Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 08:34 AM EDT

PDB ID	:	1M6B
Title	:	Structure of the HER3 (ERBB3) Extracellular Domain
Authors	:	Leahy, D.J.; Cho, H.-S.
Deposited on	:	2002-07-15
Resolution	:	2.60 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 following versions of software and data (see references (i)) were used in the production of this report:

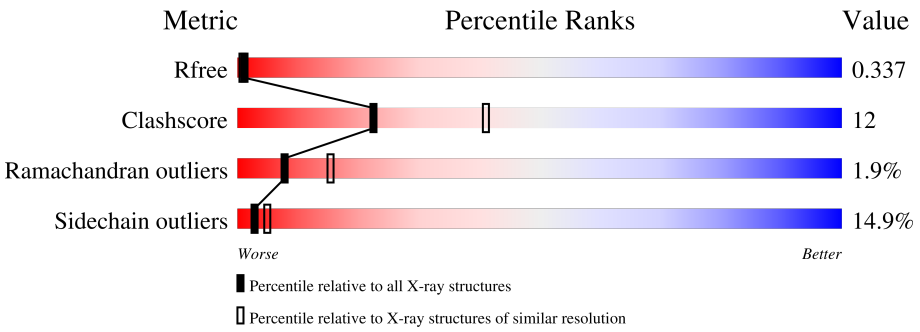
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Mol	Chain	Length	Quality of chain
1	A	621	58% 25% 5% 12%
1	B	621	64% 24% 5% • 6%
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
3	NAG	A	626	X	-	-	-
3	NAG	A	628	X	-	-	-
3	NAG	B	626	X	-	-	-
3	NAG	B	627	X	-	-	-
3	NAG	B	628	X	-	-	-
4	SO4	B	5001	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9012 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 Receptor protein-tyrosine kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4206	2603	765	784	54	0	0	0
1	B	584	4478	2766	813	840	59	0	0	0

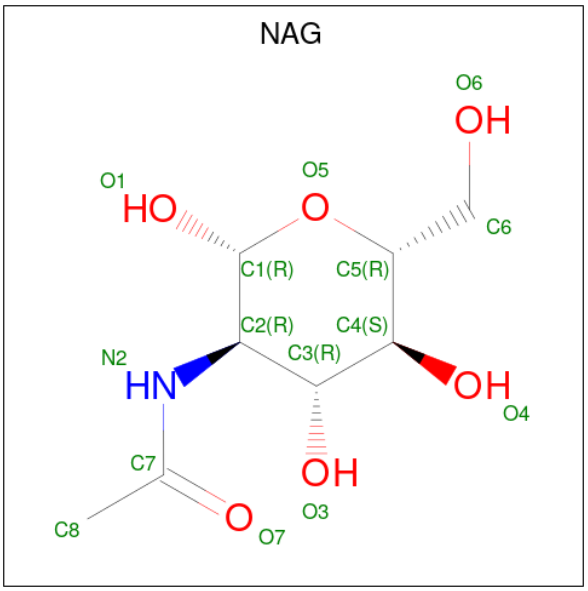
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	VAL	ILE	engineered mutation	UNP P21860
B	61	VAL	ILE	engineered mutation	UNP P21860

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

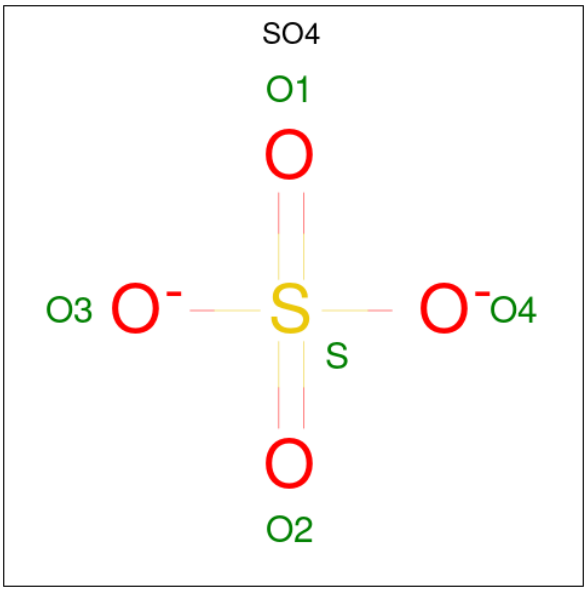
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

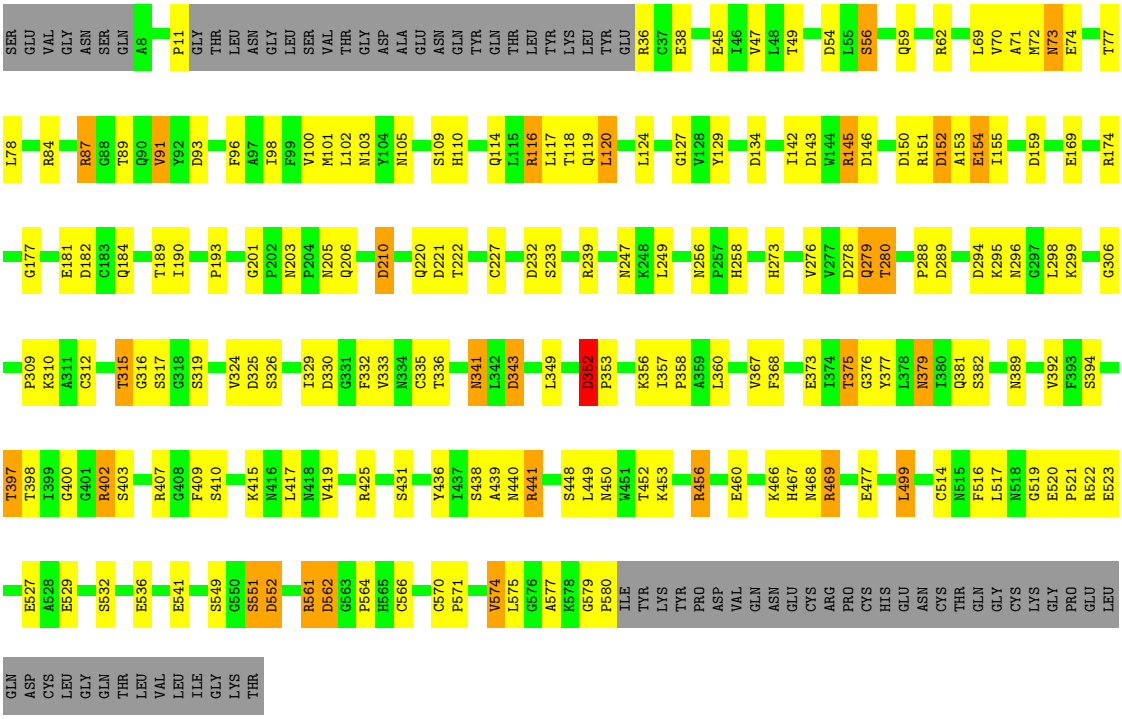
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	20	Total O 20 20	0	0
5	B	65	Total O 65 65	0	0

3 Residue-property plots (i)

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

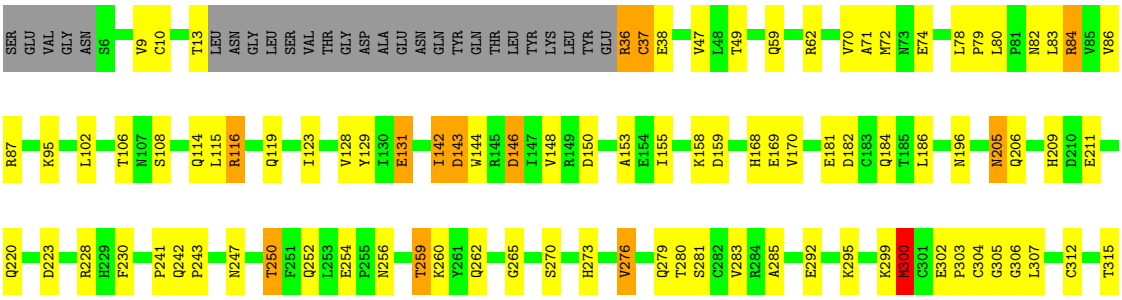
• Molecule 1: Receptor protein-tyrosine kinase erbB-3

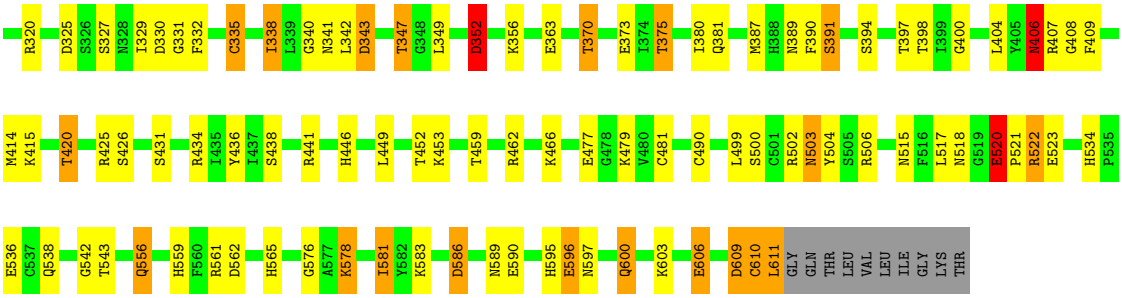
Chain A: 58% 25% 5% 12%



• Molecule 1: Receptor protein-tyrosine kinase erbB-3

Chain B: 64% 24% 5% • 6%





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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	236.26Å 49.62Å 190.86Å 90.00° 125.56° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 28.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 90.7 (28.74-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.235 , 0.294 0.299 , 0.337	Depositor DCC
R_{free} test set	2754 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 30.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9012	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: NAG, SO4

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	0.56	0/4308	0.84	15/5845 (0.3%)
1	B	0.62	1/4586 (0.0%)	0.86	8/6222 (0.1%)
All	All	0.59	1/8894 (0.0%)	0.85	23/12067 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	MET	SD-CE	5.39	2.08	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	221	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	146	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	143	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	325	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	232	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	609	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	143	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	325	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	146	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	352	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	343	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	93	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	134	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	210	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	289	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	159	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	152	ASP	CB-CG-OD2	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	343	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	159	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	278	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	562	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4206	0	3996	79	0
1	B	4478	0	4242	123	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	98	0	91	0	0
3	B	84	0	78	2	0
4	B	5	0	0	4	0
5	A	20	0	0	3	0
5	B	65	0	0	7	0
All	All	9012	0	8457	202	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 12.

All (202) 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:300:MET:CE	1:B:300:MET:SD	2.08	1.42
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.11	1.11
1:B:335:CYS:O	1:B:370:THR:HG22	1.56	1.03
1:B:452:THR:HG22	1:B:459:THR:HG21	1.42	1.00
1:B:578:LYS:HE2	1:B:578:LYS:H	1.31	0.96
1:B:247:ASN:ND2	5:B:1072:HOH:O	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:GLU:HB2	1:B:521:PRO:CD	2.00	0.90
1:B:452:THR:CG2	1:B:459:THR:HG21	2.03	0.87
1:B:168:HIS:HD2	1:B:170:VAL:HB	1.41	0.86
1:B:250:THR:HG21	1:B:254:GLU:OE2	1.75	0.86
1:B:534:HIS:HD2	1:B:536:GLU:H	1.26	0.84
1:A:330:ASP:O	1:A:333:VAL:HG23	1.77	0.83
1:A:145:ARG:HE	1:A:155:ILE:HD13	1.44	0.83
1:B:335:CYS:O	1:B:370:THR:CG2	2.28	0.82
1:B:436:TYR:CE2	1:B:438:SER:HB2	2.18	0.79
1:A:315:THR:HG21	1:A:343:ASP:HB2	1.65	0.79
1:B:452:THR:HG22	1:B:459:THR:CG2	2.12	0.78
1:A:469:ARG:NH2	1:A:477:GLU:OE2	2.16	0.76
1:A:551:SER:HB2	1:A:566:CYS:H	1.51	0.75
1:B:36:ARG:HD3	1:B:37:CYS:H	1.50	0.75
1:B:434:ARG:HG2	1:B:462:ARG:HB2	1.69	0.75
1:B:520:GLU:HB2	1:B:521:PRO:HD3	1.68	0.75
1:B:116:ARG:HG3	1:B:116:ARG:NH1	1.92	0.75
1:B:559:HIS:NE2	4:B:5001:SO4:O2	2.21	0.74
1:B:565:HIS:HD2	5:B:1058:HOH:O	1.72	0.73
1:A:87:ARG:HG2	1:A:124:LEU:HD12	1.69	0.73
1:A:456:ARG:HH11	1:A:456:ARG:HB2	1.54	0.72
1:B:534:HIS:CD2	1:B:536:GLU:H	2.08	0.72
1:B:420:THR:HG22	1:B:479:LYS:NZ	2.04	0.72
1:B:559:HIS:NE2	4:B:5001:SO4:O4	2.25	0.70
1:B:247:ASN:CG	5:B:1072:HOH:O	2.27	0.69
1:A:73:ASN:ND2	1:A:103:ASN:OD1	2.25	0.69
1:B:414:MET:O	1:B:415:LYS:HG2	1.92	0.68
1:B:243:PRO:HA	1:B:259:THR:HG23	1.77	0.67
1:B:315:THR:HG22	1:B:343:ASP:OD2	1.94	0.67
1:A:150:ASP:HB3	1:A:153:ALA:HB2	1.77	0.67
1:B:381:GLN:HG2	1:B:415:LYS:HE2	1.77	0.67
1:B:116:ARG:HH11	1:B:116:ARG:CG	1.97	0.66
1:B:586:ASP:HB2	1:B:590:GLU:H	1.60	0.66
1:A:375:THR:HA	1:A:402:ARG:HH11	1.61	0.65
1:B:209:HIS:HD2	1:B:211:GLU:H	1.41	0.65
1:B:534:HIS:CD2	1:B:536:GLU:HB2	2.32	0.65
1:B:520:GLU:CB	1:B:521:PRO:CD	2.74	0.64
1:B:150:ASP:HB3	1:B:153:ALA:HB2	1.80	0.64
1:B:520:GLU:HB2	1:B:521:PRO:HD2	1.77	0.64
1:B:420:THR:HG22	1:B:479:LYS:HZ3	1.63	0.63
1:A:552:ASP:HA	1:A:564:PRO:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ARG:CB	1:B:36:ARG:HH11	2.12	0.62
1:B:559:HIS:NE2	4:B:5001:SO4:S	2.69	0.62
1:B:220:GLN:HB2	1:B:223:ASP:OD2	2.00	0.62
1:A:551:SER:HB2	1:A:566:CYS:N	2.15	0.61
1:A:70:VAL:HB	1:A:100:VAL:HG22	1.83	0.60
5:A:1045:HOH:O	2:C:1:NAG:H81	2.00	0.60
1:A:117:LEU:HD13	1:A:120:LEU:HD22	1.83	0.60
1:A:440:ASN:HD22	1:A:468:ASN:ND2	1.99	0.60
1:B:243:PRO:HA	1:B:259:THR:CG2	2.33	0.59
1:B:302:GLU:HG3	1:B:303:PRO:HD2	1.84	0.58
1:A:315:THR:CG2	1:A:343:ASP:HB2	2.34	0.58
1:A:440:ASN:H	1:A:468:ASN:HD22	1.52	0.58
1:B:578:LYS:HE2	1:B:578:LYS:N	2.11	0.58
1:A:436:TYR:CE2	1:A:438:SER:HB2	2.40	0.57
1:B:586:ASP:HB2	1:B:590:GLU:N	2.19	0.57
1:A:341:ASN:HD22	1:A:377:TYR:H	1.52	0.57
1:B:283:VAL:HG12	1:B:285:ALA:H	1.69	0.56
1:A:332:PHE:O	1:A:335:CYS:HB2	2.06	0.56
1:B:36:ARG:HD3	1:B:37:CYS:HB2	1.87	0.56
1:B:373:GLU:HG3	1:B:398:THR:HB	1.87	0.56
1:B:304:CYS:O	1:B:306:GLY:N	2.38	0.56
1:A:72:MET:HE1	1:A:102:LEU:HB2	1.87	0.55
1:B:129:TYR:CE2	1:B:131:GLU:HB2	2.41	0.55
1:B:114:GLN:OE1	1:B:116:ARG:HD3	2.07	0.55
1:B:606:GLU:HB2	1:B:609:ASP:OD2	2.06	0.55
1:B:241:PRO:HG2	1:B:260:LYS:HG3	1.89	0.55
1:A:256:ASN:HD21	1:A:258:HIS:HB2	1.72	0.55
1:B:565:HIS:CD2	5:B:1058:HOH:O	2.55	0.55
1:A:84:ARG:HD3	1:A:119:GLN:HG3	1.88	0.54
1:A:466:LYS:HG3	1:A:467:HIS:CD2	2.42	0.54
1:A:574:VAL:O	1:A:580:PRO:HA	2.07	0.54
1:B:520:GLU:CB	1:B:521:PRO:HD3	2.34	0.54
1:B:610:CYS:O	1:B:611:LEU:O	2.25	0.54
1:A:456:ARG:HB2	1:A:456:ARG:NH1	2.20	0.54
1:B:534:HIS:HD2	1:B:536:GLU:HB2	1.73	0.54
1:B:438:SER:OG	1:B:466:LYS:HG3	2.08	0.54
1:B:36:ARG:CD	1:B:37:CYS:H	2.19	0.53
1:A:397:THR:HG22	1:A:398:THR:OG1	2.09	0.53
1:B:36:ARG:HH11	1:B:36:ARG:HB2	1.73	0.53
1:A:87:ARG:NH2	1:A:227:CYS:O	2.27	0.53
1:A:425:ARG:NH1	5:A:1025:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:HA	1:A:439:ALA:O	2.10	0.52
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.75	0.52
1:B:262:GLN:HB2	1:B:281:SER:CB	2.40	0.52
1:B:400:GLY:O	1:B:431:SER:HB2	2.09	0.52
1:A:449:LEU:HD12	1:A:499:LEU:HD12	1.92	0.51
1:A:349:LEU:HD12	1:A:382:SER:OG	2.10	0.51
1:A:341:ASN:HD22	1:A:376:GLY:HA3	1.75	0.51
1:A:201:GLY:HA3	1:A:206:GLN:OE1	2.11	0.51
1:B:80:LEU:HD13	1:B:83:LEU:HD22	1.92	0.50
1:B:146:ASP:OD1	1:B:186:LEU:HA	2.11	0.50
1:B:518:ASN:HA	1:B:522:ARG:CZ	2.40	0.50
1:B:209:HIS:CD2	1:B:211:GLU:H	2.25	0.50
1:A:440:ASN:H	1:A:468:ASN:ND2	2.09	0.50
1:A:519:GLY:O	1:A:522:ARG:HD3	2.12	0.50
1:B:47:VAL:HA	1:B:71:ALA:O	2.12	0.50
1:A:222:THR:HG22	1:A:222:THR:O	2.12	0.50
1:B:168:HIS:CD2	1:B:170:VAL:HB	2.32	0.50
1:B:609:ASP:O	1:B:610:CYS:SG	2.70	0.50
1:A:54:ASP:OD1	1:A:56:SER:HB3	2.12	0.49
1:B:247:ASN:OD1	1:B:247:ASN:C	2.50	0.49
1:A:469:ARG:HD3	5:A:1022:HOH:O	2.11	0.49
1:B:330:ASP:C	1:B:332:PHE:H	2.16	0.49
1:B:243:PRO:HD2	5:B:1065:HOH:O	2.13	0.48
1:B:446:HIS:HA	5:B:1042:HOH:O	2.14	0.48
1:A:279:GLN:CG	1:A:280:THR:H	2.25	0.48
1:A:520:GLU:HB2	1:A:521:PRO:HD3	1.96	0.48
1:A:127:GLY:HA3	1:A:154:GLU:O	2.14	0.48
1:B:143:ASP:H	1:B:184:GLN:HE22	1.61	0.48
1:A:341:ASN:ND2	1:A:376:GLY:HA3	2.28	0.48
1:B:409:PHE:CE2	1:B:436:TYR:HB2	2.49	0.48
1:A:38:GLU:OE1	1:A:62:ARG:NH1	2.47	0.47
1:A:174:ARG:HB3	1:A:184:GLN:HB3	1.96	0.47
1:A:409:PHE:CD2	1:A:436:TYR:HB2	2.49	0.47
1:B:404:LEU:HD13	1:B:408:GLY:HA2	1.96	0.47
1:B:515:ASN:HB3	1:B:518:ASN:O	2.14	0.47
1:B:583:LYS:NZ	5:B:1069:HOH:O	2.47	0.47
1:A:450:ASN:ND2	1:A:453:LYS:HD2	2.29	0.47
1:B:397:THR:HA	1:B:426:SER:O	2.13	0.47
1:B:409:PHE:CD2	1:B:436:TYR:HB2	2.49	0.47
1:B:205:ASN:ND2	1:B:206:GLN:HG3	2.29	0.47
1:B:78:LEU:HD23	1:B:115:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LEU:HD23	1:B:499:LEU:HA	1.78	0.46
1:A:373:GLU:HG3	1:A:398:THR:HB	1.97	0.46
1:A:379:ASN:HD21	1:A:381:GLN:HG3	1.81	0.46
1:A:394:SER:HB2	1:A:425:ARG:HD3	1.97	0.46
1:B:453:LYS:HE2	3:B:627:NAG:O6	2.15	0.46
1:A:72:MET:CE	1:A:102:LEU:HB2	2.46	0.46
1:B:406:ASN:HB3	1:B:407:ARG:H	1.49	0.46
1:A:449:LEU:CD1	1:A:499:LEU:HD12	2.46	0.45
1:B:506:ARG:HD3	1:B:523:GLU:OE1	2.16	0.45
1:A:368:PHE:HB2	1:A:392:VAL:CG1	2.46	0.45
1:B:595:HIS:C	1:B:597:ASN:H	2.19	0.45
1:A:376:GLY:HA2	1:A:403:SER:H	1.81	0.45
1:B:576:GLY:HA3	1:B:581:ILE:CD1	2.47	0.45
1:B:262:GLN:HB2	1:B:281:SER:HB3	1.99	0.45
1:B:205:ASN:HD22	1:B:206:GLN:HG3	1.81	0.45
1:B:380:ILE:HG21	1:B:390:PHE:CE2	2.51	0.45
1:B:420:THR:HG22	1:B:479:LYS:HZ1	1.81	0.45
1:A:309:PRO:HA	1:A:336:THR:OG1	2.17	0.45
1:B:230:PHE:HA	1:B:265:GLY:O	2.17	0.45
1:A:514:CYS:HB2	1:A:516:PHE:CE1	2.52	0.45
1:B:243:PRO:CA	1:B:259:THR:HG23	2.46	0.45
1:B:559:HIS:CD2	4:B:5001:SO4:O2	2.70	0.45
1:A:417:LEU:HD22	1:A:441:ARG:HG3	1.98	0.44
1:A:356:LYS:O	1:A:358:PRO:HD3	2.17	0.44
1:B:72:MET:CE	1:B:102:LEU:HB2	2.47	0.44
1:A:222:THR:O	1:A:222:THR:CG2	2.65	0.44
1:A:375:THR:HA	1:A:402:ARG:NH1	2.27	0.44
1:A:349:LEU:HD23	1:A:360:LEU:HD12	1.99	0.44
1:A:96:PHE:CD2	1:A:129:TYR:HB2	2.52	0.44
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.76	0.44
1:A:74:GLU:HB3	1:A:110:HIS:HB3	2.00	0.44
1:B:59:GLN:O	1:B:82:ASN:ND2	2.39	0.44
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.65	0.43
1:A:440:ASN:HD22	1:A:468:ASN:HD21	1.62	0.43
1:B:340:GLY:H	1:B:375:THR:HB	1.83	0.43
1:B:242:GLN:O	1:B:259:THR:HG23	2.17	0.43
1:B:128:VAL:HG21	1:B:144:TRP:CE3	2.54	0.43
1:A:400:GLY:HA3	1:A:402:ARG:CZ	2.48	0.43
1:B:589:ASN:HD22	1:B:589:ASN:HA	1.62	0.43
1:B:148:VAL:HG21	1:B:155:ILE:HD11	2.00	0.43
1:A:71:ALA:C	1:A:72:MET:HG2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:CG1	1:A:91:VAL:O	2.66	0.43
1:A:315:THR:CG2	1:A:316:GLY:N	2.82	0.43
1:B:503:ASN:HB2	1:B:504:TYR:H	1.62	0.43
1:B:347:THR:HG22	1:B:352:ASP:HB2	2.00	0.43
1:B:452:THR:OG1	3:B:627:NAG:H5	2.19	0.43
1:A:45:GLU:HG2	1:A:69:LEU:HD23	2.00	0.42
1:A:169:GLU:OE2	1:B:62:ARG:NH2	2.53	0.42
1:A:47:VAL:HA	1:A:71:ALA:O	2.18	0.42
1:B:70:VAL:HG21	1:B:78:LEU:HD22	2.01	0.42
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.81	0.42
1:A:579:GLY:HA2	1:A:580:PRO:HD2	1.87	0.42
1:B:262:GLN:HB2	1:B:281:SER:HB2	2.02	0.42
1:B:338:ILE:HD13	1:B:342:LEU:HD11	2.00	0.42
1:B:506:ARG:NH1	1:B:523:GLU:OE2	2.53	0.42
1:B:375:THR:O	1:B:400:GLY:HA3	2.20	0.42
1:B:143:ASP:N	1:B:184:GLN:HE22	2.17	0.41
1:B:538:GLN:HB3	1:B:556:GLN:HB3	2.01	0.41
1:A:177:GLY:HA3	1:A:182:ASP:CB	2.51	0.41
1:B:256:ASN:O	1:B:259:THR:OG1	2.38	0.41
1:B:389:ASN:OD1	1:B:391:SER:HB3	2.21	0.41
1:B:517:LEU:HD13	1:B:542:GLY:O	2.20	0.41
1:B:142:ILE:O	1:B:142:ILE:HG22	2.20	0.41
1:A:561:ARG:HG2	1:A:562:ASP:N	2.36	0.41
1:A:101:MET:CE	1:A:102:LEU:HD12	2.51	0.41
1:B:387:MET:HA	2:D:1:NAG:O6	2.20	0.41
1:B:481:CYS:SG	1:B:490:CYS:N	2.93	0.41
1:A:78:LEU:O	1:A:116:ARG:HB2	2.21	0.40
1:A:203:ASN:HB2	1:A:206:GLN:HG3	2.02	0.40
1:A:521:PRO:O	1:A:523:GLU:HG3	2.21	0.40
1:B:86:VAL:O	1:B:123:ILE:HA	2.21	0.40
1:B:276:VAL:HG21	1:B:292:GLU:HG3	2.02	0.40
1:B:84:ARG:NH2	1:B:119:GLN:HG3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/621 (88%)	482 (88%)	52 (10%)	11 (2%)	7	14
1	B	580/621 (93%)	525 (90%)	45 (8%)	10 (2%)	9	18
All	All	1125/1242 (91%)	1007 (90%)	97 (9%)	21 (2%)	8	15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	460	GLU
1	B	520	GLU
1	B	586	ASP
1	A	296	ASN
1	B	305	GLY
1	B	596	GLU
1	B	600	GLN
1	B	610	CYS
1	A	279	GLN
1	A	577	ALA
1	A	120	LEU
1	A	193	PRO
1	A	288	PRO
1	B	279	GLN
1	B	406	ASN
1	A	306	GLY
1	A	571	PRO
1	B	331	GLY
1	A	574	VAL
1	B	79	PRO

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	474/537 (88%)	398 (84%)	76 (16%)	2 4
1	B	506/537 (94%)	436 (86%)	70 (14%)	3 6
All	All	980/1074 (91%)	834 (85%)	146 (15%)	3 5

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	36	ARG
1	A	49	THR
1	A	56	SER
1	A	59	GLN
1	A	73	ASN
1	A	77	THR
1	A	87	ARG
1	A	89	THR
1	A	91	VAL
1	A	98	ILE
1	A	105	ASN
1	A	109	SER
1	A	114	GLN
1	A	116	ARG
1	A	118	THR
1	A	142	ILE
1	A	145	ARG
1	A	151	ARG
1	A	152	ASP
1	A	154	GLU
1	A	181	GLU
1	A	189	THR
1	A	190	ILE
1	A	205	ASN
1	A	210	ASP
1	A	220	GLN
1	A	233	SER
1	A	239	ARG
1	A	247	ASN
1	A	249	LEU
1	A	273	HIS
1	A	276	VAL
1	A	280	THR
1	A	294	ASP

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Mol	Chain	Res	Type
1	A	295	LYS
1	A	298	LEU
1	A	299	LYS
1	A	310	LYS
1	A	312	CYS
1	A	315	THR
1	A	319	SER
1	A	324	VAL
1	A	326	SER
1	A	329	ILE
1	A	341	ASN
1	A	352	ASP
1	A	357	ILE
1	A	367	VAL
1	A	375	THR
1	A	379	ASN
1	A	389	ASN
1	A	397	THR
1	A	402	ARG
1	A	407	ARG
1	A	410	SER
1	A	419	VAL
1	A	431	SER
1	A	441	ARG
1	A	448	SER
1	A	452	THR
1	A	456	ARG
1	A	469	ARG
1	A	499	LEU
1	A	517	LEU
1	A	527	GLU
1	A	529	GLU
1	A	532	SER
1	A	536	GLU
1	A	541	GLU
1	A	549	SER
1	A	551	SER
1	A	561	ARG
1	A	562	ASP
1	A	570	CYS
1	A	575	LEU
1	B	9	VAL

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Mol	Chain	Res	Type
1	B	10	CYS
1	B	13	THR
1	B	36	ARG
1	B	37	CYS
1	B	38	GLU
1	B	49	THR
1	B	74	GLU
1	B	84	ARG
1	B	87	ARG
1	B	95	LYS
1	B	106	THR
1	B	108	SER
1	B	116	ARG
1	B	131	GLU
1	B	142	ILE
1	B	158	LYS
1	B	169	GLU
1	B	181	GLU
1	B	182	ASP
1	B	196	ASN
1	B	205	ASN
1	B	250	THR
1	B	252	GLN
1	B	259	THR
1	B	270	SER
1	B	273	HIS
1	B	276	VAL
1	B	280	THR
1	B	295	LYS
1	B	299	LYS
1	B	300	MET
1	B	307	LEU
1	B	312	CYS
1	B	320	ARG
1	B	327	SER
1	B	329	ILE
1	B	335	CYS
1	B	338	ILE
1	B	341	ASN
1	B	347	THR
1	B	349	LEU
1	B	352	ASP

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Mol	Chain	Res	Type
1	B	356	LYS
1	B	363	GLU
1	B	370	THR
1	B	375	THR
1	B	391	SER
1	B	394	SER
1	B	406	ASN
1	B	420	THR
1	B	425	ARG
1	B	441	ARG
1	B	449	LEU
1	B	477	GLU
1	B	500	SER
1	B	502	ARG
1	B	503	ASN
1	B	520	GLU
1	B	522	ARG
1	B	543	THR
1	B	556	GLN
1	B	561	ARG
1	B	578	LYS
1	B	581	ILE
1	B	596	GLU
1	B	600	GLN
1	B	603	LYS
1	B	606	GLU
1	B	611	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	198	HIS
1	A	247	ASN
1	A	256	ASN
1	A	341	ASN
1	A	379	ASN
1	A	381	GLN
1	A	386	HIS
1	A	467	HIS
1	A	468	ASN
1	A	538	GLN

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Mol	Chain	Res	Type
1	A	565	HIS
1	B	138	HIS
1	B	168	HIS
1	B	184	GLN
1	B	205	ASN
1	B	209	HIS
1	B	229	HIS
1	B	467	HIS
1	B	534	HIS
1	B	589	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	C	1	2,1	14,14,15	0.82	0	17,19,21	1.63	4 (23%)
2	NAG	C	2	2	14,14,15	0.42	0	17,19,21	1.62	4 (23%)
2	NAG	D	1	2,1	14,14,15	0.45	0	17,19,21	1.28	2 (11%)
2	NAG	D	2	2	14,14,15	0.57	0	17,19,21	0.89	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	4.03	117.66	112.19
2	D	1	NAG	C1-O5-C5	3.38	116.77	112.19
2	C	1	NAG	C2-N2-C7	-2.93	118.73	122.90
2	C	2	NAG	C2-N2-C7	2.45	126.39	122.90
2	C	1	NAG	C4-C3-C2	2.39	114.51	111.02
2	C	2	NAG	O5-C5-C6	2.36	110.91	107.20
2	C	1	NAG	O5-C1-C2	-2.29	107.67	111.29
2	C	2	NAG	C3-C4-C5	-2.20	106.31	110.24
2	D	1	NAG	O5-C5-C6	2.16	110.60	107.20
2	C	1	NAG	O3-C3-C2	-2.09	105.13	109.47
2	D	2	NAG	O5-C5-C6	2.06	110.43	107.20

There are no chirality outliers.

All (12) 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
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

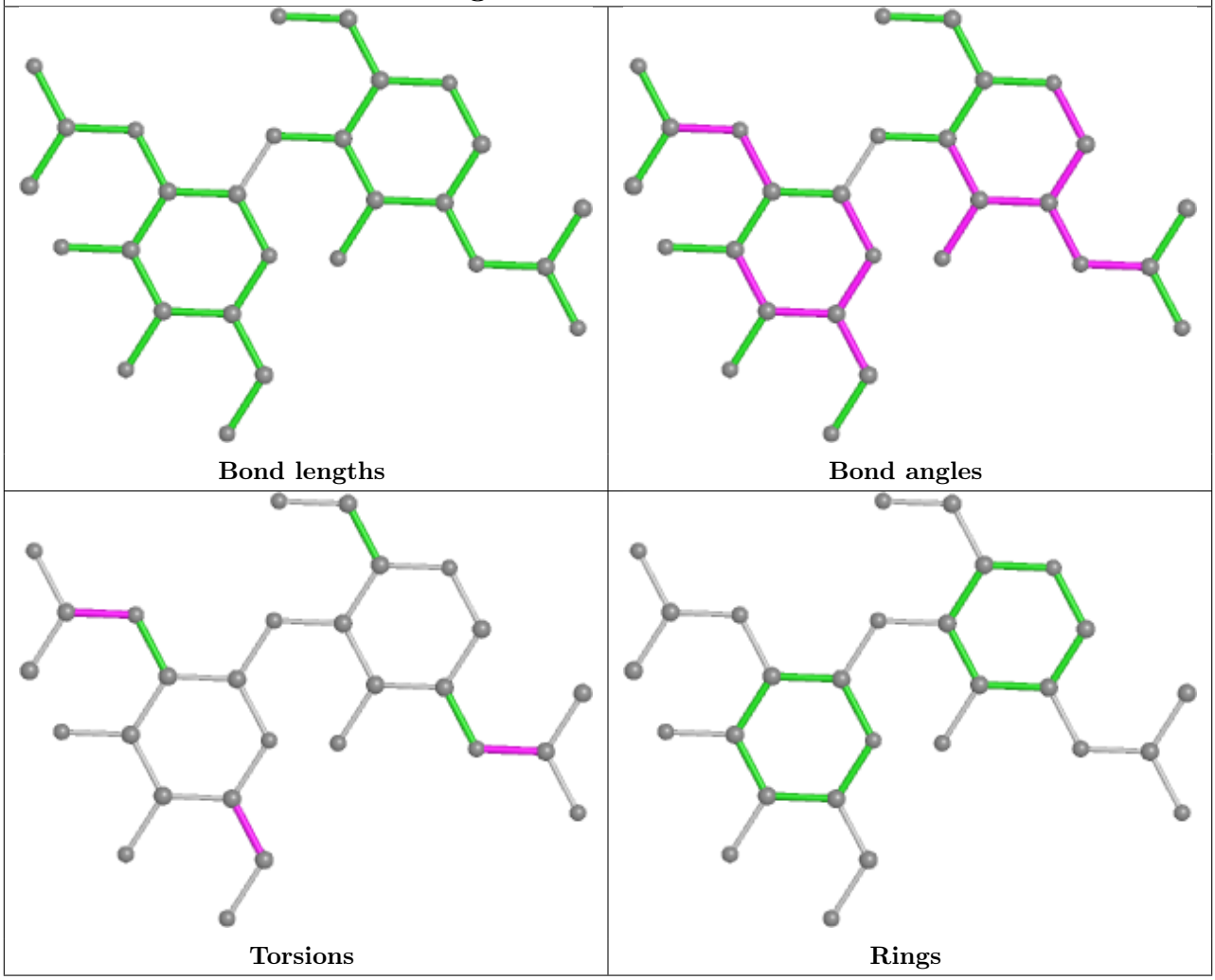
There are no ring outliers.

2 monomers are involved in 2 short contacts:

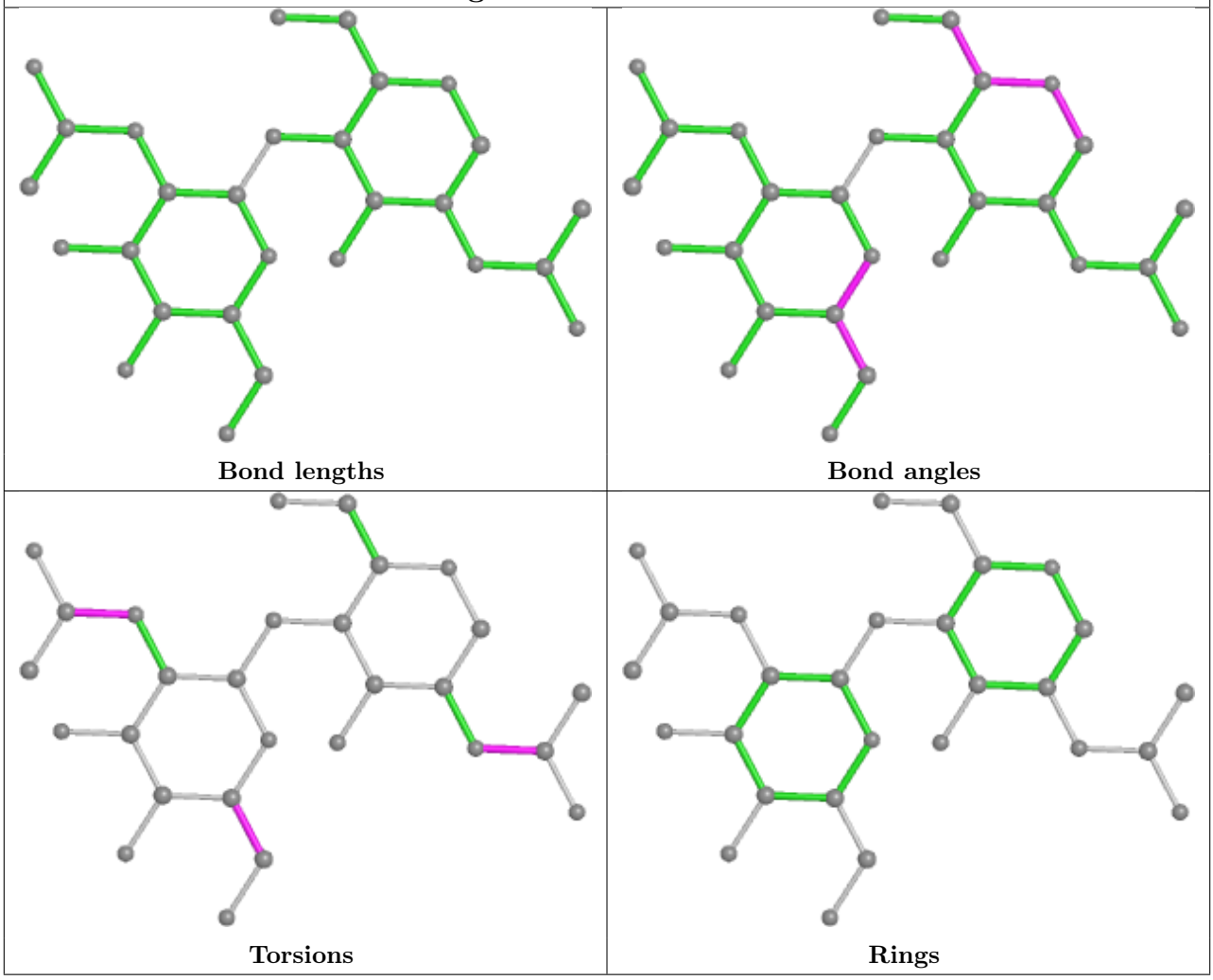
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	C	1	NAG	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	623	1	14,14,15	0.69	0	17,19,21	1.31	3 (17%)
4	SO4	B	5001	-	4,4,4	0.22	0	6,6,6	0.32	0
3	NAG	B	622	1	14,14,15	0.68	0	17,19,21	3.03	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	622	1	14,14,15	0.43	0	17,19,21	2.24	2 (11%)
3	NAG	A	630	1	14,14,15	0.67	0	17,19,21	1.68	3 (17%)
3	NAG	B	626	1	14,14,15	0.68	0	17,19,21	1.93	6 (35%)
3	NAG	B	628	1	14,14,15	0.69	0	17,19,21	1.65	2 (11%)
3	NAG	A	626	1	14,14,15	0.62	0	17,19,21	1.15	2 (11%)
3	NAG	B	627	1	14,14,15	0.57	0	17,19,21	1.52	2 (11%)
3	NAG	A	627	1	14,14,15	0.62	0	17,19,21	1.53	4 (23%)
3	NAG	A	628	1	14,14,15	0.73	0	17,19,21	1.76	4 (23%)
3	NAG	B	623	1	14,14,15	0.70	0	17,19,21	1.63	4 (23%)
3	NAG	A	629	1	14,14,15	0.79	1 (7%)	17,19,21	1.62	4 (23%)
3	NAG	B	629	1	14,14,15	1.02	1 (7%)	17,19,21	1.55	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	623	1	-	0/6/23/26	0/1/1/1
3	NAG	B	622	1	-	4/6/23/26	0/1/1/1
3	NAG	B	626	1	1/1/5/7	6/6/23/26	0/1/1/1
3	NAG	A	622	1	-	3/6/23/26	0/1/1/1
3	NAG	B	628	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	630	1	-	4/6/23/26	0/1/1/1
3	NAG	A	626	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	B	627	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	A	627	1	-	4/6/23/26	0/1/1/1
3	NAG	A	628	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	623	1	-	4/6/23/26	0/1/1/1
3	NAG	A	629	1	-	0/6/23/26	0/1/1/1
3	NAG	B	629	1	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	629	NAG	C1-C2	2.99	1.56	1.52
3	A	629	NAG	C1-C2	2.43	1.56	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	622	NAG	C2-N2-C7	-8.24	111.17	122.90
3	A	622	NAG	C1-O5-C5	7.93	122.93	112.19
3	A	630	NAG	C1-O5-C5	5.60	119.78	112.19
3	B	622	NAG	C1-O5-C5	5.59	119.76	112.19
3	A	628	NAG	O5-C1-C2	-4.98	103.42	111.29
3	B	628	NAG	C2-N2-C7	-4.91	115.91	122.90
3	B	626	NAG	C1-O5-C5	4.23	117.92	112.19
3	B	622	NAG	C4-C3-C2	3.92	116.77	111.02
3	B	626	NAG	O5-C5-C6	3.90	113.32	107.20
3	B	627	NAG	O5-C1-C2	-3.83	105.23	111.29
3	B	629	NAG	C1-O5-C5	3.79	117.33	112.19
3	B	623	NAG	C4-C3-C2	3.58	116.26	111.02
3	A	629	NAG	C1-O5-C5	3.57	117.02	112.19
3	B	622	NAG	O7-C7-N2	-3.42	115.66	121.95
3	B	627	NAG	C1-O5-C5	3.37	116.76	112.19
3	B	626	NAG	C4-C3-C2	-3.08	106.50	111.02
3	A	629	NAG	C2-N2-C7	-2.98	118.67	122.90
3	A	623	NAG	C4-C3-C2	2.92	115.30	111.02
3	B	622	NAG	C3-C4-C5	2.85	115.31	110.24
3	B	626	NAG	C3-C4-C5	-2.75	105.34	110.24
3	A	628	NAG	C4-C3-C2	2.68	114.94	111.02
3	B	629	NAG	C1-C2-N2	2.67	115.05	110.49
3	A	623	NAG	O5-C1-C2	-2.61	107.17	111.29
3	A	627	NAG	C1-O5-C5	2.56	115.66	112.19
3	A	627	NAG	O5-C1-C2	-2.51	107.33	111.29
3	A	626	NAG	C3-C4-C5	2.48	114.66	110.24
3	A	628	NAG	O5-C5-C6	2.42	111.00	107.20
3	A	629	NAG	C3-C4-C5	-2.37	106.01	110.24
3	B	623	NAG	C3-C4-C5	2.36	114.45	110.24
3	A	626	NAG	O5-C1-C2	-2.35	107.57	111.29
3	A	623	NAG	O5-C5-C6	2.34	110.87	107.20
3	A	630	NAG	C3-C4-C5	2.28	114.31	110.24
3	A	622	NAG	O4-C4-C5	2.27	114.93	109.30
3	B	626	NAG	O3-C3-C2	2.26	114.14	109.47
3	A	627	NAG	C1-C2-N2	2.25	114.34	110.49
3	B	622	NAG	C6-C5-C4	-2.24	107.75	113.00
3	B	628	NAG	C1-C2-N2	-2.21	106.71	110.49
3	B	629	NAG	C2-N2-C7	2.20	126.03	122.90
3	A	628	NAG	C1-O5-C5	2.19	115.16	112.19
3	B	623	NAG	C2-N2-C7	2.17	126.00	122.90
3	A	629	NAG	O5-C5-C6	2.15	110.57	107.20
3	B	623	NAG	C1-O5-C5	2.12	115.06	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	626	NAG	O4-C4-C5	2.07	114.44	109.30
3	A	627	NAG	O5-C5-C6	2.05	110.41	107.20
3	A	630	NAG	O5-C5-C4	2.02	115.74	110.83

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	626	NAG	C1
3	A	628	NAG	C1
3	B	626	NAG	C1
3	B	627	NAG	C1
3	B	628	NAG	C1

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	622	NAG	C8-C7-N2-C2
3	A	622	NAG	O7-C7-N2-C2
3	A	628	NAG	C8-C7-N2-C2
3	A	628	NAG	O7-C7-N2-C2
3	A	630	NAG	C8-C7-N2-C2
3	A	630	NAG	O7-C7-N2-C2
3	B	629	NAG	C1-C2-N2-C7
3	B	629	NAG	C8-C7-N2-C2
3	B	629	NAG	O7-C7-N2-C2
3	B	626	NAG	O5-C5-C6-O6
3	A	628	NAG	O5-C5-C6-O6
3	A	630	NAG	O5-C5-C6-O6
3	B	626	NAG	C8-C7-N2-C2
3	A	628	NAG	C4-C5-C6-O6
3	B	626	NAG	C4-C5-C6-O6
3	B	623	NAG	O5-C5-C6-O6
3	A	630	NAG	C4-C5-C6-O6
3	B	626	NAG	O7-C7-N2-C2
3	B	622	NAG	O5-C5-C6-O6
3	B	629	NAG	O5-C5-C6-O6
3	A	627	NAG	C8-C7-N2-C2
3	B	622	NAG	C8-C7-N2-C2
3	B	623	NAG	C8-C7-N2-C2
3	B	623	NAG	O7-C7-N2-C2
3	B	622	NAG	C4-C5-C6-O6
3	A	627	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	627	NAG	O5-C5-C6-O6
3	B	626	NAG	C1-C2-N2-C7
3	B	622	NAG	O7-C7-N2-C2
3	A	627	NAG	C4-C5-C6-O6
3	B	627	NAG	C4-C5-C6-O6
3	A	626	NAG	O5-C5-C6-O6
3	A	622	NAG	O5-C5-C6-O6
3	B	629	NAG	C4-C5-C6-O6
3	B	627	NAG	O5-C5-C6-O6
3	B	627	NAG	C8-C7-N2-C2
3	B	623	NAG	C4-C5-C6-O6
3	B	628	NAG	C8-C7-N2-C2
3	B	627	NAG	O7-C7-N2-C2
3	B	626	NAG	C3-C2-N2-C7
3	B	628	NAG	O5-C5-C6-O6
3	B	628	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5001	SO4	4	0
3	B	627	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

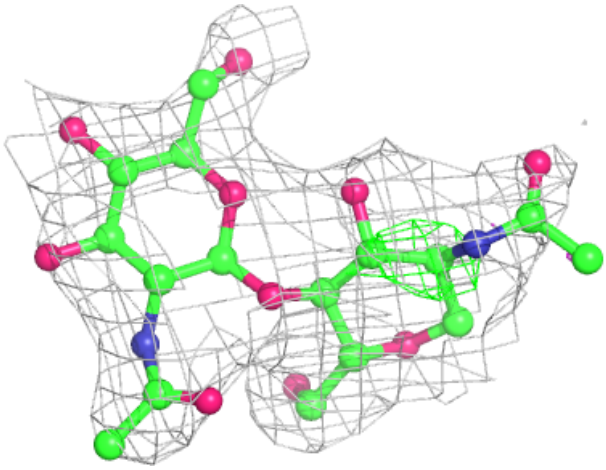
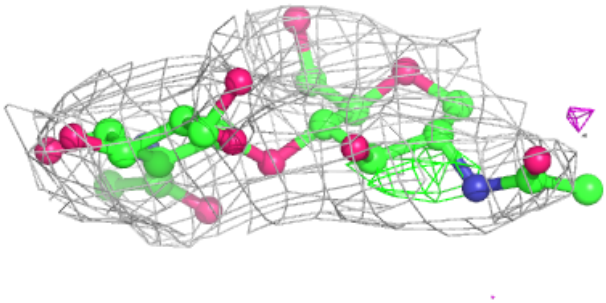
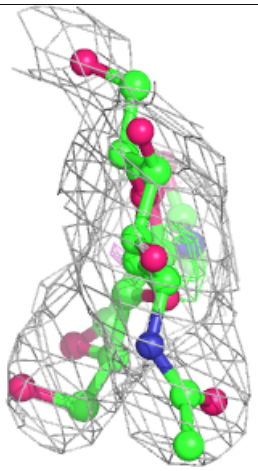
6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

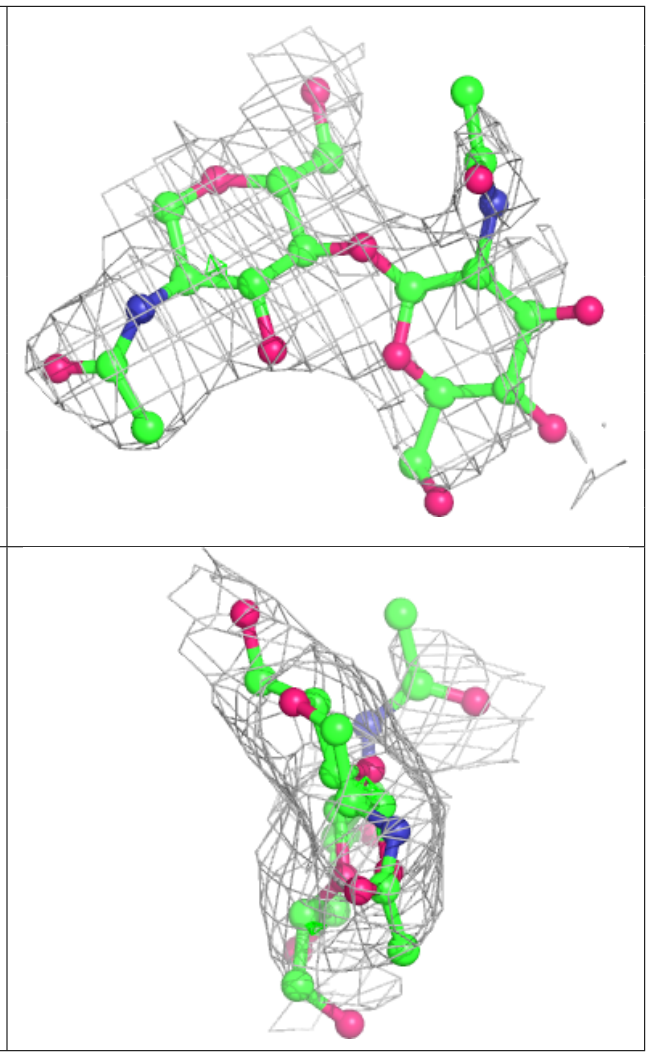
Unable to reproduce the depositors R factor - this section is therefore empty.

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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.