	120,120,120,120	0
3	NAG	B	1398	14/15	0.86	0.25	114,114,114,114	0
4	MRY	A	2002	8/8	0.87	0.24	74,74,74,74	0
4	MRY	C	2000	8/8	0.87	0.23	72,72,72,72	0
3	NAG	D	1430	14/15	0.87	0.38	119,119,119,119	0
3	NAG	C	1430	14/15	0.90	0.19	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MRY	A	2001	8/8	0.91	0.27	77,77,77,77	0
4	MRY	D	2000	8/8	0.91	0.20	80,80,80,80	0
4	MRY	A	2000	8/8	0.92	0.20	42,42,42,42	0
3	NAG	C	1674	14/15	0.92	0.13	78,78,78,78	0
3	NAG	A	1398	14/15	0.93	0.15	79,79,79,79	0
4	MRY	B	2001	8/8	0.93	0.23	75,75,75,75	0
5	NA	C	4	1/1	0.93	0.27	87,87,87,87	0
4	MRY	C	2002	8/8	0.94	0.20	60,60,60,60	0
3	NAG	A	1674	14/15	0.94	0.12	70,70,70,70	0
5	NA	B	2	1/1	0.94	0.12	60,60,60,60	0
4	MRY	A	731	8/8	0.94	0.18	65,65,65,65	0
4	MRY	B	2000	8/8	0.96	0.21	53,53,53,53	0
6	CL	A	5	1/1	0.96	0.14	71,71,71,71	0
5	NA	D	3	1/1	0.97	0.17	38,38,38,38	0
5	NA	C	1	1/1	0.98	0.14	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.