Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 10:42 pm GMT

PDB ID	:	1UZG
Title	:	CRYSTAL STRUCTURE OF THE DENGUE TYPE 3 VIRUS ENVELOPE PROTEIN
Authors	:	Modis, Y.; Harrison, S.C.
Deposited on	:	2004-03-11
Resolution	:	3.50 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:

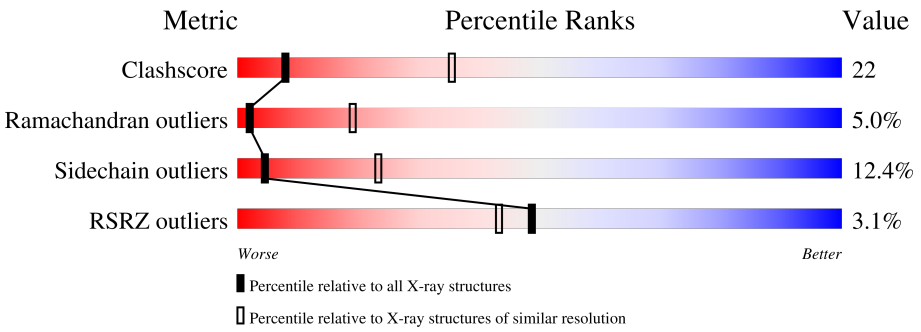
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	392	3%, 58%, 34%, 8%
1	B	392	4%, 51%, 43%, 6%
2	C	2	100%
3	D	6	17%, 50%, 33%
4	E	4	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUL	C	2	-	-	-	X
3	BMA	D	4	-	-	-	X
3	BMA	D	5	-	-	-	X
4	MAN	E	3	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6214 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 MAJOR ENVELOPE PROTEIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	3021	1902	520	578	21	0	0	0
1	B	392	3021	1902	520	578	21	0	0	0

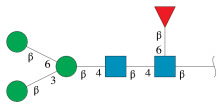
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ILE	VAL	conflict	UNP P27915
A	201	ASP	ASN	conflict	UNP P27915
B	129	ILE	VAL	conflict	UNP P27915
B	201	ASP	ASN	conflict	UNP P27915

- Molecule 2 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

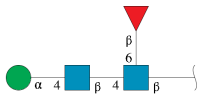
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	24	14	1	9	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



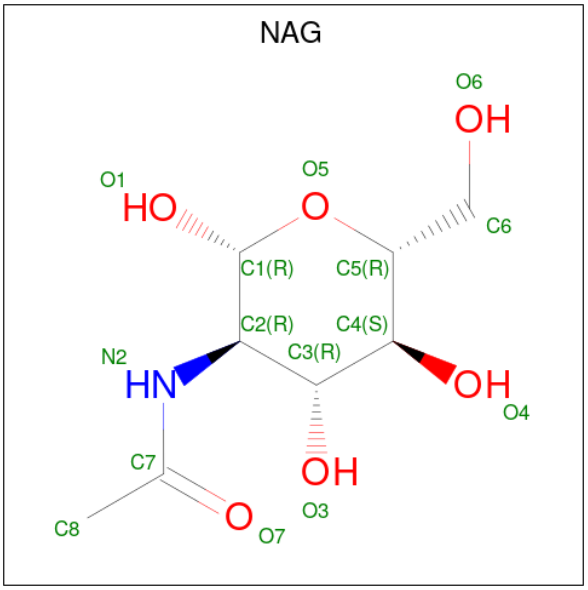
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	6	71	40	2	29	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	4	49	28	2	19	0	0	0

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	7	7	7	0	0

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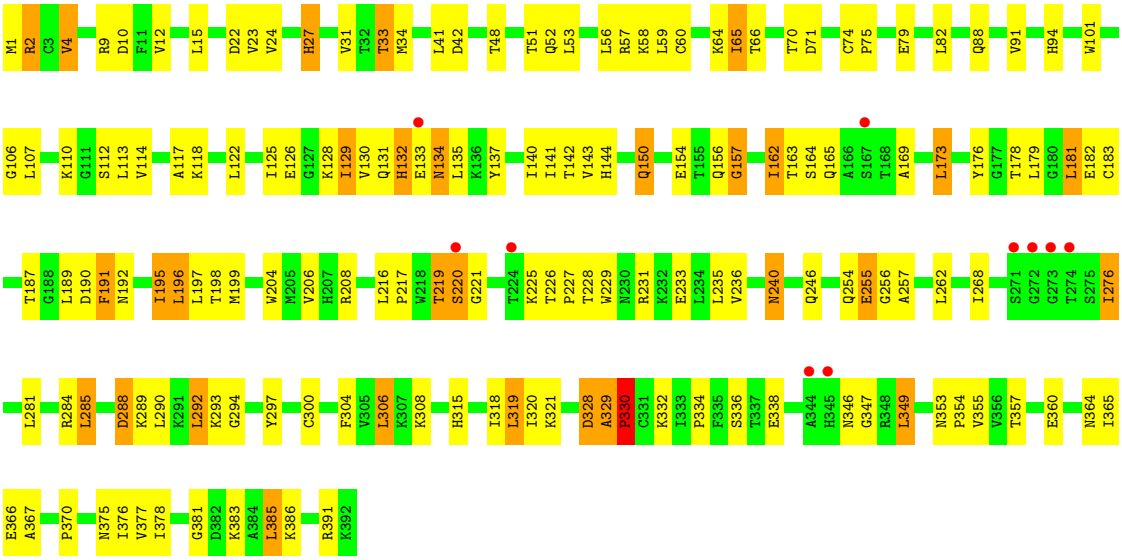
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	7	7	7	0	0

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.

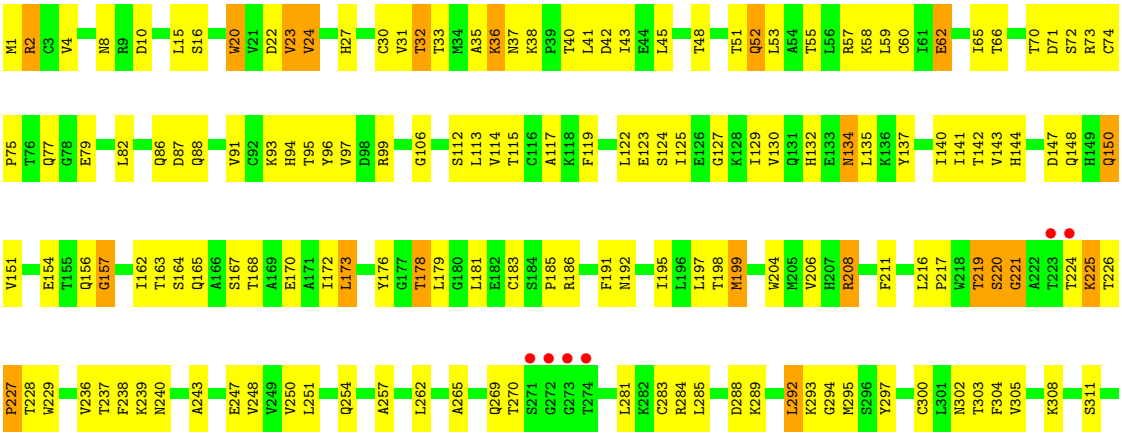
• Molecule 1: MAJOR ENVELOPE PROTEIN E

Chain A: 3% 58% 34% 8%



• Molecule 1: MAJOR ENVELOPE PROTEIN E

Chain B: 4% 51% 43% 6%

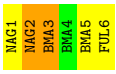


• Molecule 2: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

• Molecule 3: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2 -deoxy-beta-D-glucopyranose

Chain D: 17% 50% 33%



• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[be ta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.85Å 68.63Å 270.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.99 – 3.50 20.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.99-3.50) 91.8 (20.00-3.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.62Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.284 , 0.324 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	112.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6214	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: FUL, BMA, NAG, MAN

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	0.43	0/3077	0.72	1/4161 (0.0%)
1	B	0.43	0/3077	0.70	1/4161 (0.0%)
All	All	0.43	0/6154	0.71	2/8322 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	LYS	N-CA-C	6.76	129.26	111.00
1	A	225	LYS	N-CA-C	6.44	128.40	111.00

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	3021	0	3027	129	0
1	B	3021	0	3027	128	0
2	C	24	0	22	1	0
3	D	71	0	63	7	0
4	E	49	0	44	6	0
5	B	14	0	13	0	0
6	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	7	0	0	0	0
All	All	6214	0	6196	264	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 22.

All (264) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:HB2	1:A:370:PRO:HG3	1.46	0.96
1:B:22:ASP:HB3	1:B:284:ARG:HE	1.37	0.89
1:B:329:ALA:HB1	1:B:330:PRO:HD2	1.55	0.89
1:A:2:ARG:HH21	1:A:140:ILE:HD13	1.37	0.88
3:D:3:BMA:C6	3:D:5:BMA:C1	2.52	0.88
1:B:53:LEU:HD22	1:B:130:VAL:HG12	1.54	0.87
1:A:329:ALA:HB1	1:A:330:PRO:HD2	1.57	0.87
1:A:383:LYS:O	1:A:383:LYS:HG3	1.74	0.86
4:E:2:NAG:H5	4:E:3:MAN:H3	1.60	0.82
4:E:1:NAG:C6	4:E:4:FUL:C1	2.58	0.81
1:B:347:GLY:HA3	1:B:370:PRO:HD3	1.62	0.81
1:A:10:ASP:HB2	1:A:31:VAL:HG22	1.61	0.81
1:B:65:ILE:HD13	1:B:250:VAL:HG12	1.63	0.80
4:E:2:NAG:H62	4:E:3:MAN:H5	1.64	0.79
1:A:22:ASP:HA	1:A:284:ARG:HA	1.65	0.79
1:A:53:LEU:HD22	1:A:130:VAL:HG12	1.65	0.78
1:A:59:LEU:HD22	1:A:216:LEU:HB2	1.66	0.78
3:D:1:NAG:C6	3:D:6:FUL:C1	2.61	0.78
1:A:23:VAL:HG12	1:A:24:VAL:H	1.51	0.76
1:B:33:THR:CG2	1:B:41:LEU:HB2	2.15	0.75
1:B:43:ILE:HD13	1:B:285:LEU:HD11	1.70	0.74
1:A:268:ILE:HG23	1:A:276:ILE:O	1.88	0.73
1:B:336:SER:HB2	1:B:377:VAL:HB	1.69	0.73
1:B:113:LEU:HD23	1:B:114:VAL:N	2.04	0.72
1:A:346:ASN:HB2	1:A:370:PRO:CG	2.20	0.72
1:B:10:ASP:HB2	1:B:31:VAL:HG22	1.71	0.71
1:A:15:LEU:O	1:A:15:LEU:HG	1.89	0.71
1:A:131:GLN:O	1:A:134:ASN:HB2	1.90	0.70
1:A:142:THR:OG1	1:A:157:GLY:HA2	1.90	0.70
1:A:94:HIS:CE1	1:A:114:VAL:HB	2.27	0.70
1:A:347:GLY:HA3	1:A:370:PRO:HD3	1.71	0.70
1:A:129:ILE:HD12	1:A:208:ARG:HH12	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ALA:HB1	1:B:330:PRO:CD	2.21	0.70
1:A:2:ARG:NH2	1:A:140:ILE:HD13	2.07	0.69
1:B:60:CYS:O	1:B:216:LEU:HD22	1.92	0.69
1:B:59:LEU:HD22	1:B:216:LEU:HB2	1.73	0.69
1:B:22:ASP:HA	1:B:284:ARG:HA	1.75	0.69
1:A:27:HIS:HE1	1:A:276:ILE:HB	1.59	0.68
1:A:292:LEU:CD2	1:A:293:LYS:H	2.06	0.68
1:B:172:ILE:HG12	1:B:178:THR:HG22	1.75	0.68
1:A:94:HIS:ND1	1:A:114:VAL:HB	2.09	0.67
1:B:292:LEU:CD2	1:B:293:LYS:H	2.07	0.67
1:B:91:VAL:HG11	1:B:236:VAL:HG11	1.77	0.66
1:A:150:GLN:HB2	1:A:156:GLN:HE22	1.61	0.66
1:A:292:LEU:HD23	1:A:293:LYS:H	1.59	0.66
1:B:1:MET:HG2	1:B:144:HIS:CD2	2.31	0.66
1:A:60:CYS:HB2	1:A:229:TRP:CZ3	2.31	0.66
1:B:292:LEU:HD23	1:B:293:LYS:H	1.62	0.64
1:B:304:PHE:CZ	1:B:333:ILE:HG23	2.32	0.64
1:B:48:THR:HG23	1:B:137:TYR:CD2	2.32	0.64
1:A:349:LEU:HD23	1:A:367:ALA:HB2	1.80	0.64
1:A:60:CYS:O	1:A:216:LEU:HD22	1.98	0.64
1:A:22:ASP:HB3	1:A:284:ARG:HE	1.64	0.63
1:A:132:HIS:O	1:A:134:ASN:N	2.31	0.63
1:A:336:SER:HB2	1:A:377:VAL:HB	1.81	0.63
1:A:329:ALA:HB1	1:A:330:PRO:CD	2.28	0.62
1:A:338:GLU:HB2	1:A:375:ASN:HB2	1.83	0.61
1:A:65:ILE:HG12	1:A:117:ALA:HB1	1.83	0.60
1:A:24:VAL:O	1:A:24:VAL:HG13	2.01	0.60
1:B:219:THR:HG22	1:B:229:TRP:CZ3	2.36	0.60
1:B:32:THR:HG23	1:B:42:ASP:OD1	2.01	0.59
1:A:141:ILE:HD13	1:A:179:LEU:HD23	1.84	0.59
1:B:297:TYR:HE1	1:B:330:PRO:HB3	1.67	0.59
1:B:24:VAL:HG13	1:B:24:VAL:O	2.03	0.59
1:B:163:THR:HG22	1:B:164:SER:N	2.17	0.59
1:A:308:LYS:HB2	1:A:321:LYS:HD3	1.84	0.59
1:B:79:GLU:HA	1:B:112:SER:OG	2.03	0.59
1:B:127:GLY:HA3	1:B:211:PHE:CZ	2.38	0.58
1:A:9:ARG:HB3	1:A:315:HIS:CE1	2.39	0.58
1:B:74:CYS:HB3	1:B:75:PRO:HD2	1.85	0.58
1:A:41:LEU:HD22	1:A:179:LEU:HD22	1.86	0.58
1:B:350:ILE:HB	1:B:366:GLU:O	2.04	0.57
1:B:74:CYS:HB3	1:B:75:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:CG	1:A:142:THR:HB	2.34	0.57
1:A:306:LEU:HD13	1:A:385:LEU:HD11	1.87	0.57
1:B:48:THR:HG23	1:B:137:TYR:CE2	2.39	0.57
1:A:2:ARG:HD2	1:A:142:THR:HB	1.87	0.57
1:A:162:ILE:O	1:A:162:ILE:HG23	2.04	0.57
1:A:131:GLN:O	1:A:132:HIS:C	2.42	0.57
1:B:33:THR:HG23	1:B:41:LEU:HB2	1.84	0.57
1:B:150:GLN:O	1:B:150:GLN:HG2	2.05	0.56
1:A:346:ASN:CB	1:A:370:PRO:HG3	2.30	0.56
1:B:297:TYR:CE1	1:B:330:PRO:HB3	2.41	0.56
4:E:2:NAG:C6	4:E:3:MAN:H5	2.34	0.56
3:D:1:NAG:H61	3:D:2:NAG:O7	2.05	0.56
1:A:183:CYS:HB3	1:A:281:LEU:HD11	1.89	0.55
1:B:70:THR:HA	1:B:82:LEU:HD11	1.89	0.55
1:B:2:ARG:HH11	1:B:2:ARG:HB2	1.71	0.54
1:A:2:ARG:HB2	1:A:2:ARG:HH11	1.72	0.54
1:A:4:VAL:CG1	1:A:319:LEU:HD11	2.37	0.54
1:A:318:ILE:O	1:A:366:GLU:HA	2.07	0.54
1:B:147:ASP:HB3	1:B:150:GLN:HB2	1.89	0.54
1:B:349:LEU:HD23	1:B:367:ALA:HB2	1.90	0.54
3:D:2:NAG:O3	3:D:3:BMA:H2	2.08	0.54
1:B:204:TRP:NE1	1:B:262:LEU:HB3	2.23	0.54
1:B:16:SER:HA	1:B:36:LYS:HD3	1.90	0.54
1:A:1:MET:HA	1:A:42:ASP:OD2	2.08	0.53
1:B:23:VAL:HG12	1:B:24:VAL:H	1.73	0.53
1:B:4:VAL:HG13	1:B:319:LEU:HD11	1.90	0.53
1:A:256:GLY:HA3	1:B:254:GLN:NE2	2.23	0.53
1:B:129:ILE:HG23	1:B:129:ILE:O	2.09	0.53
1:B:75:PRO:O	1:B:77:GLN:HG3	2.10	0.52
1:A:163:THR:HG22	1:A:164:SER:N	2.24	0.52
1:B:219:THR:O	1:B:220:SER:C	2.47	0.52
1:A:110:LYS:HE2	1:B:314:GLN:HE22	1.75	0.52
1:B:204:TRP:CD2	1:B:262:LEU:HD13	2.45	0.52
1:A:297:TYR:CE1	1:A:330:PRO:HB3	2.44	0.51
1:A:48:THR:HG23	1:A:137:TYR:CD2	2.45	0.51
1:A:349:LEU:HD23	1:A:367:ALA:CB	2.41	0.51
1:A:353:ASN:O	1:A:355:VAL:HG23	2.09	0.51
1:B:97:VAL:O	1:B:99:ARG:HG2	2.09	0.51
3:D:1:NAG:H61	3:D:2:NAG:C7	2.40	0.51
1:B:65:ILE:HG13	1:B:117:ALA:HB1	1.93	0.51
1:A:128:LYS:O	1:A:195:ILE:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:VAL:O	1:B:151:VAL:HG13	2.11	0.51
3:D:3:BMA:H62	3:D:5:BMA:C1	2.38	0.51
1:B:15:LEU:HG	1:B:15:LEU:O	2.10	0.51
1:A:360:GLU:HA	1:A:360:GLU:OE1	2.12	0.50
1:B:135:LEU:HD11	1:B:191:PHE:HE2	1.76	0.50
1:A:130:VAL:O	1:A:191:PHE:HB3	2.11	0.50
4:E:2:NAG:H5	4:E:3:MAN:C3	2.38	0.50
1:B:45:LEU:HG	1:B:45:LEU:O	2.11	0.50
1:A:23:VAL:HG12	1:A:24:VAL:N	2.25	0.50
1:B:163:THR:HG22	1:B:164:SER:H	1.77	0.50
1:A:4:VAL:HG11	1:A:319:LEU:HD11	1.93	0.49
1:B:41:LEU:CD2	1:B:143:VAL:HG22	2.43	0.49
1:B:238:PHE:HE1	1:B:248:VAL:HG22	1.77	0.49
1:B:20:TRP:HA	1:B:285:LEU:O	2.13	0.49
1:B:41:LEU:HD23	1:B:143:VAL:HG22	1.94	0.49
1:B:71:ASP:HB2	1:B:82:LEU:HD21	1.95	0.49
1:A:128:LYS:HB2	1:A:196:LEU:HD23	1.95	0.48
1:A:142:THR:OG1	1:A:157:GLY:CA	2.61	0.48
1:B:113:LEU:HD23	1:B:113:LEU:C	2.33	0.48
1:B:183:CYS:HB3	1:B:281:LEU:HD11	1.96	0.48
1:B:2:ARG:HG3	1:B:142:THR:HB	1.95	0.48
1:B:59:LEU:O	1:B:124:SER:HB2	2.13	0.48
1:B:94:HIS:ND1	1:B:114:VAL:HB	2.28	0.48
1:A:2:ARG:HG3	1:A:142:THR:HB	1.96	0.48
1:A:190:ASP:C	1:A:192:ASN:H	2.16	0.48
1:B:141:ILE:HD13	1:B:179:LEU:HD23	1.95	0.48
1:B:65:ILE:HD13	1:B:250:VAL:CG1	2.39	0.48
1:A:162:ILE:HD13	1:A:162:ILE:C	2.34	0.47
1:A:143:VAL:O	1:A:150:GLN:NE2	2.47	0.47
1:B:353:ASN:N	1:B:354:PRO:HD3	2.29	0.47
1:B:52:GLN:OE1	1:B:134:ASN:ND2	2.47	0.47
4:E:2:NAG:H61	4:E:4:FUL:H5	1.96	0.47
1:A:231:ARG:HA	1:A:233:GLU:OE2	2.14	0.47
1:B:179:LEU:HD21	1:B:285:LEU:HD22	1.97	0.47
1:B:10:ASP:CB	1:B:31:VAL:HG22	2.43	0.47
1:A:12:VAL:HG21	1:A:23:VAL:HG13	1.95	0.47
1:A:349:LEU:CD2	1:A:367:ALA:HB2	2.44	0.47
1:B:93:LYS:HB2	1:B:238:PHE:CD2	2.50	0.47
1:A:179:LEU:HD11	1:A:285:LEU:HB3	1.96	0.47
1:B:97:VAL:HA	1:B:243:ALA:HB1	1.95	0.47
1:B:125:ILE:HD11	1:B:199:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:HG3	1:B:247:GLU:HB2	1.97	0.47
1:A:300:CYS:SG	1:A:332:LYS:O	2.73	0.47
1:B:304:PHE:O	1:B:385:LEU:HD22	2.16	0.46
1:A:257:ALA:HB2	1:B:257:ALA:HB2	1.97	0.46
1:A:187:THR:HG21	1:A:191:PHE:CE2	2.50	0.46
1:B:195:ILE:HG12	1:B:208:ARG:HG2	1.97	0.46
1:B:204:TRP:HD1	1:B:265:ALA:HB3	1.80	0.46
1:A:64:LYS:HB2	1:A:122:LEU:HD11	1.96	0.46
1:B:4:VAL:CG1	1:B:319:LEU:HD11	2.46	0.46
1:B:367:ALA:C	1:B:369:PRO:HD3	2.37	0.45
1:A:129:ILE:CD1	1:A:208:ARG:HH12	2.27	0.45
1:A:101:TRP:HE3	1:B:151:VAL:HG11	1.80	0.45
1:A:113:LEU:HD23	1:A:113:LEU:C	2.37	0.45
1:B:183:CYS:HA	1:B:283:CYS:HA	1.97	0.45
1:B:367:ALA:O	1:B:369:PRO:HD3	2.16	0.45
1:A:192:ASN:HA	1:A:208:ARG:HH21	1.81	0.45
1:A:219:THR:O	1:A:220:SER:C	2.55	0.45
1:B:348:ARG:HA	1:B:348:ARG:NE	2.32	0.45
1:A:195:ILE:HG13	1:A:208:ARG:HA	1.97	0.45
1:A:320:ILE:O	1:A:364:ASN:HA	2.17	0.45
1:B:88:GLN:CB	1:B:228:THR:HG23	2.47	0.45
1:A:328:ASP:O	1:A:329:ALA:HB3	2.17	0.45
1:A:2:ARG:CD	1:A:142:THR:HB	2.47	0.44
1:B:334:PRO:O	1:B:378:ILE:HA	2.17	0.44
1:A:256:GLY:HA3	1:B:254:GLN:HE21	1.81	0.44
1:A:329:ALA:O	1:A:330:PRO:C	2.55	0.44
1:B:119:PHE:CD1	1:B:119:PHE:C	2.91	0.44
1:B:311:SER:O	1:B:318:ILE:HA	2.17	0.44
1:B:35:ALA:HB3	1:B:38:LYS:HB2	1.99	0.44
1:B:329:ALA:CB	1:B:330:PRO:CD	2.92	0.44
1:B:380:ILE:O	1:B:382:ASP:N	2.50	0.44
1:A:33:THR:HG23	1:A:41:LEU:HD12	2.00	0.44
1:A:70:THR:OG1	1:A:71:ASP:N	2.50	0.44
1:A:376:ILE:O	1:A:386:LYS:HA	2.17	0.44
1:B:225:LYS:C	1:B:227:PRO:HD3	2.38	0.44
1:B:349:LEU:HD23	1:B:367:ALA:CB	2.48	0.44
1:A:74:CYS:HB3	1:A:75:PRO:CD	2.47	0.44
1:B:36:LYS:O	1:B:38:LYS:HG2	2.17	0.44
1:B:352:ALA:C	1:B:354:PRO:HD3	2.39	0.44
1:A:125:ILE:HG22	1:A:126:GLU:N	2.32	0.43
1:A:91:VAL:HG11	1:A:236:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASN:HB2	1:B:324:TYR:CE1	2.53	0.43
1:A:217:PRO:HG2	1:A:235:LEU:HD22	2.00	0.43
1:A:169:ALA:O	1:A:181:LEU:HD12	2.19	0.43
1:A:1:MET:HG2	1:A:144:HIS:CD2	2.54	0.43
1:A:288:ASP:C	1:A:290:LEU:H	2.22	0.43
1:B:289:LYS:NZ	1:B:289:LYS:HB3	2.33	0.43
1:A:88:GLN:CB	1:A:228:THR:HG23	2.49	0.43
1:B:329:ALA:O	1:B:330:PRO:C	2.57	0.43
1:B:338:GLU:HB2	1:B:375:ASN:HB2	2.00	0.43
1:B:37:ASN:O	1:B:292:LEU:HD12	2.19	0.42
1:A:226:THR:N	1:A:227:PRO:HD3	2.34	0.42
1:B:391:ARG:O	1:B:392:LYS:HB3	2.20	0.42
1:A:182:GLU:O	1:A:182:GLU:HG2	2.19	0.42
1:A:254:GLN:O	1:A:255:GLU:C	2.57	0.42
1:B:162:ILE:N	1:B:162:ILE:HD12	2.34	0.42
1:A:33:THR:CG2	1:A:41:LEU:HB2	2.49	0.42
1:A:143:VAL:HG21	1:A:173:LEU:HD13	2.02	0.42
1:B:148:GLN:HG3	1:B:362:PRO:HD2	2.02	0.42
3:D:2:NAG:H4	3:D:3:BMA:O2	2.19	0.42
1:A:125:ILE:HG23	1:A:198:THR:O	2.20	0.42
1:A:216:LEU:HA	1:A:217:PRO:HD3	1.87	0.42
1:B:58:LYS:HE3	1:B:221:GLY:HA2	2.01	0.42
1:A:118:LYS:NZ	2:C:1:NAG:H81	2.35	0.42
1:A:190:ASP:OD1	1:A:192:ASN:HB2	2.20	0.42
1:A:292:LEU:HD22	1:A:293:LYS:H	1.84	0.42
1:A:304:PHE:CD1	1:A:378:ILE:HG22	2.55	0.41
1:A:338:GLU:HB2	1:A:375:ASN:O	2.20	0.41
1:B:33:THR:O	1:B:40:THR:HA	2.20	0.41
1:A:385:LEU:HD23	1:A:386:LYS:N	2.35	0.41
1:B:2:ARG:NH1	1:B:2:ARG:CB	2.83	0.41
1:A:4:VAL:HG11	1:A:319:LEU:CD1	2.50	0.41
1:B:295:MET:C	1:B:297:TYR:H	2.24	0.41
1:A:110:LYS:CE	1:B:314:GLN:HE22	2.33	0.41
1:B:94:HIS:CE1	1:B:114:VAL:HB	2.55	0.41
1:B:95:THR:C	1:B:96:TYR:HD1	2.23	0.41
1:B:163:THR:CG2	1:B:164:SER:N	2.82	0.41
1:A:204:TRP:CD2	1:A:262:LEU:HD13	2.56	0.41
1:A:347:GLY:CA	1:A:370:PRO:HD3	2.45	0.41
1:A:2:ARG:HG3	1:A:2:ARG:H	1.61	0.41
1:A:59:LEU:HD13	1:A:216:LEU:HD12	2.02	0.41
1:A:70:THR:HA	1:A:82:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:HA	1:A:112:SER:HB2	2.02	0.41
1:A:173:LEU:HB2	1:A:176:TYR:HB2	2.02	0.41
1:B:2:ARG:HH21	1:B:140:ILE:HD13	1.85	0.41
1:B:125:ILE:HD11	1:B:199:MET:CE	2.50	0.41
1:B:173:LEU:HB2	1:B:176:TYR:HB2	2.02	0.41
1:B:300:CYS:SG	1:B:332:LYS:O	2.79	0.41
1:B:378:ILE:HD12	1:B:387:ILE:HD11	2.02	0.41
1:A:162:ILE:HG13	1:A:183:CYS:HB2	2.02	0.41
1:A:353:ASN:N	1:A:354:PRO:HD3	2.35	0.41
1:B:72:SER:HB3	1:B:113:LEU:HG	2.03	0.41
1:A:23:VAL:CG1	1:A:31:VAL:HG11	2.51	0.40
1:A:240:ASN:HB2	1:A:246:GLN:HG3	2.03	0.40
1:A:255:GLU:O	1:A:256:GLY:C	2.60	0.40
1:A:354:PRO:HB3	1:A:365:ILE:CD1	2.51	0.40
1:B:2:ARG:HH11	1:B:2:ARG:CB	2.34	0.40
1:B:226:THR:N	1:B:227:PRO:HD3	2.36	0.40
1:A:383:LYS:O	1:A:383:LYS:CG	2.55	0.40
1:B:140:ILE:CG1	1:B:157:GLY:HA3	2.51	0.40
1:B:179:LEU:HD11	1:B:285:LEU:HD22	2.03	0.40
1:B:349:LEU:CD2	1:B:367:ALA:HB2	2.50	0.40
1:B:197:LEU:HD23	1:B:198:THR:O	2.21	0.40
1:B:216:LEU:HA	1:B:217:PRO:HD3	1.72	0.40
1:A:2:ARG:HH21	1:A:140:ILE:CD1	2.21	0.40
1:A:48:THR:HG23	1:A:137:TYR:CE2	2.57	0.40
1:A:41:LEU:CD2	1:A:179:LEU:HD22	2.51	0.40
1:A:125:ILE:CG2	1:A:126:GLU:N	2.84	0.40
1:B:62:GLU:HB3	1:B:122:LEU:HB2	2.02	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	390/392 (100%)	300 (77%)	70 (18%)	20 (5%)	2 19
1	B	390/392 (100%)	301 (77%)	70 (18%)	19 (5%)	2 19
All	All	780/784 (100%)	601 (77%)	140 (18%)	39 (5%)	2 19

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	132	HIS
1	A	288	ASP
1	A	381	GLY
1	B	51	THR
1	B	288	ASP
1	B	381	GLY
1	A	133	GLU
1	A	150	GLN
1	A	221	GLY
1	A	294	GLY
1	A	329	ALA
1	B	132	HIS
1	B	167	SER
1	B	221	GLY
1	B	294	GLY
1	B	329	ALA
1	A	157	GLY
1	A	199	MET
1	A	220	SER
1	A	289	LYS
1	B	199	MET
1	B	220	SER
1	B	269	GLN
1	A	255	GLU
1	B	20	TRP
1	B	240	ASN
1	A	240	ASN
1	B	157	GLY
1	B	185	PRO
1	A	4	VAL
1	A	191	PHE
1	B	150	GLN
1	A	330	PRO
1	A	334	PRO

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Mol	Chain	Res	Type
1	B	106	GLY
1	B	227	PRO
1	A	106	GLY
1	B	24	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	331/331 (100%)	294 (89%)	37 (11%)	6 27
1	B	331/331 (100%)	286 (86%)	45 (14%)	3 20
All	All	662/662 (100%)	580 (88%)	82 (12%)	4 23

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	27	HIS
1	A	33	THR
1	A	34	MET
1	A	52	GLN
1	A	56	LEU
1	A	57	ARG
1	A	58	LYS
1	A	65	ILE
1	A	66	THR
1	A	107	LEU
1	A	129	ILE
1	A	134	ASN
1	A	135	LEU
1	A	154	GLU
1	A	162	ILE
1	A	165	GLN
1	A	173	LEU
1	A	178	THR

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Mol	Chain	Res	Type
1	A	181	LEU
1	A	189	LEU
1	A	195	ILE
1	A	196	LEU
1	A	197	LEU
1	A	206	VAL
1	A	219	THR
1	A	276	ILE
1	A	285	LEU
1	A	292	LEU
1	A	306	LEU
1	A	319	LEU
1	A	328	ASP
1	A	330	PRO
1	A	349	LEU
1	A	357	THR
1	A	385	LEU
1	A	391	ARG
1	B	2	ARG
1	B	8	ASN
1	B	23	VAL
1	B	27	HIS
1	B	30	CYS
1	B	32	THR
1	B	36	LYS
1	B	52	GLN
1	B	55	THR
1	B	57	ARG
1	B	62	GLU
1	B	66	THR
1	B	73	ARG
1	B	86	GLN
1	B	87	ASP
1	B	115	THR
1	B	123	GLU
1	B	134	ASN
1	B	154	GLU
1	B	156	GLN
1	B	165	GLN
1	B	168	THR
1	B	170	GLU
1	B	173	LEU

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Mol	Chain	Res	Type
1	B	178	THR
1	B	181	LEU
1	B	186	ARG
1	B	192	ASN
1	B	206	VAL
1	B	208	ARG
1	B	219	THR
1	B	224	THR
1	B	237	THR
1	B	251	LEU
1	B	270	THR
1	B	292	LEU
1	B	303	THR
1	B	305	VAL
1	B	308	LYS
1	B	330	PRO
1	B	335	PHE
1	B	348	ARG
1	B	349	LEU
1	B	376	ILE
1	B	390	TYR

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	27	HIS
1	A	148	GLN
1	A	156	GLN
1	A	207	HIS
1	A	240	ASN
1	A	246	GLN
1	A	254	GLN
1	A	269	GLN
1	A	346	ASN
1	A	388	ASN
1	B	8	ASN
1	B	27	HIS
1	B	77	GLN
1	B	148	GLN
1	B	156	GLN
1	B	240	ASN
1	B	246	GLN

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Mol	Chain	Res	Type
1	B	254	GLN
1	B	314	GLN
1	B	346	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)

12 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	1,2	14,14,15	0.66	0	17,19,21	0.73	0
2	FUL	C	2	2	10,10,11	0.71	0	14,14,16	0.82	1 (7%)
3	NAG	D	1	1,3	14,14,15	0.50	0	17,19,21	0.71	0
3	NAG	D	2	3	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
3	BMA	D	3	3	11,11,12	0.51	0	15,15,17	1.08	2 (13%)
3	BMA	D	4	3	11,11,12	0.60	0	15,15,17	0.62	0
3	BMA	D	5	3	11,11,12	0.84	0	15,15,17	0.67	0
3	FUL	D	6	3	10,10,11	0.69	0	14,14,16	0.99	0
4	NAG	E	1	1,4	14,14,15	0.59	0	17,19,21	0.83	0
4	NAG	E	2	4	14,14,15	0.81	0	17,19,21	1.02	1 (5%)
4	MAN	E	3	4	11,11,12	0.69	0	15,15,17	1.26	2 (13%)
4	FUL	E	4	4	10,10,11	0.87	0	14,14,16	0.80	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	C	1	1,2	-	3/6/23/26	0/1/1/1
2	FUL	C	2	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	BMA	D	4	3	-	2/2/19/22	0/1/1/1
3	BMA	D	5	3	-	2/2/19/22	0/1/1/1
3	FUL	D	6	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	6/6/23/26	0/1/1/1
4	MAN	E	3	4	-	0/2/19/22	0/1/1/1
4	FUL	E	4	4	-	-	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	3	MAN	C1-C2-C3	3.47	113.94	109.67
4	E	2	NAG	O4-C4-C5	2.63	115.83	109.30
3	D	2	NAG	C4-C3-C2	2.48	114.66	111.02
3	D	3	BMA	C3-C4-C5	-2.47	105.84	110.24
2	C	2	FUL	C1-C2-C3	2.40	112.62	109.67
4	E	3	MAN	C1-O5-C5	2.28	115.28	112.19
3	D	3	BMA	O5-C5-C6	2.14	110.56	107.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	C1-C2-N2-C7
3	D	5	BMA	O5-C5-C6-O6
3	D	4	BMA	C4-C5-C6-O6
3	D	5	BMA	C4-C5-C6-O6
3	D	4	BMA	O5-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	O5-C5-C6-O6

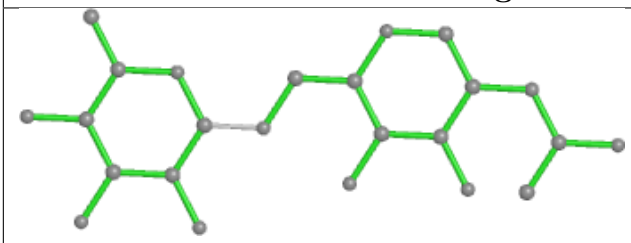
There are no ring outliers.

10 monomers are involved in 14 short contacts:

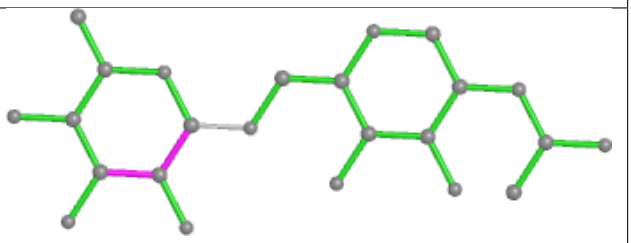
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	5	0
4	E	1	NAG	1	0
3	D	1	NAG	3	0
4	E	3	MAN	4	0
2	C	1	NAG	1	0
4	E	4	FUL	2	0
3	D	2	NAG	4	0
3	D	6	FUL	1	0
3	D	3	BMA	4	0
3	D	5	BMA	2	0

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

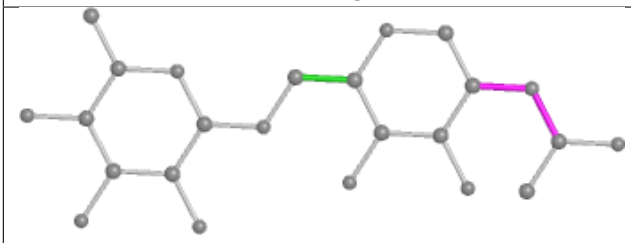
Oligosaccharide Chain C



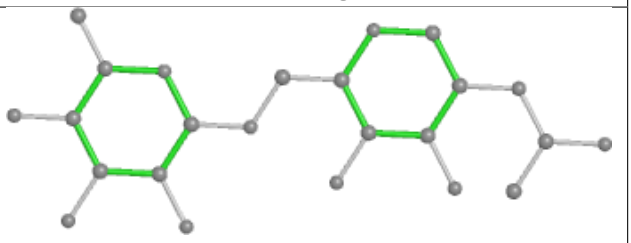
Bond lengths



Bond angles

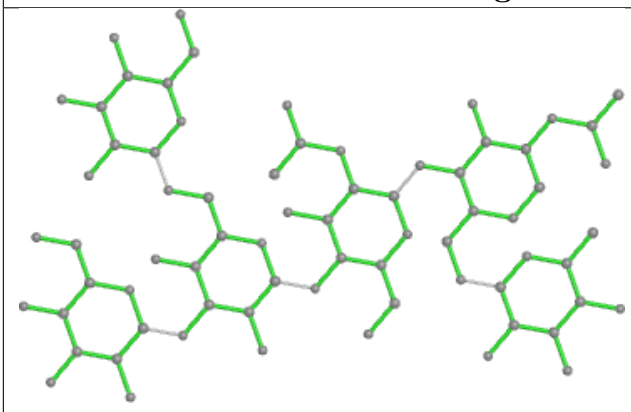


Torsions

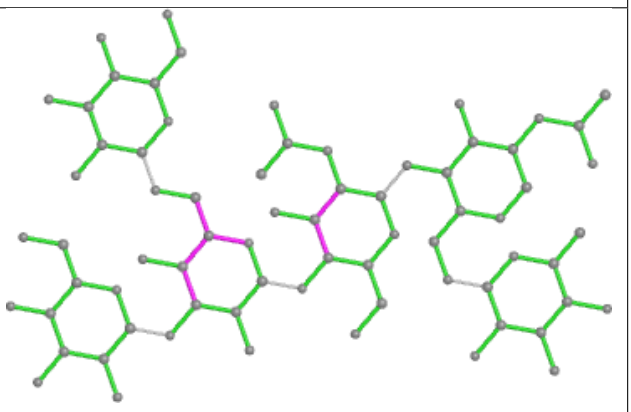


Rings

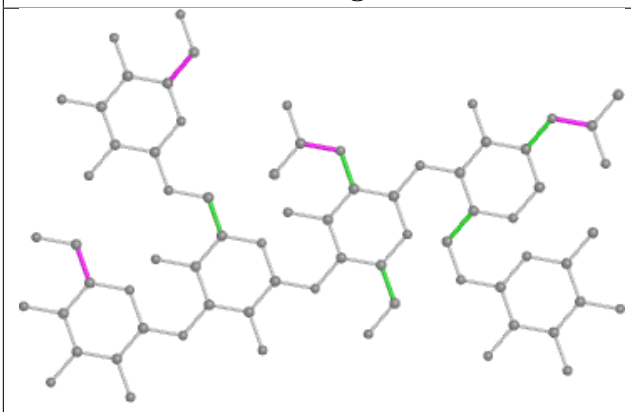
Oligosaccharide Chain D



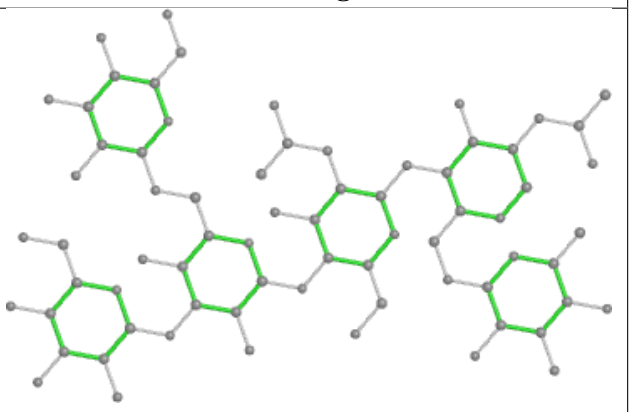
Bond lengths



Bond angles

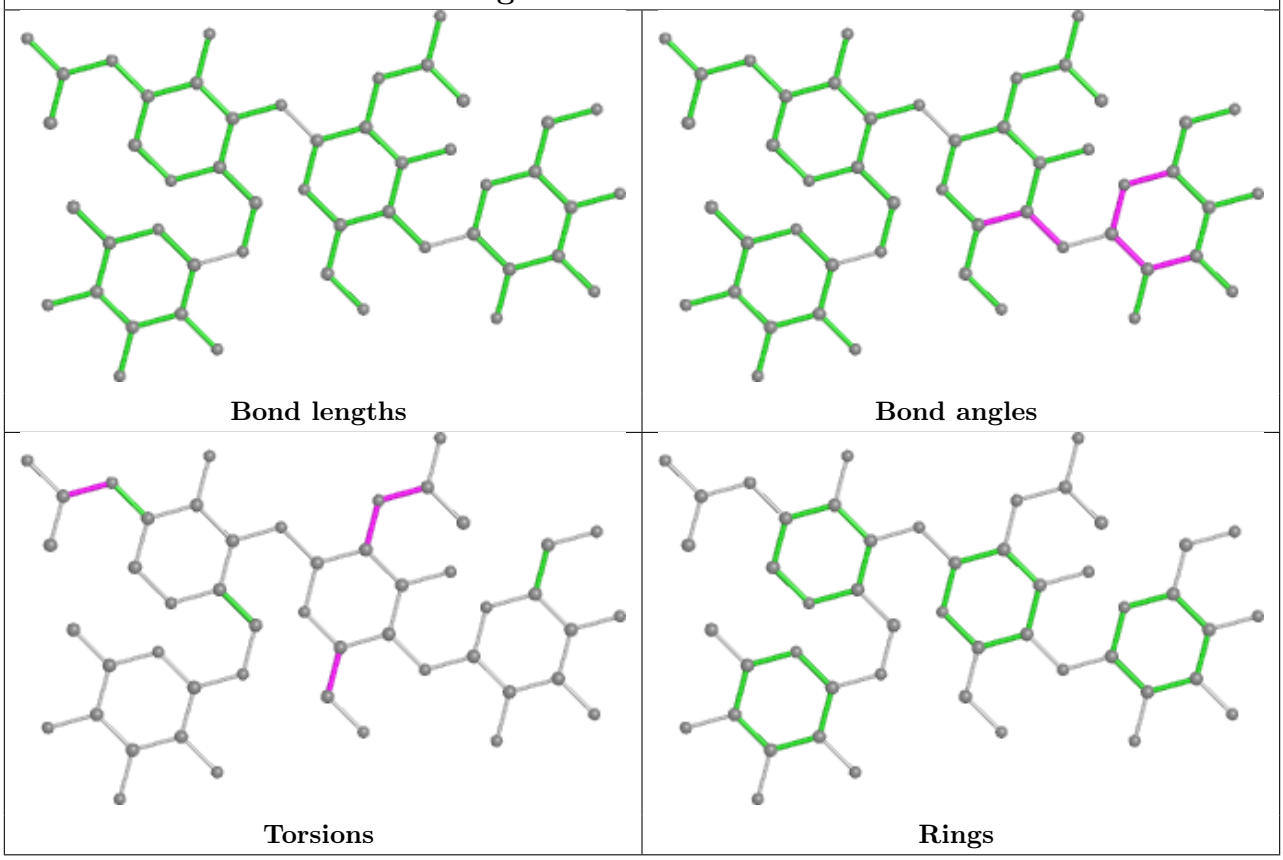


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	1393	1	14,14,15	0.63	0	17,19,21	0.66	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
5	NAG	B	1393	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1393	NAG	C8-C7-N2-C2
5	B	1393	NAG	O7-C7-N2-C2
5	B	1393	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	392/392 (100%)	-0.29	10 (2%)	56	49	40, 69, 119, 134	0
1	B	392/392 (100%)	-0.22	14 (3%)	42	38	41, 71, 121, 134	0
All	All	784/784 (100%)	-0.26	24 (3%)	49	43	40, 70, 120, 134	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	LYS	7.6
1	A	345	HIS	5.7
1	B	340	GLY	5.7
1	B	342	GLY	4.6
1	B	341	GLN	4.2
1	B	345	HIS	4.0
1	B	272	GLY	3.3
1	B	274	THR	3.1
1	B	273	GLY	3.1
1	B	339	ASP	3.1
1	B	344	ALA	3.0
1	A	272	GLY	2.9
1	B	223	THR	2.9
1	A	133	GLU	2.8
1	A	220	SER	2.7
1	A	224	THR	2.7
1	A	271	SER	2.6
1	B	224	THR	2.4
1	A	274	THR	2.3
1	B	382	ASP	2.3
1	A	344	ALA	2.3
1	B	271	SER	2.3
1	A	167	SER	2.1
1	A	273	GLY	2.0

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

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

6.3 Carbohydrates (i)

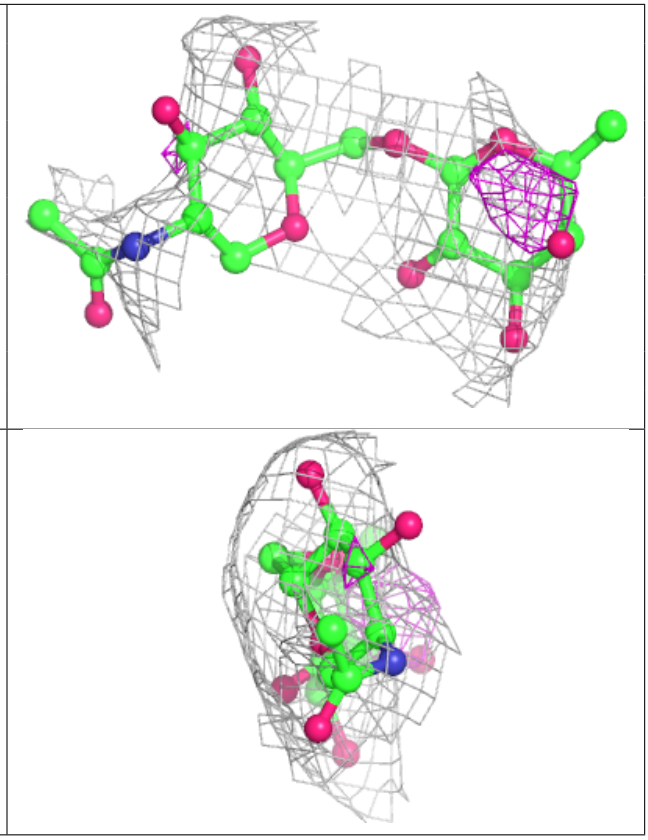
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	D	4	11/12	0.65	0.43	128,132,133,133	0
3	BMA	D	5	11/12	0.66	0.69	128,128,129,130	0
2	FUL	C	2	10/11	0.70	0.63	135,136,137,137	0
2	NAG	C	1	14/15	0.76	0.38	125,134,136,136	0
4	MAN	E	3	11/12	0.76	0.44	133,136,136,136	0
3	BMA	D	3	11/12	0.83	0.20	127,129,131,131	0
4	NAG	E	2	14/15	0.84	0.61	131,133,136,136	0
4	NAG	E	1	14/15	0.87	0.36	108,121,131,132	0
3	NAG	D	1	14/15	0.89	0.26	109,120,127,128	0
3	NAG	D	2	14/15	0.90	0.37	131,133,135,135	0
4	FUL	E	4	10/11	0.93	0.33	97,101,101,102	0
3	FUL	D	6	10/11	0.95	0.31	99,101,103,103	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.

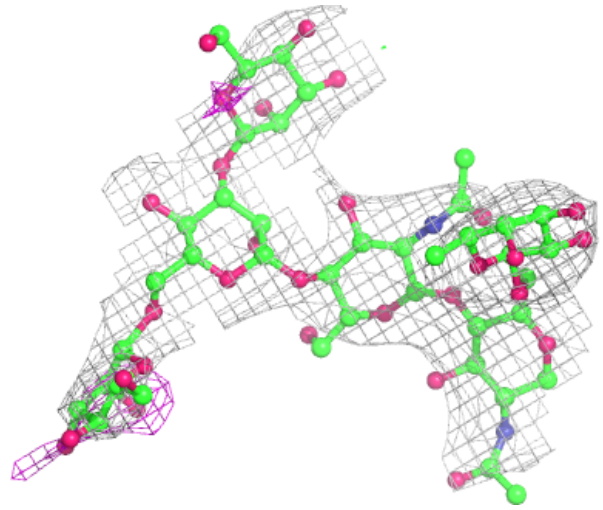
Electron density around Chain C:

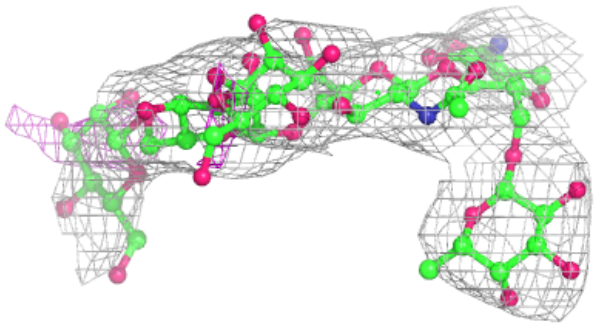
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

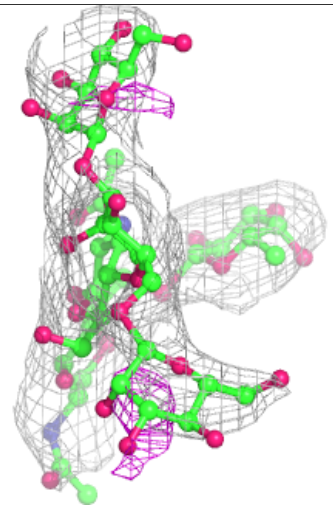


Electron density around Chain D:

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

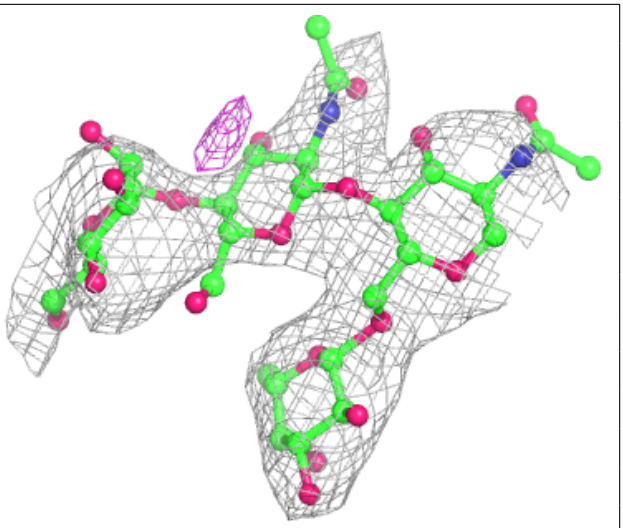


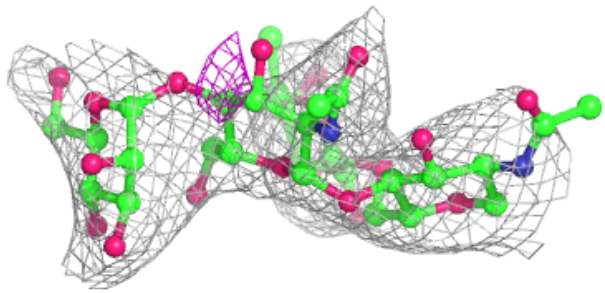


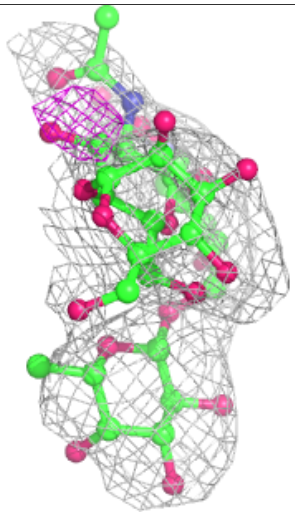


Electron density around Chain E:

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







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
5	NAG	B	1393	14/15	0.88	0.22	124,134,134,135	0

6.5 Other polymers (i)

There are no such residues in this entry.