Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 09:02 PM EST

PDB ID	:	3EHN
Title	:	BT1043 with N-acetyllactosamine
Authors	:	Smith, T.J.; Koropatkin, N.M.
Deposited on	:	2008-09-13
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

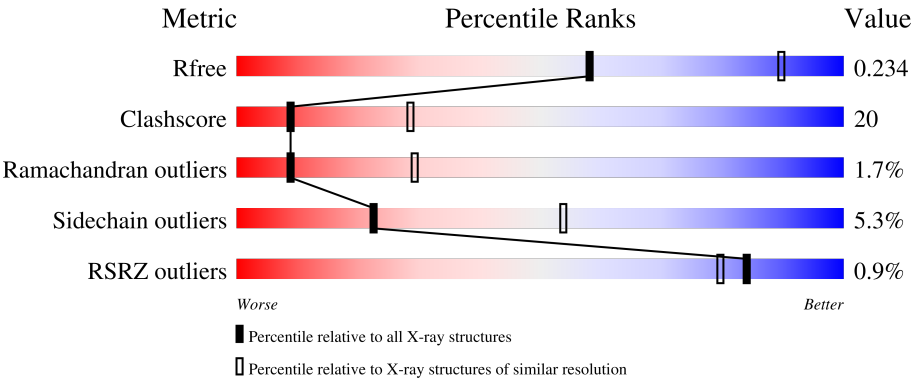
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	532	69% 25%
1	B	532	2% 51% 42%
2	C	2	50% 50%
2	D	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDG	C	1	X	-	-	-
2	NDG	D	1	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8275 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4058	2581	677	787	13			
1	B	512	Total	C	N	O	S	0	0	0
			4039	2571	674	781	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP Q8A8X4
A	16	ALA	-	expression tag	UNP Q8A8X4
A	17	SER	-	expression tag	UNP Q8A8X4
A	226	VAL	ALA	conflict	UNP Q8A8X4
B	15	MET	-	expression tag	UNP Q8A8X4
B	16	ALA	-	expression tag	UNP Q8A8X4
B	17	SER	-	expression tag	UNP Q8A8X4
B	226	VAL	ALA	conflict	UNP Q8A8X4

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	D	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is water.

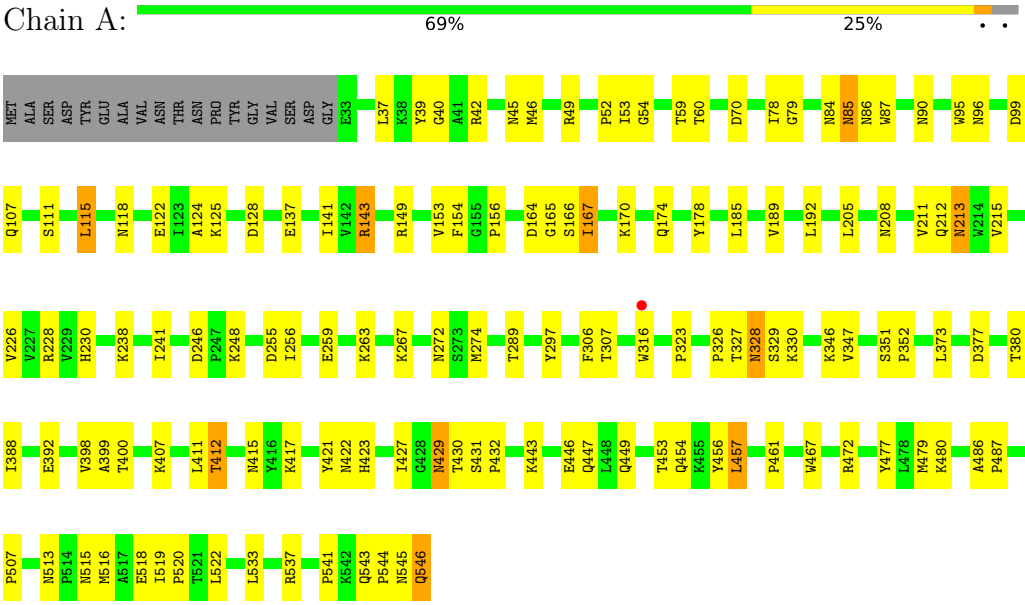
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	B	26	Total O 26 26	0	0

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.

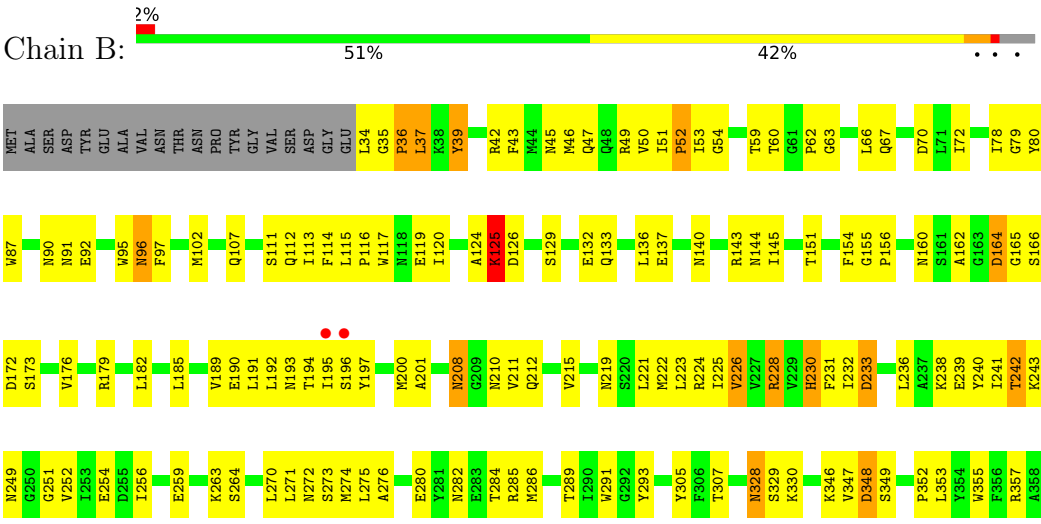
• Molecule 1: SusD homolog

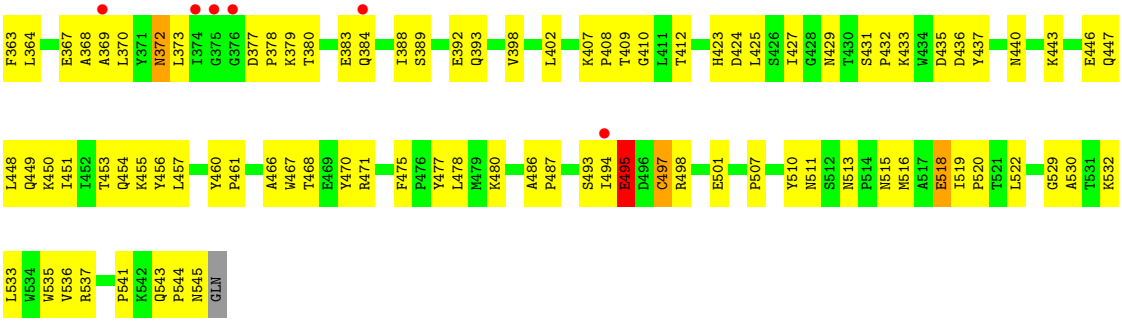
Chain A:



• Molecule 1: SusD homolog

Chain B:





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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	156.09Å 156.09Å 156.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.36 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.80) 97.1 (49.36-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.246 0.185 , 0.234	Depositor DCC
R_{free} test set	3215 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.047 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8275	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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

5.1 Standard geometry

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

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	0.39	0/4164	0.62	0/5659
1	B	0.35	0/4145	0.58	0/5635
All	All	0.37	0/8309	0.60	0/11294

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

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	4058	0	3906	104	0
1	B	4039	0	3892	222	0
2	C	26	0	20	2	0
2	D	26	0	21	0	0
3	A	100	0	0	4	0
3	B	26	0	0	1	0
All	All	8275	0	7839	325	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 20.

All (325) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:ILE:H	1:B:494:ILE:HD12	1.30	0.97
1:A:377:ASP:HB3	1:A:380:THR:HG23	1.47	0.96
1:A:59:THR:HG22	1:A:60:THR:H	1.29	0.95
1:A:494:ILE:HD12	1:A:494:ILE:H	1.28	0.93
1:B:85:ASN:HD22	1:B:86:ASN:H	1.17	0.93
1:B:282:ASN:HD22	1:B:285:ARG:HH22	1.09	0.92
1:A:59:THR:HG22	1:A:60:THR:N	1.89	0.86
1:B:454:GLN:HA	1:B:457:LEU:HD23	1.57	0.85
1:A:103:ASN:O	1:A:107:GLN:HG3	1.77	0.84
1:B:85:ASN:HD22	1:B:86:ASN:N	1.75	0.84
1:B:125:LYS:HG3	1:B:126:ASP:H	1.42	0.84
1:A:208:ASN:HD22	1:A:267:LYS:NZ	1.77	0.82
1:A:256:ILE:O	1:A:259:GLU:HG2	1.81	0.80
1:A:241:ILE:HD13	1:A:373:LEU:HB3	1.64	0.79
1:B:408:PRO:HG3	1:B:429:ASN:ND2	1.98	0.79
1:B:468:THR:HA	1:B:471:ARG:HH21	1.48	0.78
1:A:42:ARG:HG3	3:A:635:HOH:O	1.82	0.77
1:B:133:GLN:HB3	1:B:191:LEU:HD11	1.65	0.77
1:B:437:TYR:CE2	1:B:443:LYS:HG3	2.20	0.76
1:A:328:ASN:HD22	1:A:329:SER:H	1.33	0.76
1:A:386:ILE:HD11	1:A:454:GLN:HG3	1.66	0.76
1:B:185:LEU:O	1:B:189:VAL:HG23	1.88	0.74
1:B:226:VAL:HG11	1:B:241:ILE:HB	1.69	0.74
1:A:208:ASN:HD22	1:A:267:LYS:HZ3	1.36	0.73
1:A:384:GLN:HE21	1:A:384:GLN:HA	1.53	0.73
1:A:85:ASN:HD22	1:A:86:ASN:H	1.37	0.73
1:B:328:ASN:HD22	1:B:329:SER:H	1.36	0.72
1:B:516:MET:O	1:B:519:ILE:HG12	1.92	0.70
1:B:85:ASN:ND2	1:B:87:TRP:H	1.89	0.70
1:B:125:LYS:HG3	1:B:126:ASP:N	2.06	0.69
1:B:328:ASN:HD22	1:B:329:SER:N	1.90	0.69
1:A:137:GLU:O	1:A:141:ILE:HG13	1.93	0.69
1:A:519:ILE:HB	1:A:520:PRO:HD3	1.75	0.69
1:A:328:ASN:HD22	1:A:329:SER:N	1.91	0.69
1:B:222:MET:O	1:B:226:VAL:HG23	1.92	0.69
1:B:78:ILE:HG21	1:B:467:TRP:HA	1.75	0.68
1:B:494:ILE:H	1:B:494:ILE:CD1	2.04	0.68
1:A:486:ALA:HB3	1:A:487:PRO:HD3	1.76	0.68
1:A:388:ILE:O	1:A:392:GLU:HG3	1.93	0.68
1:B:494:ILE:HD12	1:B:494:ILE:N	2.08	0.67
1:B:107:GLN:HA	1:B:111:SER:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ILE:HG12	1:B:221:LEU:HD22	1.75	0.67
1:B:59:THR:HG22	1:B:60:THR:HG23	1.77	0.67
1:B:246:ASP:OD1	1:B:248:LYS:HG2	1.95	0.66
1:A:85:ASN:ND2	1:A:86:ASN:H	1.92	0.66
1:A:263:LYS:HB3	1:A:352:PRO:HB3	1.78	0.66
1:A:494:ILE:H	1:A:494:ILE:CD1	2.05	0.66
1:B:59:THR:HG22	1:B:60:THR:N	2.11	0.66
1:B:240:TYR:HA	1:B:243:LYS:HD3	1.77	0.66
1:B:182:LEU:HD13	1:B:236:LEU:HD11	1.77	0.65
1:A:411:LEU:O	1:A:422:ASN:HA	1.96	0.65
1:B:537:ARG:HH21	1:B:541:PRO:HG2	1.61	0.65
1:B:507:PRO:O	1:B:510:TYR:HB2	1.97	0.65
1:B:468:THR:CA	1:B:471:ARG:HH21	2.09	0.64
1:B:282:ASN:HD22	1:B:285:ARG:NH2	1.90	0.64
1:A:221:LEU:O	1:A:225:ILE:HG13	1.96	0.64
1:B:282:ASN:ND2	1:B:285:ARG:HH22	1.90	0.64
1:B:437:TYR:HA	1:B:446:GLU:OE2	1.98	0.63
1:B:453:THR:O	1:B:456:TYR:HB3	1.97	0.63
1:B:453:THR:O	1:B:457:LEU:HD22	1.99	0.63
1:A:95:TRP:N	1:A:95:TRP:CD1	2.67	0.63
1:A:472:ARG:O	1:A:537:ARG:HG2	1.99	0.63
1:B:256:ILE:O	1:B:259:GLU:HG2	1.99	0.63
1:B:84:ASN:O	1:B:85:ASN:HB2	1.97	0.62
1:B:201:ALA:HB1	1:B:208:ASN:ND2	2.14	0.62
1:B:532:LYS:HD2	1:B:536:VAL:HG11	1.81	0.62
1:B:275:LEU:HD11	1:B:349:SER:N	2.14	0.62
1:B:223:LEU:O	1:B:226:VAL:HB	1.99	0.62
1:B:236:LEU:O	1:B:239:GLU:HB3	2.00	0.62
1:B:433:LYS:HD3	1:B:436:ASP:HB2	1.80	0.62
1:A:443:LYS:O	1:A:447:GLN:HG3	2.00	0.61
1:B:284:THR:HG23	3:B:702:HOH:O	2.01	0.61
1:B:59:THR:HG22	1:B:60:THR:H	1.64	0.61
1:B:293:TYR:HE1	1:B:429:ASN:HD21	1.49	0.61
1:A:107:GLN:HA	1:A:111:SER:OG	2.00	0.60
1:B:369:ALA:O	1:B:378:PRO:HG3	2.01	0.60
1:B:443:LYS:O	1:B:447:GLN:HG3	2.01	0.60
1:B:125:LYS:CG	1:B:126:ASP:H	2.12	0.60
1:B:179:ARG:NH1	1:B:236:LEU:HD22	2.17	0.59
1:B:221:LEU:O	1:B:225:ILE:HG13	2.02	0.59
1:B:537:ARG:NH2	1:B:541:PRO:HG2	2.17	0.59
1:B:328:ASN:HD21	1:B:330:LYS:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ALA:HB3	1:B:487:PRO:HD3	1.83	0.59
1:A:185:LEU:O	1:A:189:VAL:HG23	2.02	0.59
1:A:494:ILE:HD12	1:A:494:ILE:N	2.10	0.59
1:A:238:LYS:HA	1:A:241:ILE:HG22	1.85	0.58
1:A:170:LYS:HE3	1:A:518:GLU:OE1	2.03	0.58
1:B:370:LEU:HD11	1:B:447:GLN:HB3	1.84	0.58
1:B:379:LYS:O	1:B:383:GLU:HG3	2.02	0.58
1:B:45:ASN:O	1:B:49:ARG:HG2	2.02	0.58
1:B:46:MET:CE	1:B:117:TRP:HB2	2.35	0.57
1:B:328:ASN:ND2	1:B:329:SER:N	2.52	0.57
1:B:85:ASN:ND2	1:B:86:ASN:N	2.49	0.57
1:A:398:VAL:HG13	1:A:399:ALA:N	2.20	0.57
1:B:191:LEU:HD23	1:B:191:LEU:O	2.06	0.56
1:A:328:ASN:ND2	1:A:329:SER:N	2.53	0.56
1:B:125:LYS:HE3	1:B:126:ASP:OD2	2.06	0.56
1:B:173:SER:HB3	1:B:522:LEU:HD22	1.88	0.56
1:A:85:ASN:HD22	1:A:86:ASN:N	2.03	0.56
1:B:195:ILE:HG22	1:B:196:SER:N	2.21	0.56
1:B:228:ARG:NH1	1:B:228:ARG:HB2	2.21	0.56
1:B:275:LEU:HD23	1:B:347:VAL:HG13	1.87	0.56
1:B:408:PRO:HG2	1:B:425:LEU:O	2.06	0.56
1:B:154:PHE:O	1:B:156:PRO:HD2	2.06	0.56
1:B:275:LEU:HD21	1:B:348:ASP:HA	1.88	0.55
1:B:468:THR:HA	1:B:471:ARG:NH2	2.19	0.55
1:B:95:TRP:CG	1:B:486:ALA:HB1	2.41	0.55
1:B:513:ASN:OD1	1:B:515:ASN:HB2	2.06	0.55
1:B:307:THR:CG2	1:B:346:LYS:HG2	2.37	0.55
1:B:328:ASN:ND2	1:B:330:LYS:H	2.05	0.55
1:B:532:LYS:HB3	1:B:536:VAL:HG21	1.88	0.55
1:A:189:VAL:HG13	1:A:215:VAL:HG13	1.87	0.55
1:B:113:ILE:O	1:B:116:PRO:HG2	2.07	0.55
1:B:179:ARG:HA	1:B:182:LEU:HD12	1.87	0.54
1:A:306:PHE:O	1:A:346:LYS:HE3	2.08	0.54
1:B:368:ALA:HB1	1:B:373:LEU:HB2	1.90	0.54
1:B:519:ILE:HB	1:B:520:PRO:HD3	1.88	0.54
1:A:39:TYR:OH	1:A:124:ALA:HB2	2.08	0.54
1:A:59:THR:CG2	1:A:60:THR:N	2.61	0.54
1:B:276:ALA:O	1:B:280:GLU:HB2	2.07	0.54
1:B:359:SER:HB3	1:B:388:ILE:HG22	1.88	0.54
1:B:448:LEU:HD23	1:B:537:ARG:HH12	1.72	0.54
1:A:78:ILE:HG21	1:A:467:TRP:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:GLU:HG3	1:B:530:ALA:O	2.07	0.54
1:B:66:LEU:HD22	1:B:273:SER:OG	2.07	0.54
1:B:224:ARG:NH1	1:B:360:GLU:OE1	2.42	0.53
1:B:78:ILE:CG2	1:B:467:TRP:HA	2.38	0.53
1:A:99:ASP:OD1	1:A:507:PRO:HD2	2.08	0.53
1:A:384:GLN:HA	1:A:384:GLN:NE2	2.22	0.53
1:B:45:ASN:HD22	1:B:116:PRO:HB3	1.73	0.53
1:A:208:ASN:ND2	1:A:267:LYS:NZ	2.54	0.53
1:B:232:ILE:HG22	1:B:232:ILE:O	2.09	0.53
1:A:84:ASN:O	1:A:85:ASN:HB2	2.08	0.53
1:A:400:THR:HG21	1:B:330:LYS:HE3	1.91	0.53
1:A:453:THR:O	1:A:456:TYR:HB3	2.08	0.52
1:B:407:LYS:HB3	1:B:408:PRO:HD2	1.92	0.52
1:B:478:LEU:O	1:B:498:ARG:NH1	2.43	0.52
1:A:85:ASN:ND2	1:A:86:ASN:N	2.56	0.52
1:B:431:SER:HB2	1:B:432:PRO:CD	2.40	0.52
1:B:248:LYS:HG3	1:B:249:ASN:ND2	2.25	0.52
1:B:167:ILE:HD13	1:B:167:ILE:C	2.30	0.51
1:A:167:ILE:C	1:A:167:ILE:HD13	2.31	0.51
1:A:407:LYS:HE3	1:A:429:ASN:O	2.10	0.51
1:A:516:MET:O	1:A:519:ILE:HG12	2.10	0.51
1:B:95:TRP:CD1	1:B:95:TRP:N	2.75	0.51
1:B:230:HIS:C	1:B:230:HIS:HD1	2.13	0.51
1:A:328:ASN:ND2	1:A:330:LYS:H	2.08	0.51
1:B:125:LYS:HB2	1:B:125:LYS:NZ	2.25	0.51
1:B:389:SER:O	1:B:393:GLN:HG2	2.10	0.51
1:B:91:ASN:HB2	1:B:92:GLU:OE1	2.10	0.51
1:B:211:VAL:O	1:B:215:VAL:HG23	2.10	0.51
1:B:370:LEU:C	1:B:372:ASN:H	2.13	0.51
1:B:388:ILE:O	1:B:392:GLU:HG3	2.11	0.51
1:B:447:GLN:O	1:B:451:ILE:HG13	2.11	0.51
1:B:537:ARG:HH21	1:B:541:PRO:CG	2.24	0.51
1:B:383:GLU:OE2	1:B:402:LEU:HD13	2.10	0.51
1:B:42:ARG:O	1:B:46:MET:HG3	2.11	0.50
1:B:433:LYS:HG2	1:B:435:ASP:H	1.77	0.50
1:A:95:TRP:N	1:A:95:TRP:HD1	2.08	0.50
1:B:448:LEU:CD2	1:B:537:ARG:HH12	2.25	0.50
1:B:498:ARG:HH11	1:B:498:ARG:HG3	1.76	0.50
1:A:79:GLY:HA3	1:A:289:THR:HB	1.93	0.50
1:B:223:LEU:HG	1:B:364:LEU:HD13	1.92	0.50
1:B:151:THR:O	1:B:155:GLY:HA2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:GLU:HG2	1:A:522:LEU:HG	1.94	0.49
1:B:409:THR:HG22	1:B:410:GLY:O	2.12	0.49
1:B:59:THR:CG2	1:B:60:THR:H	2.17	0.49
1:A:246:ASP:OD2	1:A:248:LYS:HE3	2.12	0.49
1:B:357:ARG:NH2	1:B:392:GLU:HB3	2.27	0.49
1:B:228:ARG:HD2	1:B:535:TRP:CD1	2.47	0.49
1:B:230:HIS:C	1:B:230:HIS:ND1	2.66	0.49
1:B:498:ARG:NH1	1:B:498:ARG:HG3	2.27	0.49
1:B:107:GLN:O	1:B:112:GLN:HB2	2.13	0.48
1:B:286:MET:HE3	1:B:291:TRP:HB2	1.95	0.48
1:B:533:LEU:HD12	1:B:535:TRP:CH2	2.48	0.48
1:A:46:MET:HE1	1:A:143:ARG:HB2	1.95	0.48
1:B:170:LYS:HE2	1:B:518:GLU:OE1	2.13	0.48
1:A:118:ASN:O	1:A:122:GLU:HG3	2.14	0.48
1:A:328:ASN:ND2	1:A:329:SER:H	2.07	0.48
1:B:78:ILE:CD1	1:B:466:ALA:HB3	2.42	0.48
1:B:125:LYS:CG	1:B:126:ASP:N	2.73	0.48
1:B:252:VAL:O	1:B:254:GLU:HG3	2.13	0.48
1:B:429:ASN:OD1	1:B:477:TYR:HD2	1.97	0.48
1:B:219:ASN:HB2	1:B:251:GLY:O	2.14	0.47
1:B:54:GLY:HA3	1:B:62:PRO:HG2	1.97	0.47
1:B:427:ILE:HD13	1:B:545:ASN:O	2.14	0.47
1:A:192:LEU:HD22	1:A:211:VAL:HG13	1.97	0.47
1:A:398:VAL:HG13	1:A:399:ALA:H	1.79	0.47
1:B:226:VAL:HG11	1:B:241:ILE:HD12	1.96	0.47
1:B:423:HIS:CD2	1:B:480:LYS:H	2.33	0.47
1:B:212:GLN:OE1	1:B:212:GLN:HA	2.15	0.47
1:B:368:ALA:O	1:B:372:ASN:N	2.48	0.47
1:B:192:LEU:HD22	1:B:211:VAL:HG13	1.97	0.47
1:B:248:LYS:NZ	1:B:249:ASN:HD21	2.12	0.47
1:B:79:GLY:HA3	1:B:289:THR:HB	1.97	0.47
1:B:226:VAL:CG1	1:B:241:ILE:HB	2.43	0.46
1:B:241:ILE:HG23	1:B:242:THR:N	2.31	0.46
1:A:246:ASP:OD1	1:A:248:LYS:HG2	2.15	0.46
1:B:36:PRO:O	1:B:37:LEU:HD12	2.16	0.46
1:B:172:ASP:HB3	1:B:176:VAL:HB	1.96	0.46
1:A:174:GLN:OE1	1:A:533:LEU:HB3	2.15	0.46
1:A:421:TYR:OH	1:A:479:MET:HB3	2.16	0.46
1:B:362:TYR:CE2	1:B:384:GLN:HG2	2.51	0.46
1:B:431:SER:HB2	1:B:432:PRO:HD2	1.98	0.46
1:B:446:GLU:O	1:B:450:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASN:HD22	1:A:430:THR:H	1.64	0.45
1:B:129:SER:O	1:B:133:GLN:HG2	2.16	0.45
1:B:189:VAL:HG12	1:B:193:ASN:HD21	1.80	0.45
1:B:189:VAL:HG12	1:B:193:ASN:ND2	2.31	0.45
1:A:213:ASN:HD22	1:A:213:ASN:HA	1.61	0.45
1:B:35:GLY:N	1:B:36:PRO:CD	2.79	0.45
1:B:238:LYS:HA	1:B:241:ILE:HG21	1.97	0.45
1:B:367:GLU:HG3	1:B:448:LEU:CD1	2.47	0.45
1:B:511:ASN:N	1:B:511:ASN:ND2	2.64	0.45
1:A:178:TYR:CD2	1:A:225:ILE:HG23	2.51	0.45
1:B:537:ARG:HH21	1:B:541:PRO:CD	2.30	0.45
1:B:477:TYR:CD1	1:B:543:GLN:HB2	2.51	0.45
1:B:228:ARG:HD2	1:B:535:TRP:CG	2.52	0.45
1:B:272:ASN:OD1	1:B:274:MET:HB2	2.17	0.45
1:B:347:VAL:HG22	1:B:348:ASP:N	2.31	0.45
1:B:449:GLN:HA	1:B:475:PHE:CD2	2.52	0.45
1:A:412:THR:HG23	1:A:415:ASN:HD22	1.81	0.45
1:B:43:PHE:O	1:B:47:GLN:HG3	2.16	0.45
1:A:297:TYR:CE2	1:A:432:PRO:HD3	2.53	0.44
1:B:111:SER:O	1:B:114:PHE:HB3	2.17	0.44
1:B:424:ASP:HB3	1:B:427:ILE:CD1	2.48	0.44
1:A:208:ASN:ND2	1:A:267:LYS:HZ1	2.16	0.44
1:B:42:ARG:HE	1:B:119:GLU:CD	2.20	0.44
1:B:230:HIS:HE1	1:B:231:PHE:CZ	2.34	0.44
1:B:543:GLN:HA	1:B:544:PRO:HD3	1.85	0.44
1:B:228:ARG:HB2	1:B:228:ARG:HH11	1.79	0.44
1:A:208:ASN:HD22	1:A:267:LYS:HZ1	1.62	0.44
1:B:51:ILE:HG22	1:B:353:LEU:HD13	2.00	0.44
1:B:63:GLY:HA2	1:B:273:SER:HB2	1.99	0.44
1:B:363:PHE:CD2	1:B:455:LYS:HA	2.52	0.44
1:A:377:ASP:HB3	1:A:380:THR:CG2	2.34	0.44
1:A:545:ASN:O	1:A:546:GLN:CB	2.65	0.44
1:B:493:SER:OG	1:B:495:GLU:HB2	2.18	0.44
1:B:46:MET:SD	1:B:120:ILE:HD12	2.58	0.43
1:B:238:LYS:HA	1:B:241:ILE:CG2	2.48	0.43
1:B:96:ASN:HD22	1:B:96:ASN:C	2.21	0.43
1:B:189:VAL:O	1:B:193:ASN:ND2	2.51	0.43
1:A:347:VAL:HG23	1:A:351:SER:CB	2.48	0.43
1:B:190:GLU:O	1:B:194:THR:HG23	2.18	0.43
1:B:377:ASP:HB3	1:B:380:THR:OG1	2.18	0.43
1:B:384:GLN:HA	1:B:384:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HH12	2:C:1:NDG:H8C3	1.83	0.43
1:B:230:HIS:ND1	1:B:230:HIS:O	2.50	0.43
1:B:240:TYR:HA	1:B:243:LYS:CD	2.46	0.43
1:B:34:LEU:HD11	1:B:132:GLU:OE2	2.18	0.43
1:B:264:SER:HB2	1:B:270:LEU:O	2.18	0.43
1:B:470:TYR:HA	1:B:475:PHE:O	2.19	0.43
1:A:238:LYS:HA	1:A:241:ILE:CG2	2.49	0.43
1:A:431:SER:HB2	1:A:432:PRO:CD	2.49	0.43
1:B:228:ARG:O	1:B:228:ARG:HG3	2.18	0.43
1:B:477:TYR:CE1	1:B:543:GLN:HB2	2.54	0.43
1:B:533:LEU:HD12	1:B:535:TRP:CZ2	2.53	0.43
1:A:111:SER:O	1:A:115:LEU:HD22	2.19	0.43
1:B:271:LEU:O	1:B:272:ASN:C	2.56	0.43
1:B:305:TYR:HE1	1:B:393:GLN:CD	2.22	0.43
1:B:307:THR:HG22	1:B:346:LYS:HG2	2.00	0.43
1:A:45:ASN:O	1:A:49:ARG:HG2	2.18	0.43
1:A:477:TYR:CG	1:A:543:GLN:HB2	2.54	0.43
1:B:39:TYR:CD2	1:B:120:ILE:HG23	2.54	0.43
1:B:67:GLN:CG	1:B:72:ILE:HG23	2.49	0.42
1:A:453:THR:O	1:A:457:LEU:HD22	2.18	0.42
1:B:95:TRP:N	1:B:95:TRP:HD1	2.16	0.42
1:A:85:ASN:ND2	1:A:87:TRP:H	2.17	0.42
1:A:149:ARG:O	1:A:153:VAL:HG23	2.19	0.42
1:A:272:ASN:OD1	1:A:274:MET:HB2	2.19	0.42
1:A:446:GLU:O	1:A:449:GLN:HB3	2.20	0.42
1:B:160:ASN:C	1:B:162:ALA:H	2.22	0.42
1:B:224:ARG:HH11	1:B:360:GLU:CD	2.22	0.42
1:A:513:ASN:OD1	1:A:515:ASN:HB2	2.20	0.42
1:B:195:ILE:HG23	1:B:197:TYR:CE1	2.54	0.42
1:B:435:ASP:HA	1:B:437:TYR:HE1	1.84	0.42
1:A:101:ARG:NH1	2:C:1:NDG:H8C3	2.35	0.42
1:A:417:LYS:H	1:A:417:LYS:HG2	1.69	0.42
1:B:96:ASN:C	1:B:96:ASN:ND2	2.72	0.42
1:B:238:LYS:C	1:B:241:ILE:HG22	2.40	0.42
1:A:53:ILE:HG13	1:A:54:GLY:N	2.34	0.42
1:A:154:PHE:HB3	1:A:505:PHE:CZ	2.54	0.42
1:B:145:ILE:CG1	1:B:221:LEU:HD22	2.48	0.42
1:A:537:ARG:HD2	3:A:673:HOH:O	2.19	0.42
1:B:53:ILE:CD1	1:B:272:ASN:HA	2.50	0.42
1:B:46:MET:HE1	1:B:117:TRP:HB2	2.01	0.42
1:B:164:ASP:C	1:B:166:SER:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:CG2	1:A:467:TRP:HA	2.50	0.41
1:B:293:TYR:CE2	1:B:425:LEU:HD21	2.54	0.41
1:B:398:VAL:O	1:B:402:LEU:HG	2.19	0.41
1:A:156:PRO:HD3	3:A:618:HOH:O	2.21	0.41
1:B:85:ASN:ND2	1:B:86:ASN:H	1.98	0.41
1:B:95:TRP:CD2	1:B:486:ALA:HB1	2.55	0.41
1:B:97:PHE:HB3	1:B:102:MET:SD	2.60	0.41
1:B:136:LEU:O	1:B:140:ASN:ND2	2.53	0.41
1:A:537:ARG:NH2	1:A:541:PRO:CD	2.83	0.41
1:B:50:VAL:HG21	1:B:355:TRP:CZ2	2.55	0.41
1:B:140:ASN:O	1:B:144:ASN:ND2	2.53	0.41
1:B:407:LYS:N	1:B:407:LYS:HD2	2.36	0.41
1:B:124:ALA:HB3	1:B:136:LEU:HB2	2.03	0.41
1:B:78:ILE:HG21	1:B:467:TRP:CA	2.48	0.41
1:B:460:TYR:HA	1:B:461:PRO:HA	1.79	0.41
1:A:412:THR:HG23	1:A:415:ASN:ND2	2.36	0.41
1:A:545:ASN:O	1:A:546:GLN:HB2	2.20	0.41
1:B:124:ALA:O	1:B:125:LYS:C	2.57	0.41
1:A:326:PRO:O	1:A:327:THR:C	2.59	0.41
1:A:423:HIS:CD2	1:A:480:LYS:H	2.38	0.41
1:B:192:LEU:HD22	1:B:211:VAL:CG1	2.51	0.41
1:A:223:LEU:O	1:A:226:VAL:HG22	2.21	0.41
1:B:263:LYS:HB3	1:B:352:PRO:HB3	2.02	0.41
1:B:433:LYS:HE2	1:B:435:ASP:HB2	2.02	0.41
1:B:501:GLU:HB2	1:B:529:GLY:O	2.20	0.41
1:A:46:MET:CE	1:A:143:ARG:HB2	2.51	0.41
1:B:114:PHE:O	1:B:115:LEU:C	2.59	0.41
1:B:232:ILE:O	1:B:233:ASP:HB2	2.20	0.40
1:A:205:LEU:HD22	3:A:604:HOH:O	2.21	0.40
1:A:307:THR:HG22	1:A:346:LYS:HG2	2.03	0.40
1:B:115:LEU:H	1:B:115:LEU:HD22	1.87	0.40
1:B:137:GLU:O	1:B:140:ASN:HB2	2.22	0.40
1:B:226:VAL:HG11	1:B:241:ILE:CB	2.47	0.40
1:B:179:ARG:HH11	1:B:179:ARG:HG2	1.87	0.40
1:A:223:LEU:HA	1:A:226:VAL:HG22	2.04	0.40
1:A:164:ASP:C	1:A:166:SER:H	2.24	0.40
1:A:543:GLN:HA	1:A:544:PRO:HD3	1.91	0.40
1:B:42:ARG:HE	1:B:119:GLU:HB3	1.86	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	512/532 (96%)	476 (93%)	31 (6%)	5 (1%)	15 44
1	B	510/532 (96%)	442 (87%)	56 (11%)	12 (2%)	6 20
All	All	1022/1064 (96%)	918 (90%)	87 (8%)	17 (2%)	9 29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	ASN
1	B	372	ASN
1	A	40	GLY
1	B	52	PRO
1	B	125	LYS
1	B	233	ASP
1	A	52	PRO
1	B	210	ASN
1	B	497	CYS
1	A	165	GLY
1	A	316	TRP
1	B	495	GLU
1	B	200	MET
1	A	427	ILE
1	B	36	PRO
1	B	165	GLY
1	B	226	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	433/448 (97%)	410 (95%)	23 (5%)	22 54
1	B	431/448 (96%)	408 (95%)	23 (5%)	22 54
All	All	864/896 (96%)	818 (95%)	46 (5%)	22 54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	70	ASP
1	A	85	ASN
1	A	90	ASN
1	A	96	ASN
1	A	115	LEU
1	A	125	LYS
1	A	128	ASP
1	A	143	ARG
1	A	167	ILE
1	A	212	GLN
1	A	213	ASN
1	A	228	ARG
1	A	230	HIS
1	A	255	ASP
1	A	323	PRO
1	A	328	ASN
1	A	412	THR
1	A	429	ASN
1	A	457	LEU
1	A	461	PRO
1	A	495	GLU
1	A	546	GLN
1	B	37	LEU
1	B	39	TYR
1	B	52	PRO
1	B	70	ASP
1	B	80	TYR
1	B	85	ASN
1	B	90	ASN
1	B	96	ASN
1	B	125	LYS
1	B	143	ARG
1	B	164	ASP

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Mol	Chain	Res	Type
1	B	167	ILE
1	B	208	ASN
1	B	228	ARG
1	B	230	HIS
1	B	242	THR
1	B	328	ASN
1	B	348	ASP
1	B	412	THR
1	B	440	ASN
1	B	495	GLU
1	B	497	CYS
1	B	518	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	85	ASN
1	A	96	ASN
1	A	107	GLN
1	A	112	GLN
1	A	160	ASN
1	A	208	ASN
1	A	213	ASN
1	A	249	ASN
1	A	282	ASN
1	A	328	ASN
1	A	384	GLN
1	A	387	ASN
1	A	391	GLN
1	A	415	ASN
1	A	423	HIS
1	A	429	ASN
1	A	511	ASN
1	A	515	ASN
1	B	48	GLN
1	B	64	ASN
1	B	85	ASN
1	B	90	ASN
1	B	96	ASN
1	B	112	GLN
1	B	133	GLN

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Mol	Chain	Res	Type
1	B	193	ASN
1	B	202	GLN
1	B	208	ASN
1	B	213	ASN
1	B	249	ASN
1	B	282	ASN
1	B	328	ASN
1	B	384	GLN
1	B	423	HIS
1	B	429	ASN
1	B	511	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	NDG	C	1	2	15,15,15	2.04	3 (20%)	21,21,21	3.09	10 (47%)
2	GAL	C	2	2	11,11,12	1.23	1 (9%)	15,15,17	0.92	1 (6%)
2	NDG	D	1	2	15,15,15	2.01	4 (26%)	21,21,21	3.16	10 (47%)
2	GAL	D	2	2	11,11,12	1.02	0	15,15,17	0.90	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	NDG	C	1	2	1/1/6/7	3/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	NDG	D	1	2	1/1/6/7	3/6/26/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NDG	C2-N2	-6.17	1.36	1.45
2	C	1	NDG	C2-N2	-5.91	1.36	1.45
2	C	1	NDG	O4-C4	3.10	1.50	1.43
2	C	1	NDG	C4-C5	2.82	1.59	1.53
2	D	1	NDG	C6-C5	2.62	1.60	1.51
2	C	2	GAL	O5-C1	2.56	1.47	1.43
2	D	1	NDG	C4-C5	2.05	1.57	1.53
2	D	1	NDG	O5-C5	2.01	1.49	1.44

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NDG	O5-C1-C2	6.62	116.17	109.52
2	C	1	NDG	O5-C1-C2	6.59	116.14	109.52
2	C	1	NDG	C2-N2-C7	6.08	137.96	123.18
2	D	1	NDG	O4-C4-C3	5.85	123.86	110.35
2	D	1	NDG	C2-N2-C7	5.42	136.35	123.18
2	D	1	NDG	O5-C5-C4	4.61	118.07	109.69
2	C	1	NDG	C1-C2-C3	-4.60	104.28	110.54
2	C	1	NDG	O5-C5-C6	4.44	117.47	106.44
2	C	1	NDG	O1-C1-C2	4.03	117.59	109.22
2	D	1	NDG	O1-C1-C2	3.97	117.46	109.22
2	D	1	NDG	C1-C2-C3	-3.92	105.20	110.54
2	C	1	NDG	O4-C4-C3	3.55	118.56	110.35
2	C	1	NDG	O3-C3-C2	3.39	116.50	109.66
2	D	1	NDG	C8-C7-N2	3.38	121.82	116.10
2	D	1	NDG	O3-C3-C2	3.16	116.03	109.66
2	C	1	NDG	O5-C5-C4	3.13	115.38	109.69
2	C	1	NDG	C8-C7-N2	2.97	121.14	116.10
2	D	1	NDG	O7-C7-N2	-2.87	116.67	121.95
2	C	1	NDG	O7-C7-N2	-2.72	116.96	121.95
2	D	1	NDG	O5-C5-C6	2.50	112.65	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GAL	C6-C5-C4	-2.04	108.22	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NDG	C1
2	D	1	NDG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NDG	C8-C7-N2-C2
2	C	1	NDG	O7-C7-N2-C2
2	D	1	NDG	C8-C7-N2-C2
2	D	1	NDG	O7-C7-N2-C2
2	C	1	NDG	O5-C5-C6-O6
2	D	1	NDG	O5-C5-C6-O6

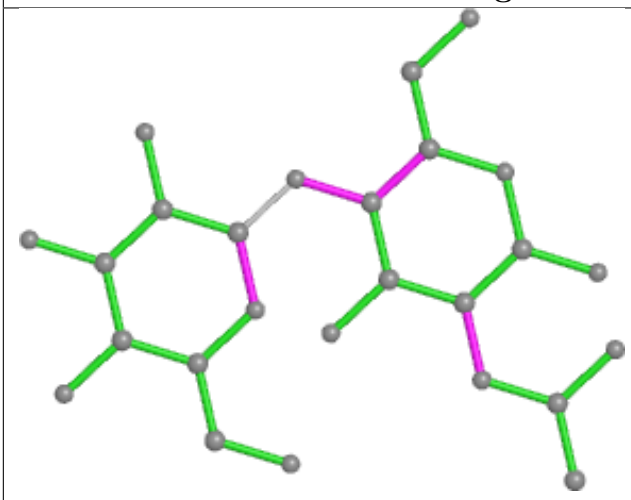
There are no ring outliers.

1 monomer is involved in 2 short contacts:

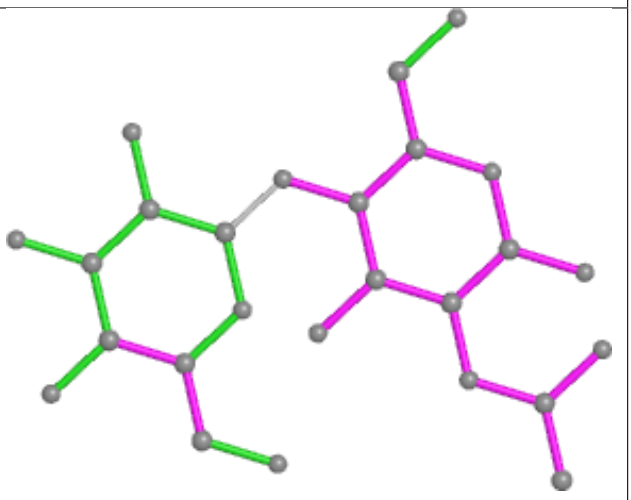
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NDG	2	0

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

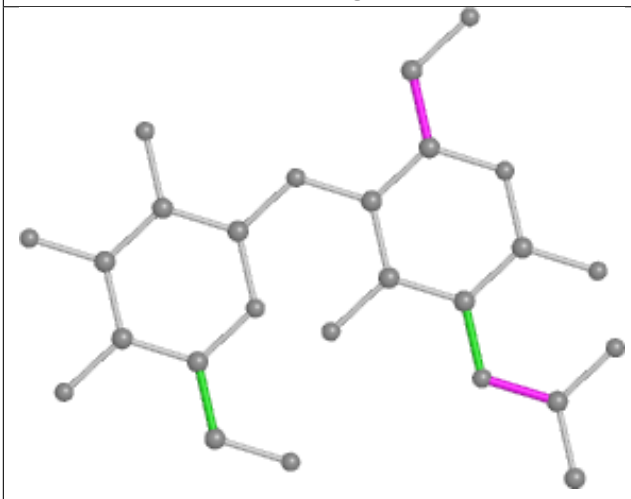
Oligosaccharide Chain C



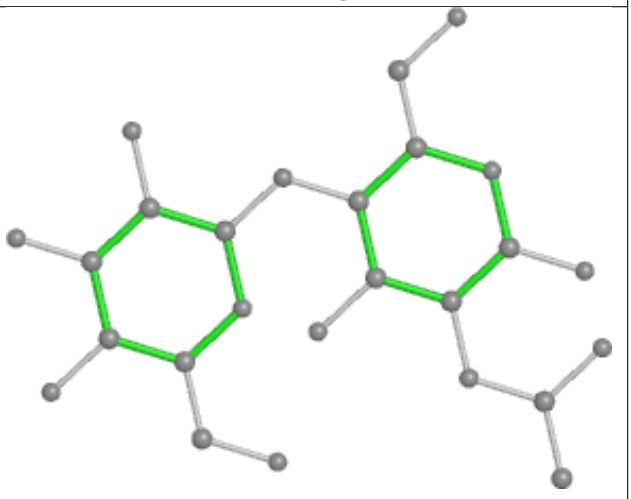
Bond lengths



Bond angles

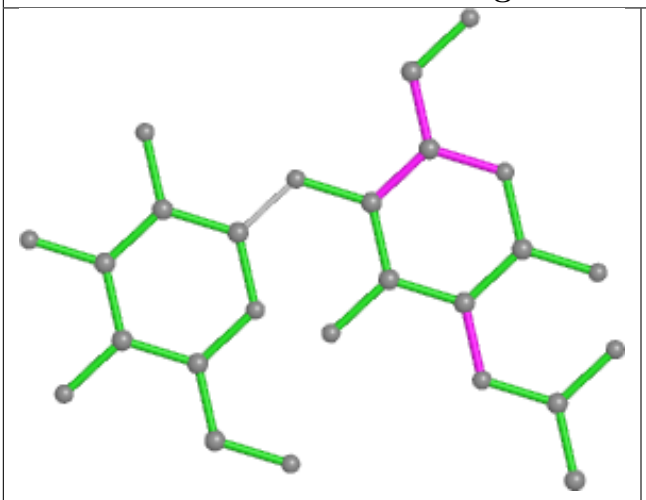


Torsions

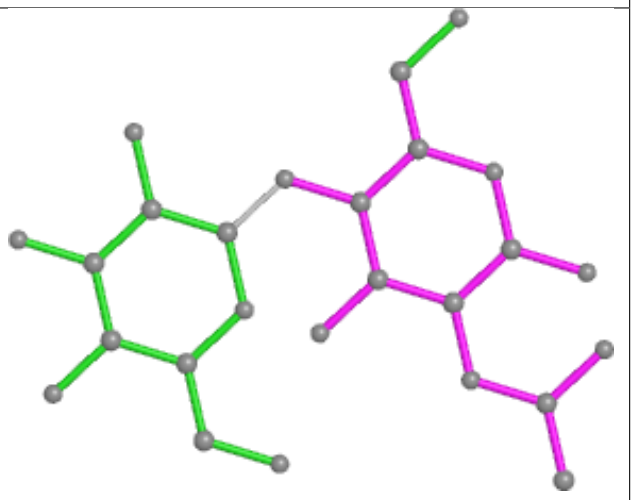


Rings

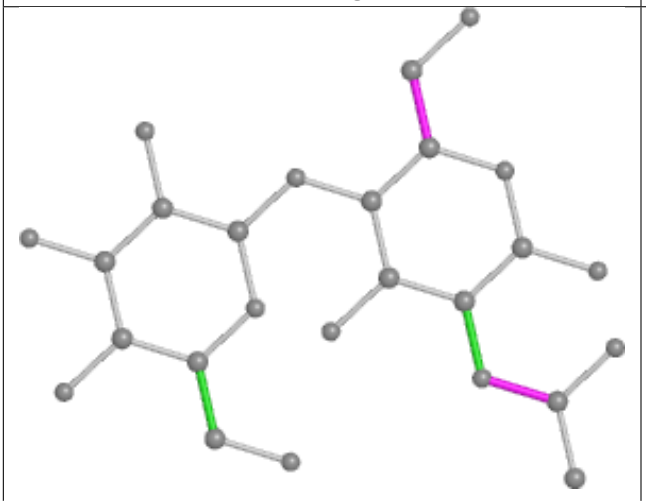
Oligosaccharide Chain D



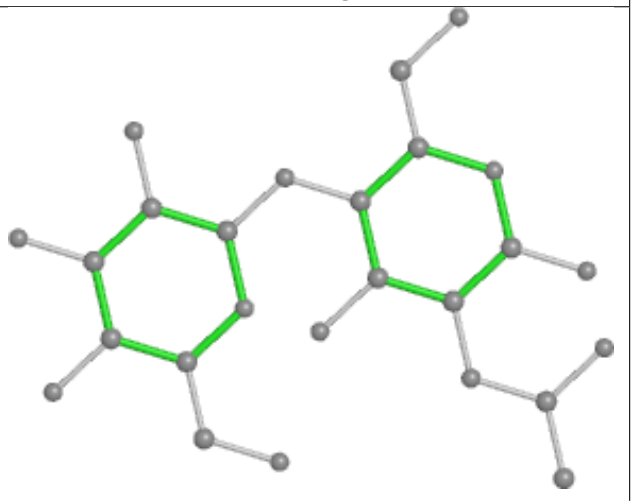
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	514/532 (96%)	-0.63	1 (0%)	95	94	9, 22, 44, 72	0
1	B	512/532 (96%)	-0.12	8 (1%)	72	66	26, 52, 66, 72	0
All	All	1026/1064 (96%)	-0.38	9 (0%)	84	80	9, 37, 64, 72	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	ALA	3.6
1	A	316	TRP	3.3
1	B	375	GLY	3.1
1	B	376	GLY	3.0
1	B	195	ILE	2.7
1	B	494	ILE	2.7
1	B	196	SER	2.3
1	B	374	ILE	2.2
1	B	384	GLN	2.2

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

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

6.3 Carbohydrates

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, 95^{th} 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	GAL	D	2	11/12	0.85	0.22	55,59,64,64	0

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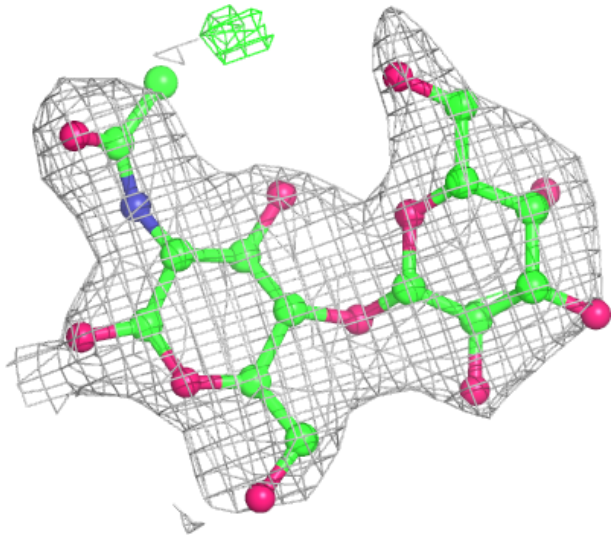
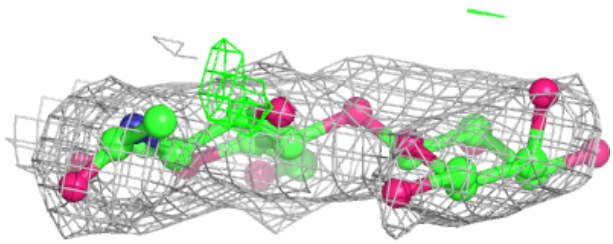
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NDG	D	1	15/15	0.90	0.24	45,50,54,58	0
2	GAL	C	2	11/12	0.92	0.22	44,46,47,48	0
2	NDG	C	1	15/15	0.94	0.20	27,30,34,39	0

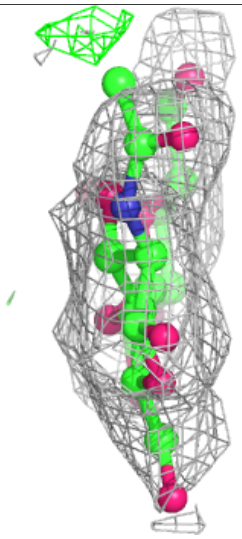
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

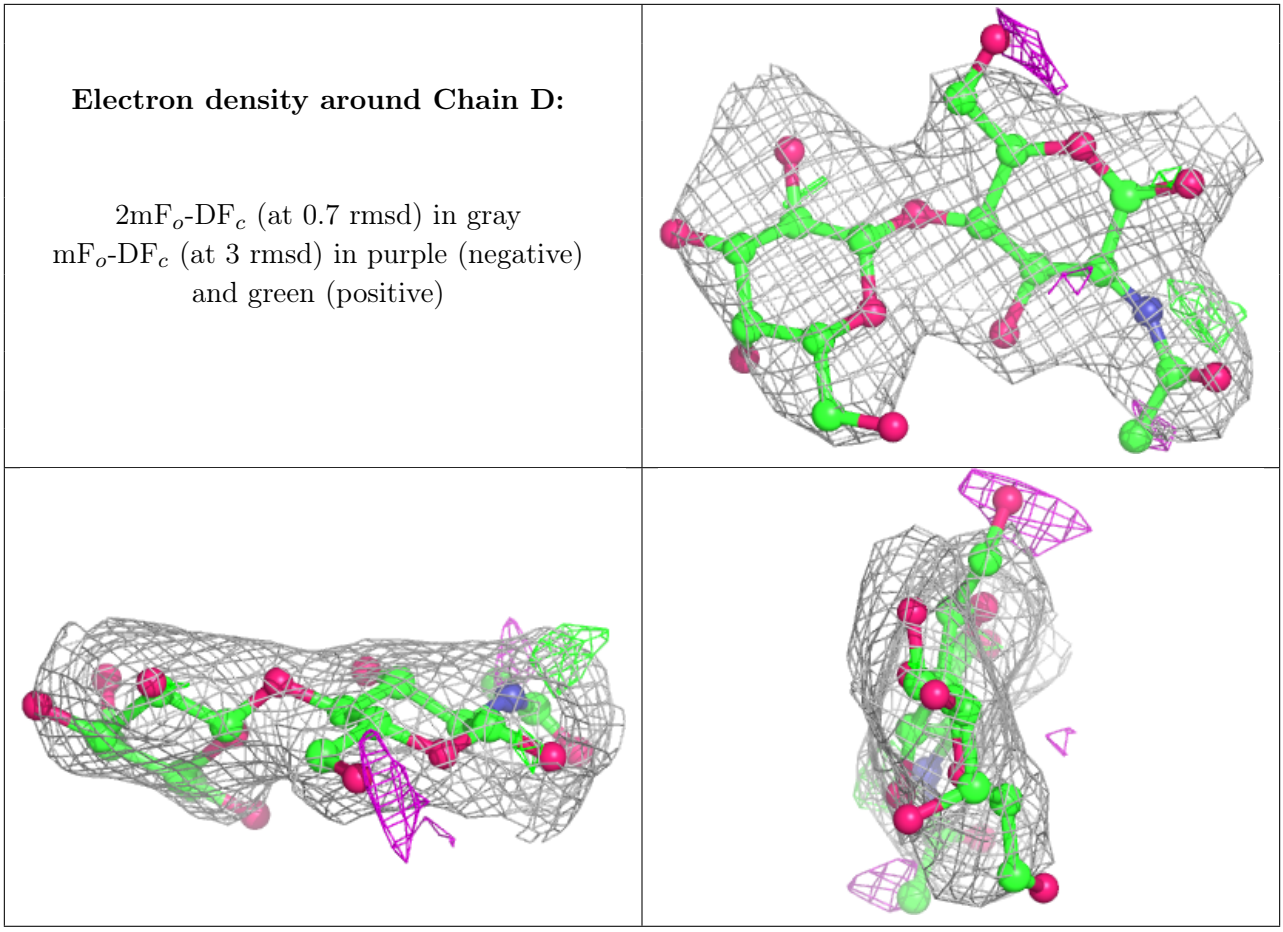






Electron density around Chain D:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.