Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 08:59 PM EDT

PDB ID	:	4U4F
Title	:	Structure of GluA2* in complex with partial agonist (S)-5-Nitrowillardiine
Authors	:	Yelshanskaya, M.V.; Li, M.; Sobolevsky, A.I.
Deposited on	:	2014-07-23
Resolution	:	4.79 Å(reported)

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

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

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

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

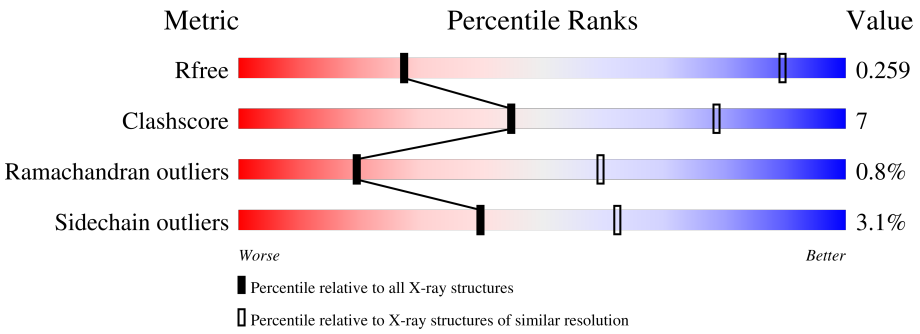
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 4.79 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	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)
Ramachandran outliers	138981	1105 (5.80-3.80)
Sidechain outliers	138945	1085 (5.80-3.80)

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%

Mol	Chain	Length	Quality of chain
1	A	822	77% 16% • 7%
1	B	822	73% 19% • 7%
1	C	822	74% 18% • 7%
1	D	822	77% 16% • 7%
2	E	2	50% 50%
2	F	2	50% 50%
2	G	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24067 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	768	5979	3836	990	1125	28	0	0	0
1	B	768	5974	3831	990	1125	28	0	0	0
1	C	768	5974	3831	990	1125	28	0	0	0
1	D	768	5974	3831	990	1125	28	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491

Continued on next page...

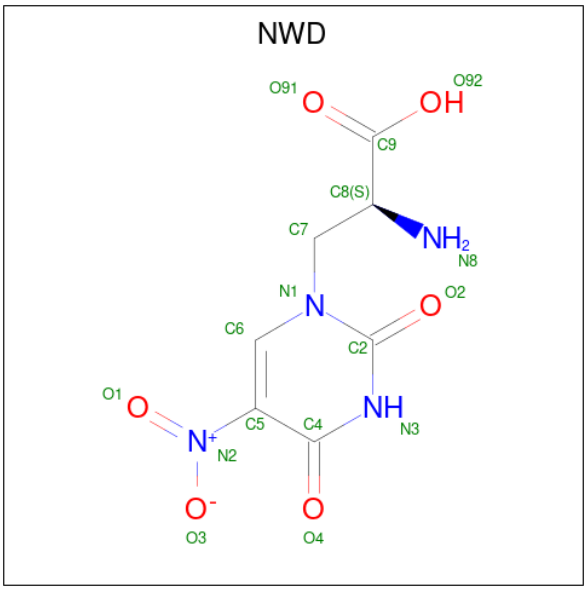
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	831	ARG	-	expression tag	UNP P19491

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

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

- Molecule 3 is 3-(5-nitro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-L-alanine (three-letter code: NWD) (formula: $C_7H_8N_4O_6$).



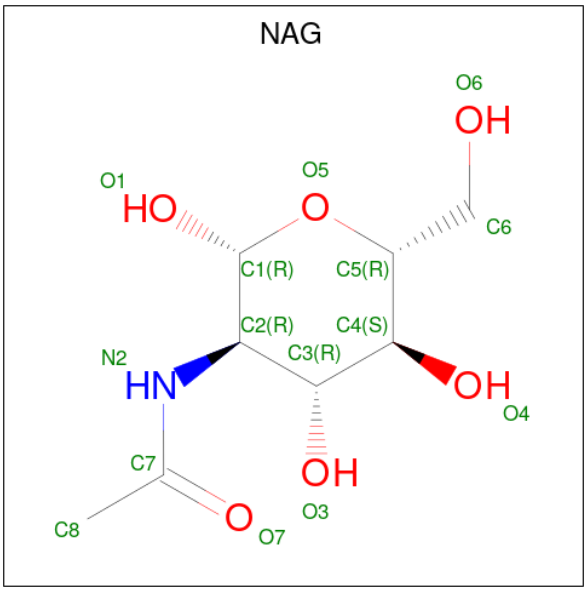
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	7	4	6	0	0
			Total	C	N	O		
3	B	1	17	7	4	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	17	7	4	6	0	0
			Total	C	N	O		
3	D	1	17	7	4	6	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



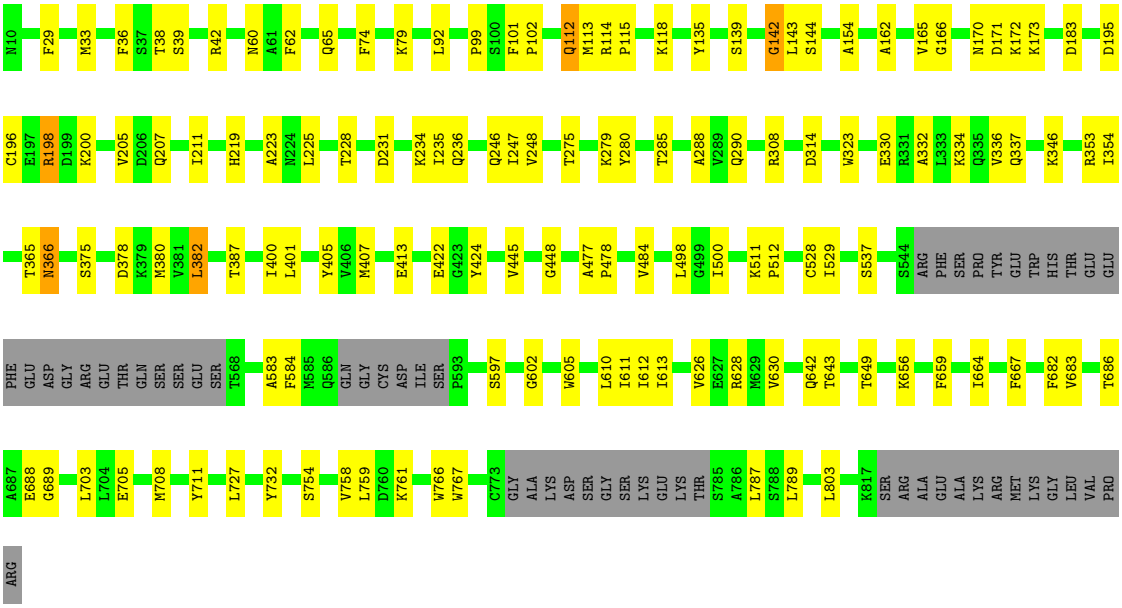
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	D	1	14	8	1	5	0	0

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.

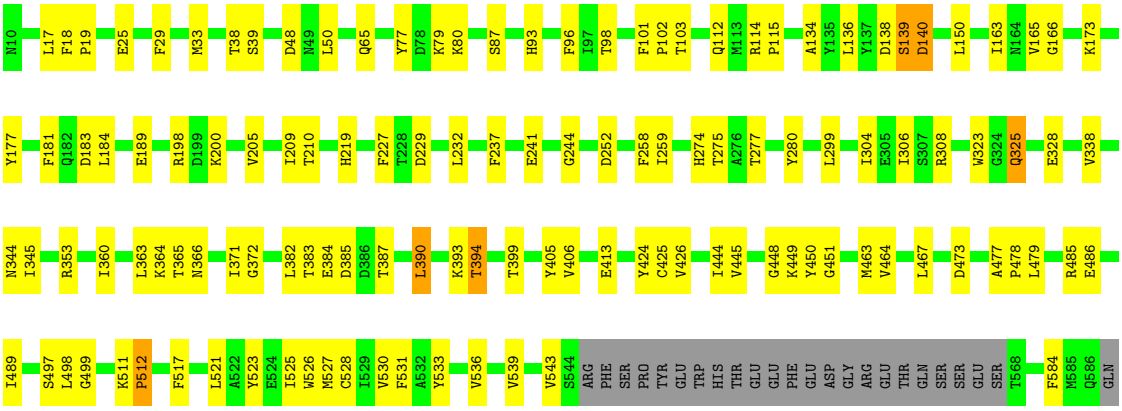
- Molecule 1: Glutamate receptor 2

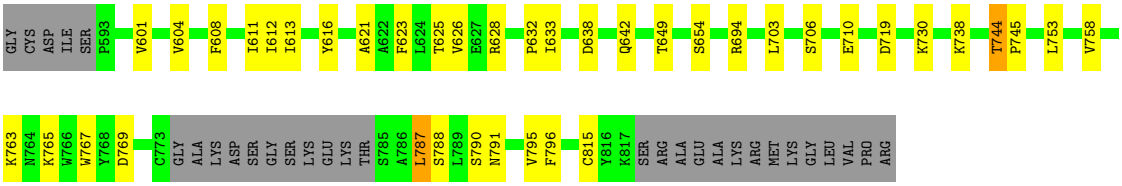
Chain A:



- Molecule 1: Glutamate receptor 2

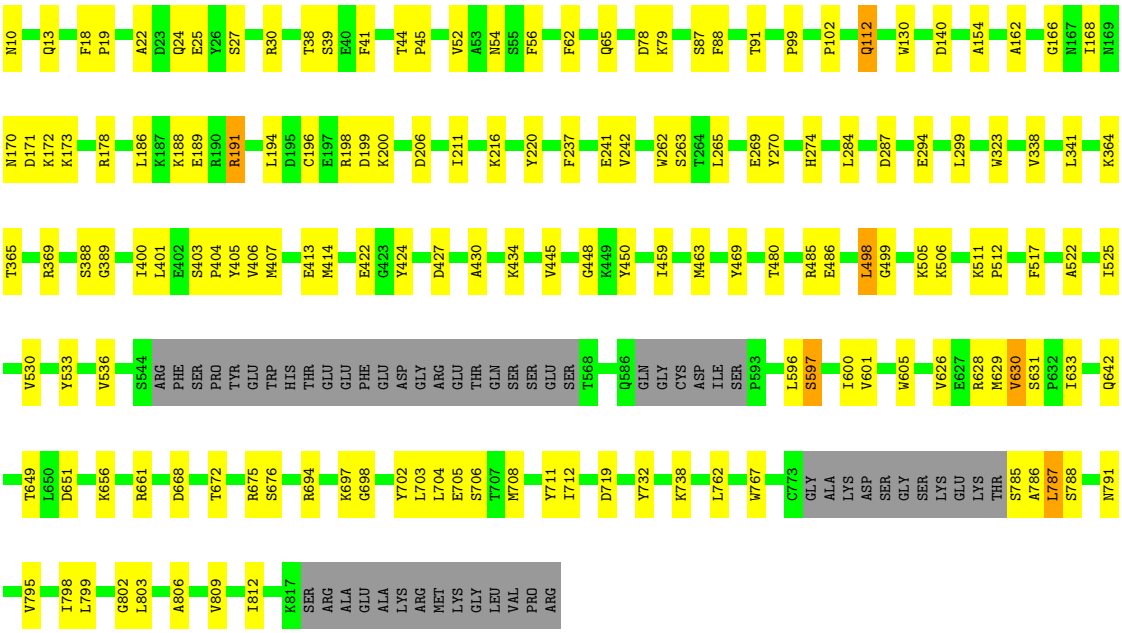
Chain B:





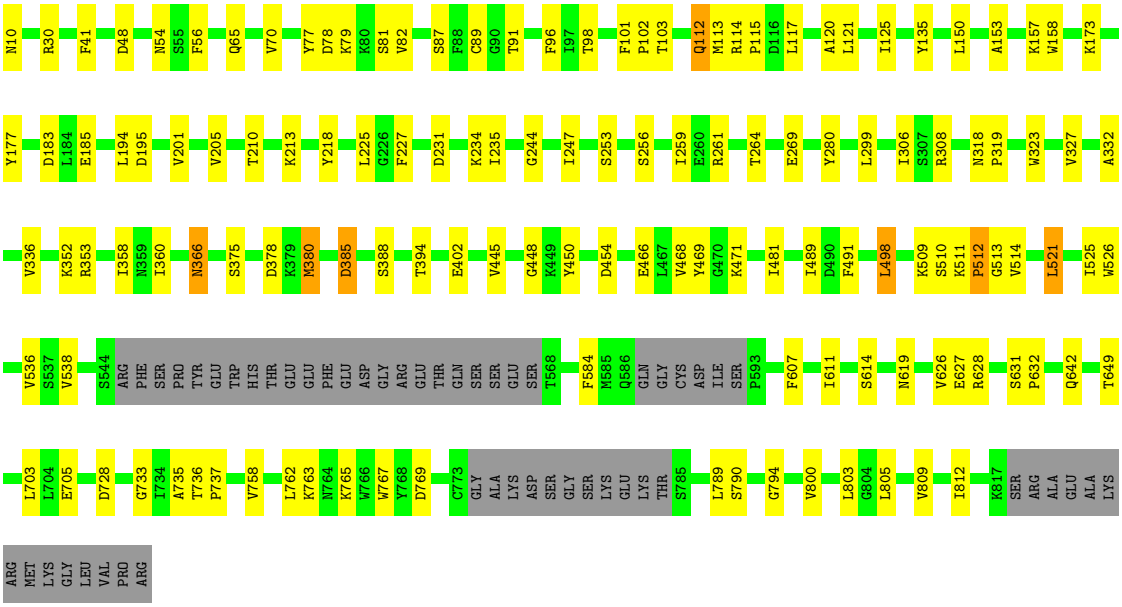
- Molecule 1: Glutamate receptor 2

Chain C:



- Molecule 1: Glutamate receptor 2

Chain D:



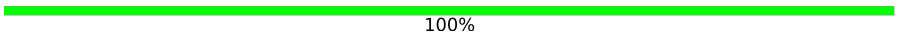
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:

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

Chain G: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	141.37Å 166.57Å 566.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.95 – 4.79 49.85 – 4.79	Depositor EDS
% Data completeness (in resolution range)	89.8 (39.95-4.79) 89.8 (49.85-4.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 4.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.228 , 0.262 0.229 , 0.259	Depositor DCC
R_{free} test set	1515 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	268.8	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 127.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	24067	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: NWD, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.23	0/6100	0.42	0/8249
1	B	0.24	0/6094	0.41	0/8241
1	C	0.22	0/6094	0.41	0/8241
1	D	0.22	0/6094	0.40	0/8241
All	All	0.23	0/24382	0.41	0/32972

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5979	0	5913	73	0
1	B	5974	0	5909	100	0
1	C	5974	0	5908	93	0
1	D	5974	0	5908	80	0
2	E	28	0	25	2	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	A	17	0	7	0	0
3	B	17	0	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	17	0	7	0	0
3	D	17	0	7	0	0
4	D	14	0	13	0	0
All	All	24067	0	23754	312	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 7.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:LYS:HB3	1:C:719:ASP:HB2	1.50	0.92
1:C:505:LYS:HD2	1:C:506:LYS:HG2	1.55	0.87
1:B:512:PRO:HA	1:B:790:SER:HB2	1.58	0.84
1:A:101:PHE:HA	1:A:114:ARG:HD3	1.66	0.78
1:C:166:GLY:HA2	1:C:200:LYS:HE2	1.72	0.71
1:B:744:THR:HG23	1:B:745:PRO:HD3	1.70	0.71
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.71	0.71
1:A:789:LEU:HD13	1:D:525:ILE:HG12	1.74	0.69
1:C:241:GLU:OE2	1:C:364:LYS:NZ	2.26	0.68
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.76	0.68
1:C:186:LEU:HD21	1:D:157:LYS:HE2	1.76	0.67
1:D:48:ASP:OD2	1:D:65:GLN:NE2	2.28	0.67
1:A:166:GLY:HA2	1:A:200:LYS:HE2	1.77	0.67
1:D:102:PRO:HD3	1:D:114:ARG:HD2	1.77	0.66
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.78	0.65
1:A:610:LEU:HD12	1:A:613:ILE:HD11	1.78	0.65
1:C:601:VAL:HG22	1:D:803:LEU:HD23	1.78	0.65
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.78	0.65
1:C:369:ARG:NH1	1:C:388:SER:OG	2.30	0.65
1:B:165:VAL:O	1:B:200:LYS:NZ	2.30	0.64
1:D:366:ASN:OD1	1:D:366:ASN:N	2.31	0.63
1:B:304:ILE:HG21	1:B:328:GLU:HG2	1.80	0.63
1:D:135:TYR:OH	1:D:195:ASP:OD2	2.16	0.63
1:C:87:SER:OG	1:D:54:ASN:OD1	2.17	0.62
1:A:170:ASN:HA	1:A:173:LYS:HB2	1.80	0.62
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.81	0.61
1:A:196:CYS:HB3	1:A:200:LYS:HB3	1.81	0.61
1:C:38:THR:OG1	1:C:39:SER:N	2.33	0.61
1:D:114:ARG:NH1	1:D:280:TYR:OH	2.34	0.60
1:D:70:VAL:O	1:D:308:ARG:NH1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:PRO:HA	1:C:112:GLN:HG2	1.84	0.60
1:D:213:LYS:NZ	1:D:218:TYR:OH	2.30	0.60
1:C:530:VAL:HA	1:C:533:TYR:HB3	1.84	0.59
1:A:330:GLU:HG2	1:A:334:LYS:HE2	1.85	0.59
1:A:758:VAL:HA	1:A:761:LYS:HB3	1.84	0.59
1:A:611:ILE:HG21	1:B:795:VAL:HG21	1.84	0.59
1:C:54:ASN:OD1	1:D:87:SER:OG	2.21	0.59
1:B:134:ALA:HB2	1:B:189:GLU:HG2	1.85	0.59
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.84	0.58
1:B:486:GLU:O	1:B:738:LYS:NZ	2.33	0.58
1:C:78:ASP:OD1	1:C:79:LYS:N	2.35	0.58
1:A:135:TYR:OH	1:A:195:ASP:OD2	2.18	0.57
1:A:231:ASP:HB3	1:A:234:LYS:HE2	1.87	0.57
1:C:787:LEU:HD13	1:C:788:SER:H	1.70	0.57
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.87	0.57
1:A:803:LEU:HD21	1:D:536:VAL:HG22	1.87	0.56
1:A:205:VAL:HG13	1:A:235:ILE:HD12	1.88	0.56
1:B:517:PHE:HB2	1:B:791:ASN:OD1	2.05	0.56
1:B:528:CYS:HA	1:B:531:PHE:HB2	1.88	0.56
1:A:236:GLN:NE2	1:A:365:THR:O	2.37	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.88	0.55
1:C:27:SER:HB3	1:C:270:TYR:HB3	1.87	0.55
1:D:521:LEU:HD23	1:D:525:ILE:HB	1.89	0.55
1:A:113:MET:HG3	1:A:288:ALA:HB2	1.88	0.55
1:A:337:GLN:HE22	2:E:1:NAG:H2	1.72	0.54
1:A:407:MET:N	1:A:422:GLU:O	2.33	0.54
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.89	0.54
1:B:633:ILE:HG23	1:B:638:ASP:HB2	1.89	0.54
1:B:198:ARG:HH22	1:B:229:ASP:HB3	1.73	0.54
1:A:346:LYS:HD2	1:A:354:ILE:HD11	1.90	0.53
1:A:602:GLY:HA2	1:A:605:TRP:HB3	1.89	0.53
1:A:198:ARG:HD3	1:A:279:LYS:HE3	1.88	0.53
1:B:17:LEU:HG	1:B:50:LEU:HD21	1.89	0.53
1:C:168:ILE:HD13	1:C:173:LYS:HG3	1.90	0.53
1:B:399:THR:HG23	1:B:444:ILE:HD13	1.91	0.53
1:A:754:SER:HB2	1:A:759:LEU:HD12	1.89	0.53
1:A:228:THR:OG1	1:A:246:GLN:NE2	2.41	0.53
1:D:402:GLU:OE1	1:D:450:TYR:OH	2.26	0.53
1:B:258:PHE:HD1	1:B:259:ILE:HD12	1.74	0.53
1:B:79:LYS:HE3	1:B:139:SER:HB2	1.90	0.52
1:A:225:LEU:HD13	1:A:247:ILE:HD11	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:VAL:HA	1:B:533:TYR:HB3	1.92	0.52
1:A:142:GLY:O	1:A:144:SER:N	2.41	0.52
1:B:79:LYS:HZ2	1:B:140:ASP:HA	1.74	0.52
1:D:185:GLU:OE1	1:D:213:LYS:NZ	2.43	0.52
1:D:225:LEU:HB3	1:D:247:ILE:HB	1.92	0.52
1:D:626:VAL:O	1:D:627:GLU:HG2	2.10	0.52
1:A:683:VAL:HG11	1:A:689:GLY:HA2	1.91	0.51
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.45	0.51
1:D:332:ALA:O	1:D:336:VAL:HG23	2.11	0.51
1:C:162:ALA:HB3	1:D:150:LEU:HD13	1.91	0.51
1:A:366:ASN:OD1	1:A:366:ASN:N	2.31	0.51
1:B:344:ASN:O	1:B:353:ARG:NH2	2.43	0.51
1:C:651:ASP:OD1	1:C:656:LYS:NZ	2.43	0.51
1:D:113:MET:O	1:D:353:ARG:NH1	2.44	0.51
1:C:505:LYS:HG2	1:C:698:GLY:N	2.26	0.51
1:B:521:LEU:HD22	1:B:526:TRP:CD2	2.46	0.51
1:A:511:LYS:HG2	1:A:512:PRO:HD2	1.92	0.51
1:B:383:THR:O	1:B:385:ASP:N	2.44	0.51
1:D:102:PRO:HA	1:D:112:GLN:HG2	1.93	0.51
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.76	0.50
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.93	0.50
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.94	0.50
1:A:114:ARG:NH2	1:A:280:TYR:OH	2.44	0.50
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.93	0.50
1:C:171:ASP:OD1	1:C:172:LYS:N	2.45	0.50
1:D:78:ASP:N	1:D:81:SER:OG	2.44	0.50
1:B:450:TYR:HE2	1:B:478:PRO:HG2	1.76	0.49
1:C:220:TYR:HB2	1:C:242:VAL:HG22	1.95	0.49
1:D:10:ASN:HB2	1:D:41:PHE:HA	1.93	0.49
1:C:694:ARG:NE	1:C:719:ASP:OD1	2.43	0.49
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.94	0.49
1:A:528:CYS:HB3	1:B:796:PHE:CZ	2.48	0.49
1:C:188:LYS:HD3	1:C:469:TYR:CZ	2.48	0.49
1:C:196:CYS:HB3	1:C:200:LYS:HB3	1.95	0.49
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.48	0.49
1:A:405:TYR:HA	1:A:424:TYR:HB3	1.94	0.48
1:D:509:LYS:O	1:D:511:LYS:N	2.46	0.48
1:A:537:SER:HB3	1:A:583:ALA:HB2	1.94	0.48
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.95	0.48
1:B:477:ALA:O	1:B:479:LEU:N	2.45	0.48
1:D:809:VAL:HG13	1:D:812:ILE:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:THR:OG1	1:B:277:THR:O	2.28	0.48
1:C:22:ALA:HB1	1:C:25:GLU:HB2	1.95	0.48
1:C:154:ALA:HB1	1:D:183:ASP:HB3	1.94	0.48
1:B:601:VAL:HG22	1:C:803:LEU:HD23	1.95	0.48
1:B:628:ARG:HG2	1:C:628:ARG:HH12	1.77	0.48
1:A:445:VAL:HG13	1:A:448:GLY:HA2	1.94	0.48
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.95	0.48
1:C:445:VAL:HG13	1:C:448:GLY:HA2	1.96	0.48
1:A:207:GLN:O	1:A:211:ILE:HG13	2.14	0.47
1:D:231:ASP:HB3	1:D:234:LYS:HE2	1.96	0.47
1:B:103:THR:N	1:B:112:GLN:OE1	2.38	0.47
1:B:449:LYS:HG2	1:B:450:TYR:H	1.78	0.47
1:B:694:ARG:NE	1:B:719:ASP:OD1	2.48	0.47
1:C:294:GLU:HG3	1:C:338:VAL:HG11	1.96	0.47
1:C:596:LEU:HB3	1:D:809:VAL:HG11	1.96	0.47
1:D:498:LEU:HD23	1:D:705:GLU:HB3	1.95	0.47
1:D:173:LYS:HG2	1:D:177:TYR:HE2	1.79	0.47
1:B:29:PHE:O	1:B:33:MET:HG2	2.13	0.47
1:C:112:GLN:H	1:C:112:GLN:HE21	1.63	0.47
1:C:505:LYS:HZ2	1:C:697:LYS:HA	1.79	0.47
1:D:173:LYS:NZ	1:D:177:TYR:OH	2.46	0.47
1:B:338:VAL:HG23	1:B:345:ILE:HD12	1.97	0.47
1:B:626:VAL:HB	1:C:628:ARG:HE	1.79	0.47
1:D:521:LEU:HD22	1:D:526:TRP:CD2	2.49	0.47
1:A:29:PHE:O	1:A:33:MET:HG2	2.15	0.47
1:A:422:GLU:HG2	1:A:766:TRP:HH2	1.80	0.47
1:A:667:PHE:CE1	1:A:727:LEU:HB3	2.50	0.47
1:D:103:THR:O	1:D:352:LYS:NZ	2.48	0.46
1:B:521:LEU:HD23	1:B:525:ILE:HB	1.97	0.46
1:C:498:LEU:HD23	1:C:705:GLU:HB3	1.97	0.46
1:B:753:LEU:HD22	1:B:758:VAL:HG21	1.97	0.46
1:C:705:GLU:OE1	1:C:732:TYR:OH	2.27	0.46
1:C:711:TYR:HB2	1:C:767:TRP:NE1	2.31	0.46
1:D:445:VAL:HG13	1:D:448:GLY:HA2	1.97	0.46
1:A:337:GLN:NE2	2:E:1:NAG:H2	2.31	0.46
1:B:114:ARG:NH1	1:B:280:TYR:OH	2.48	0.46
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.96	0.46
1:C:629:MET:O	1:C:631:SER:N	2.48	0.46
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.70	0.46
1:D:800:VAL:HA	1:D:803:LEU:HB2	1.97	0.46
1:C:427:ASP:HB2	1:C:762:LEU:HD21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.51	0.46
1:B:608:PHE:CD1	1:C:799:LEU:HD22	2.50	0.46
1:A:171:ASP:OD1	1:A:172:LYS:N	2.49	0.46
1:C:597:SER:O	1:C:600:ILE:HG12	2.15	0.46
1:D:512:PRO:HB2	1:D:513:GLY:H	1.54	0.46
1:B:138:ASP:HB3	1:B:166:GLY:HA3	1.98	0.46
1:C:517:PHE:HB2	1:C:791:ASN:OD1	2.16	0.46
1:A:79:LYS:HD3	1:A:139:SER:O	2.16	0.45
1:A:683:VAL:HB	1:A:688:GLU:HB3	1.98	0.45
1:B:763:LYS:O	1:B:767:TRP:HB2	2.16	0.45
1:B:451:GLY:O	1:B:485:ARG:NH2	2.50	0.45
1:C:198:ARG:NH2	1:C:199:ASP:OD1	2.49	0.45
1:C:480:THR:O	1:C:485:ARG:NH1	2.44	0.45
1:B:450:TYR:HA	1:B:463:MET:HE2	1.98	0.45
1:D:89:CYS:SG	1:D:96:PHE:HB2	2.57	0.45
1:A:705:GLU:OE1	1:A:732:TYR:OH	2.21	0.45
1:C:52:VAL:HG22	1:C:78:ASP:HB2	1.98	0.45
1:C:178:ARG:HA	1:C:211:ILE:HD11	1.98	0.45
1:D:607:PHE:O	1:D:611:ILE:HG12	2.16	0.45
1:D:763:LYS:O	1:D:767:TRP:HB2	2.16	0.45
1:C:30:ARG:NH2	1:C:269:GLU:OE2	2.49	0.45
1:B:406:VAL:HG23	1:B:425:CYS:HB2	1.98	0.45
1:B:499:GLY:O	1:B:706:SER:N	2.50	0.45
1:B:521:LEU:HB2	1:B:616:TYR:CD1	2.52	0.45
1:A:38:THR:OG1	1:A:39:SER:N	2.50	0.45
1:C:708:MET:O	1:C:712:ILE:HG12	2.17	0.45
1:B:788:SER:C	1:B:790:SER:H	2.20	0.44
1:C:130:TRP:CE2	1:C:191:ARG:HD3	2.52	0.44
1:D:481:ILE:HD11	1:D:733:GLY:HA3	1.98	0.44
1:B:539:VAL:HG21	1:C:803:LEU:HB3	1.99	0.44
1:A:711:TYR:HB2	1:A:767:TRP:NE1	2.32	0.44
1:B:205:VAL:O	1:B:209:ILE:HG13	2.17	0.44
1:C:407:MET:N	1:C:422:GLU:O	2.43	0.44
1:A:332:ALA:O	1:A:336:VAL:HG23	2.17	0.44
1:C:188:LYS:HD2	1:C:459:ILE:HG23	1.99	0.44
1:C:626:VAL:O	1:C:630:VAL:HG23	2.18	0.44
1:A:382:LEU:HD22	1:A:382:LEU:O	2.18	0.44
1:B:366:ASN:OD1	1:B:366:ASN:N	2.46	0.44
1:A:529:ILE:HD12	1:A:612:ILE:HG21	1.99	0.44
1:B:372:GLY:HA3	1:B:382:LEU:HA	2.00	0.44
1:C:450:TYR:O	1:C:463:MET:N	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.99	0.44
1:D:758:VAL:O	1:D:762:LEU:HB2	2.17	0.44
1:A:195:ASP:HA	1:A:223:ALA:HB3	2.00	0.44
1:B:539:VAL:O	1:B:543:VAL:HG23	2.18	0.44
1:B:604:VAL:HG11	1:C:802:GLY:HA3	2.00	0.44
1:C:18:PHE:HA	1:C:19:PRO:HD3	1.90	0.44
1:C:486:GLU:O	1:C:738:LYS:NZ	2.51	0.44
1:A:422:GLU:HG2	1:A:766:TRP:CH2	2.53	0.44
1:B:232:LEU:HD22	1:B:363:LEU:HD22	2.00	0.44
1:C:91:THR:HG21	1:D:56:PHE:CZ	2.53	0.44
1:B:18:PHE:HA	1:B:19:PRO:HD3	1.86	0.43
1:D:728:ASP:N	1:D:728:ASP:OD1	2.50	0.43
1:B:48:ASP:OD2	1:B:65:GLN:NE2	2.41	0.43
1:B:102:PRO:HD3	1:B:114:ARG:HD2	1.98	0.43
1:B:173:LYS:HZ1	1:B:200:LYS:HE3	1.82	0.43
1:C:511:LYS:HG2	1:C:512:PRO:HD2	2.01	0.43
1:C:795:VAL:O	1:C:798:ILE:HG22	2.18	0.43
1:D:466:GLU:HG2	1:D:471:LYS:HD2	2.00	0.43
1:B:638:ASP:OD1	1:B:638:ASP:N	2.52	0.43
1:A:118:LYS:HB2	1:A:118:LYS:HE3	1.80	0.43
1:B:523:TYR:O	1:B:527:MET:HG2	2.19	0.43
1:C:62:PHE:CE2	1:C:88:PHE:HB3	2.53	0.43
1:D:299:LEU:HD13	1:D:306:ILE:HG21	2.01	0.43
1:C:44:THR:HA	1:C:45:PRO:HD3	1.89	0.43
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.99	0.43
1:D:765:LYS:HA	1:D:769:ASP:HB2	2.01	0.43
1:D:121:LEU:O	1:D:125:ILE:HG13	2.18	0.43
1:D:491:PHE:CE1	1:D:735:ALA:HB2	2.54	0.43
1:C:405:TYR:HA	1:C:424:TYR:HB3	2.00	0.43
1:C:499:GLY:O	1:C:706:SER:N	2.47	0.43
1:D:96:PHE:HE1	1:D:98:THR:HB	1.84	0.43
1:A:62:PHE:HE2	1:A:92:LEU:HD12	1.84	0.43
1:A:101:PHE:HA	1:A:102:PRO:HD3	1.87	0.43
1:A:102:PRO:HA	1:A:112:GLN:HG2	1.99	0.43
1:A:610:LEU:HD21	1:B:613:ILE:HG21	2.01	0.42
1:D:201:VAL:O	1:D:205:VAL:HG23	2.19	0.42
1:D:253:SER:HA	1:D:256:SER:HB3	2.00	0.42
1:A:686:THR:HG21	1:A:708:MET:SD	2.59	0.42
1:B:445:VAL:HG13	1:B:448:GLY:HA2	2.02	0.42
1:B:601:VAL:HG23	1:C:806:ALA:HB3	2.00	0.42
1:A:405:TYR:CD2	1:A:478:PRO:HG3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:OG1	1:B:39:SER:N	2.52	0.42
1:B:79:LYS:HZ1	1:B:80:LYS:HE3	1.85	0.42
1:D:512:PRO:HA	1:D:790:SER:HB2	2.01	0.42
1:A:36:PHE:CZ	1:A:290:GLN:HB2	2.54	0.42
1:A:99:PRO:O	1:A:114:ARG:HD2	2.20	0.42
1:A:400:ILE:HG22	1:A:477:ALA:HB1	2.01	0.42
1:C:400:ILE:HA	1:C:445:VAL:HG12	2.02	0.42
1:B:219:HIS:ND1	1:B:241:GLU:O	2.46	0.42
1:B:654:SER:OG	1:B:730:LYS:NZ	2.40	0.42
1:B:325:GLN:H	1:B:325:GLN:CD	2.23	0.42
1:B:464:VAL:HG13	1:B:489:ILE:HD13	2.02	0.42
1:D:385:ASP:OD1	1:D:385:ASP:N	2.52	0.42
1:B:628:ARG:HG2	1:C:628:ARG:NH1	2.35	0.42
1:C:13:GLN:HG3	1:C:44:THR:O	2.20	0.42
1:C:672:THR:HG23	1:C:675:ARG:NH2	2.35	0.42
1:A:162:ALA:HB3	1:B:150:LEU:HD13	2.01	0.42
1:C:56:PHE:CE1	1:D:91:THR:HG21	2.55	0.42
1:D:114:ARG:HA	1:D:115:PRO:HD3	1.90	0.42
1:D:380:MET:HE3	1:D:380:MET:HB2	1.93	0.41
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.55	0.41
1:B:79:LYS:NZ	1:B:80:LYS:HE3	2.34	0.41
1:B:96:PHE:HE1	1:B:98:THR:HB	1.85	0.41
1:B:706:SER:O	1:B:710:GLU:HG2	2.20	0.41
1:B:115:PRO:HA	1:B:353:ARG:HB2	2.02	0.41
1:C:287:ASP:OD2	1:C:341:LEU:N	2.52	0.41
1:D:261:ARG:NH2	1:D:264:THR:OG1	2.53	0.41
1:B:184:LEU:HA	1:B:184:LEU:HD23	1.82	0.41
1:A:500:ILE:O	1:A:727:LEU:HG	2.20	0.41
1:D:30:ARG:HH22	1:D:269:GLU:HG3	1.84	0.41
1:D:360:ILE:HG12	1:D:380:MET:HE1	2.02	0.41
1:A:656:LYS:HE3	1:A:682:PHE:CZ	2.56	0.41
1:A:115:PRO:HA	1:A:353:ARG:HB2	2.01	0.41
1:B:787:LEU:HD22	1:B:787:LEU:HA	1.92	0.41
1:C:401:LEU:HD23	1:C:406:VAL:HG12	2.03	0.41
1:C:702:TYR:CE2	1:C:704:LEU:HB3	2.56	0.41
1:A:154:ALA:HB1	1:B:183:ASP:HB3	2.03	0.41
1:B:521:LEU:HB2	1:B:616:TYR:HD1	1.84	0.41
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.88	0.41
1:B:181:PHE:HA	1:B:184:LEU:HB2	2.02	0.41
1:B:200:LYS:HD2	1:B:200:LYS:HA	1.88	0.41
1:B:364:LYS:HB3	1:B:365:THR:H	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:LEU:HD23	1:B:467:LEU:HA	1.90	0.41
1:B:621:ALA:O	1:B:625:THR:OG1	2.28	0.41
1:C:24:GLN:HG3	1:C:262:TRP:HZ2	1.85	0.41
1:C:403:SER:HA	1:C:404:PRO:HA	1.72	0.41
1:A:626:VAL:O	1:A:630:VAL:HG23	2.21	0.41
1:A:787:LEU:HB2	1:D:619:ASN:ND2	2.35	0.41
1:B:406:VAL:HG22	1:B:426:VAL:HG23	2.03	0.41
1:C:30:ARG:HH22	1:C:269:GLU:HG3	1.86	0.41
1:D:101:PHE:HA	1:D:114:ARG:HD2	2.03	0.41
1:D:805:LEU:O	1:D:809:VAL:HG23	2.21	0.41
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.56	0.40
1:A:659:PHE:CE2	1:A:703:LEU:HD13	2.56	0.40
1:B:25:GLU:OE1	1:B:25:GLU:N	2.53	0.40
1:B:173:LYS:HG2	1:B:177:TYR:HE2	1.86	0.40
1:C:10:ASN:HB2	1:C:41:PHE:HA	2.03	0.40
1:C:91:THR:HG21	1:D:56:PHE:CE2	2.56	0.40
1:B:511:LYS:HA	1:B:512:PRO:HD3	1.90	0.40
1:C:265:LEU:O	1:C:274:HIS:ND1	2.45	0.40
1:C:430:ALA:O	1:C:434:LYS:N	2.53	0.40
1:C:522:ALA:HB3	1:C:525:ILE:HG13	2.02	0.40
1:D:468:VAL:HG23	1:D:469:TYR:CD1	2.57	0.40
1:D:489:ILE:HG22	1:D:737:PRO:HA	2.02	0.40
1:A:803:LEU:HD23	1:A:803:LEU:HA	1.96	0.40
1:D:153:ALA:HA	1:D:158:TRP:HB2	2.04	0.40
1:D:247:ILE:HD13	1:D:358:ILE:HG12	2.03	0.40
1:D:318:ASN:HA	1:D:319:PRO:HA	1.84	0.40
1:D:375:SER:HB3	1:D:378:ASP:HB2	2.02	0.40
1:D:514:VAL:HG13	1:D:794:GLY:HA3	2.03	0.40
1:B:623:PHE:CZ	1:C:786:ALA:HA	2.56	0.40
1:C:237:PHE:CD1	1:C:365:THR:HG23	2.56	0.40
1:A:528:CYS:HB3	1:B:796:PHE:HZ	1.86	0.40
1:A:628:ARG:NH2	1:D:628:ARG:HG2	2.37	0.40
1:B:136:LEU:HD22	1:B:163:ILE:HB	2.04	0.40
1:B:237:PHE:HB2	1:D:210:THR:HG22	2.04	0.40
1:B:360:ILE:HG22	1:B:371:ILE:HG12	2.03	0.40
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	760/822 (92%)	693 (91%)	61 (8%)	6 (1%)	19	59
1	B	760/822 (92%)	703 (92%)	50 (7%)	7 (1%)	17	56
1	C	760/822 (92%)	698 (92%)	57 (8%)	5 (1%)	22	62
1	D	760/822 (92%)	702 (92%)	52 (7%)	6 (1%)	19	59
All	All	3040/3288 (92%)	2796 (92%)	220 (7%)	24 (1%)	19	59

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	512	PRO
1	C	597	SER
1	D	512	PRO
1	A	143	LEU
1	B	390	LEU
1	B	393	LYS
1	C	140	ASP
1	C	630	VAL
1	D	510	SER
1	A	597	SER
1	B	384	GLU
1	D	385	ASP
1	A	584	PHE
1	B	394	THR
1	B	584	PHE
1	B	632	PRO
1	C	633	ILE
1	A	142	GLY
1	A	198	ARG
1	A	387	THR
1	D	82	VAL
1	D	584	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	632	PRO
1	C	389	GLY

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	636/702 (91%)	615 (97%)	21 (3%)	38	61
1	B	635/702 (90%)	613 (96%)	22 (4%)	36	60
1	C	635/702 (90%)	617 (97%)	18 (3%)	43	65
1	D	635/702 (90%)	616 (97%)	19 (3%)	41	63
All	All	2541/2808 (90%)	2461 (97%)	80 (3%)	40	62

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	60	ASN
1	A	65	GLN
1	A	112	GLN
1	A	165	VAL
1	A	183	ASP
1	A	219	HIS
1	A	248	VAL
1	A	275	THR
1	A	308	ARG
1	A	314	ASP
1	A	323	TRP
1	A	366	ASN
1	A	380	MET
1	A	382	LEU
1	A	401	LEU
1	A	413	GLU
1	A	484	VAL
1	A	498	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	642	GLN
1	A	643	THR
1	B	87	SER
1	B	93	HIS
1	B	139	SER
1	B	140	ASP
1	B	210	THR
1	B	252	ASP
1	B	274	HIS
1	B	308	ARG
1	B	323	TRP
1	B	325	GLN
1	B	387	THR
1	B	390	LEU
1	B	394	THR
1	B	413	GLU
1	B	473	ASP
1	B	497	SER
1	B	498	LEU
1	B	612	ILE
1	B	642	GLN
1	B	744	THR
1	B	787	LEU
1	B	815	CYS
1	C	65	GLN
1	C	112	GLN
1	C	189	GLU
1	C	191	ARG
1	C	194	LEU
1	C	206	ASP
1	C	216	LYS
1	C	263	SER
1	C	323	TRP
1	C	413	GLU
1	C	414	MET
1	C	498	LEU
1	C	642	GLN
1	C	661	ARG
1	C	668	ASP
1	C	676	SER
1	C	785	SER
1	C	787	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	79	LYS
1	D	112	GLN
1	D	194	LEU
1	D	235	ILE
1	D	259	ILE
1	D	323	TRP
1	D	327	VAL
1	D	366	ASN
1	D	380	MET
1	D	388	SER
1	D	394	THR
1	D	454	ASP
1	D	498	LEU
1	D	521	LEU
1	D	538	VAL
1	D	614	SER
1	D	631	SER
1	D	642	GLN
1	D	736	THR

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

Mol	Chain	Res	Type
1	A	337	GLN
1	A	344	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)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	0.77	0
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	0.76	0
2	NAG	F	1	1,2	14,14,15	0.68	0	17,19,21	0.97	1 (5%)
2	NAG	F	2	2	14,14,15	0.54	0	17,19,21	0.71	0
2	NAG	G	1	1,2	14,14,15	0.52	0	17,19,21	0.89	0
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C4-C3-C2	2.03	113.99	111.02

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6

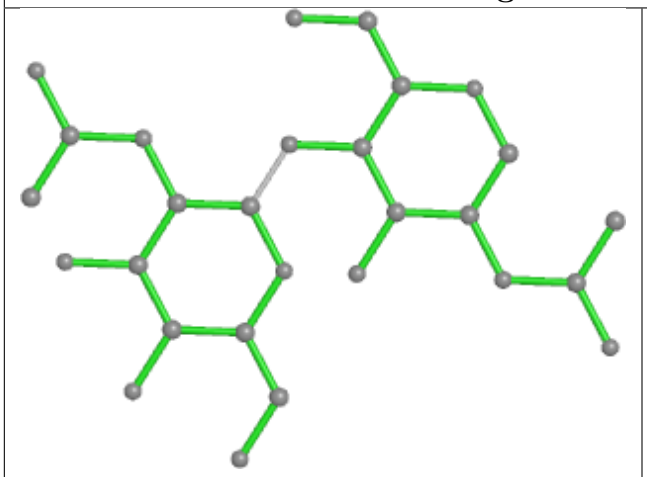
There are no ring outliers.

1 monomer is involved in 2 short contacts:

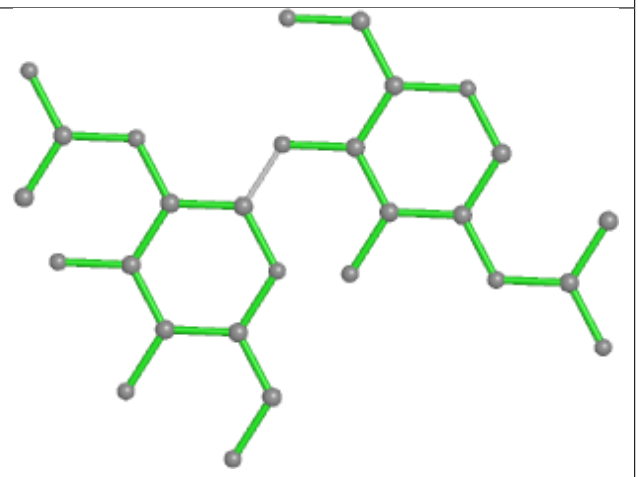
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0

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

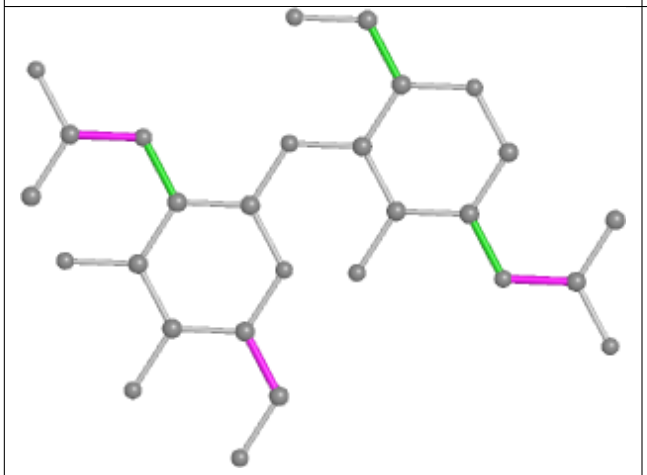
Oligosaccharide Chain E



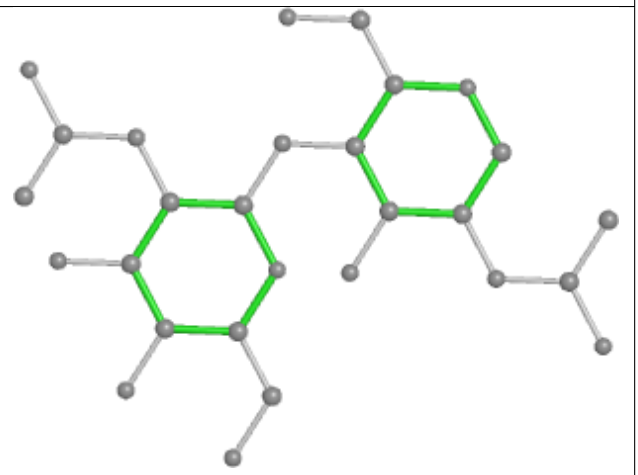
Bond lengths



Bond angles

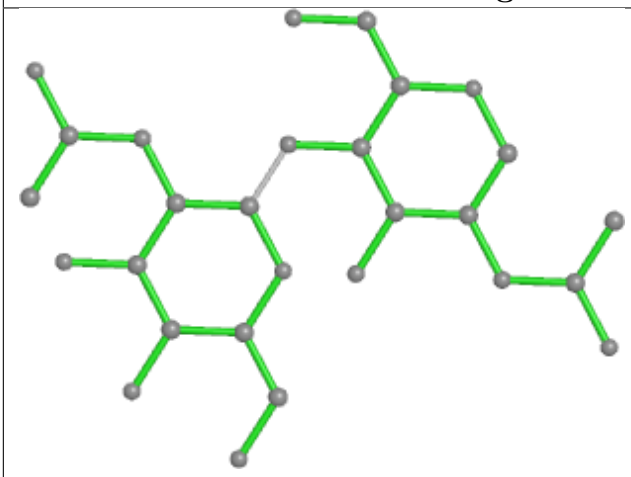


Torsions

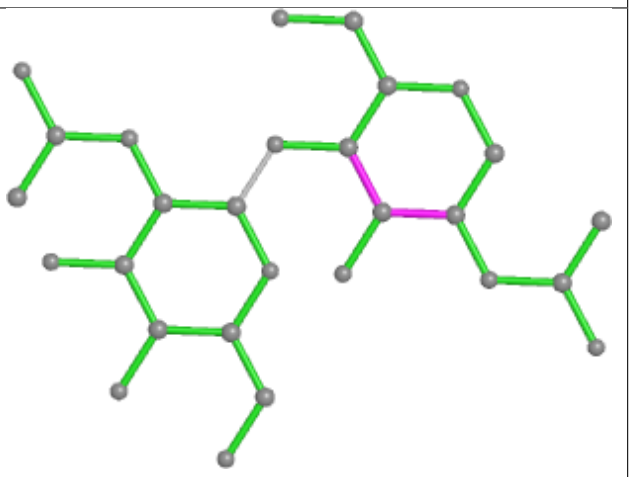


Rings

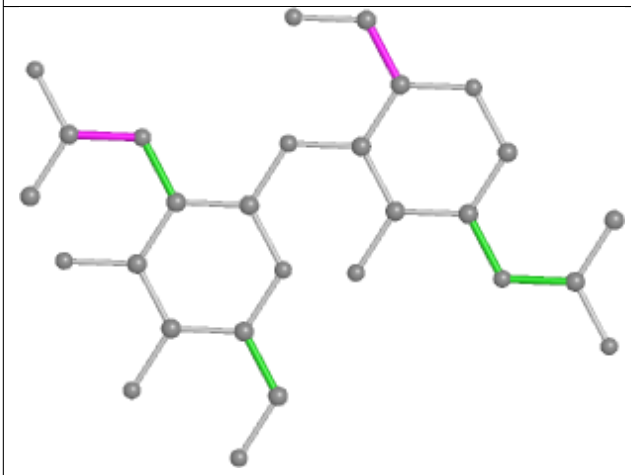
Oligosaccharide Chain F



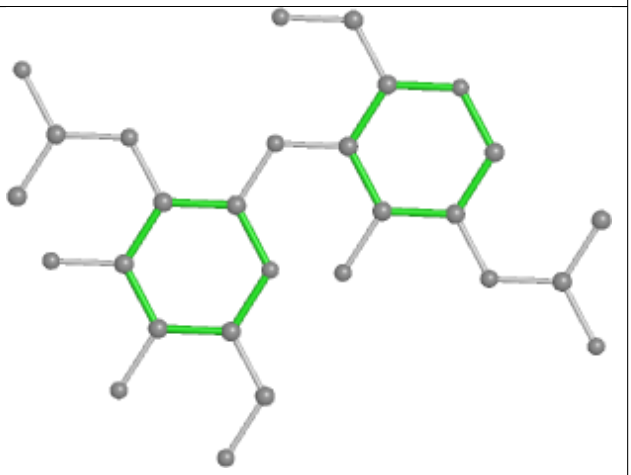
Bond lengths



Bond angles

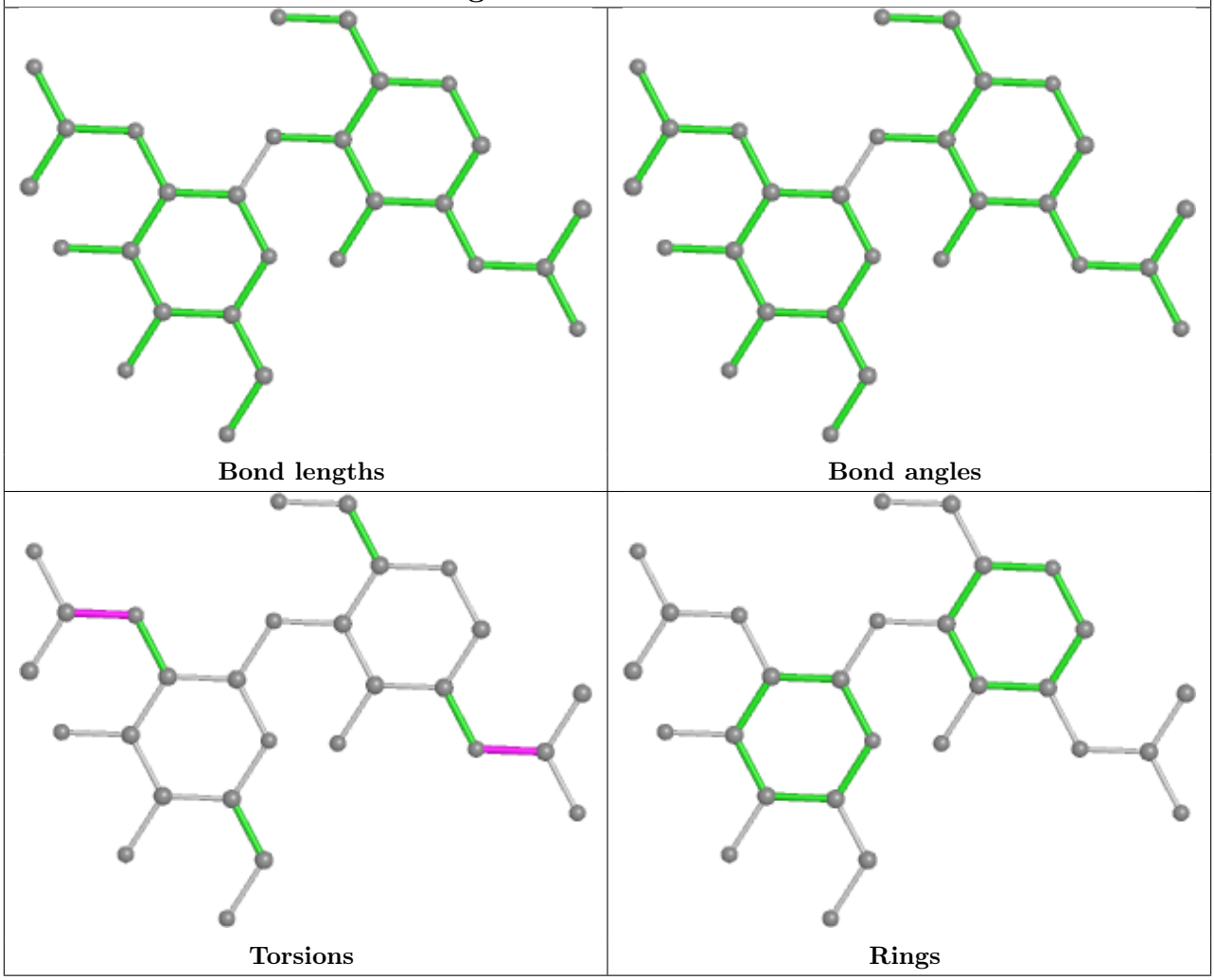


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
4	NAG	D	901	1	14,14,15	0.52	0	17,19,21	1.07	2 (11%)
3	NWD	D	902	-	14,17,17	2.19	5 (35%)	16,24,24	3.40	5 (31%)
3	NWD	C	903	-	14,17,17	2.15	4 (28%)	16,24,24	3.39	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NWD	A	903	-	14,17,17	2.18	5 (35%)	16,24,24	3.57	6 (37%)
3	NWD	B	903	-	14,17,17	2.22	5 (35%)	16,24,24	3.56	6 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	901	1	-	4/6/23/26	0/1/1/1
3	NWD	D	902	-	-	2/10/12/12	0/1/1/1
3	NWD	C	903	-	-	4/10/12/12	0/1/1/1
3	NWD	A	903	-	-	2/10/12/12	0/1/1/1
3	NWD	B	903	-	-	2/10/12/12	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	NWD	C6-N1	4.07	1.45	1.37
3	B	903	NWD	C6-N1	3.92	1.44	1.37
3	A	903	NWD	C2-N1	3.89	1.43	1.37
3	D	902	NWD	C2-N1	3.89	1.43	1.37
3	A	903	NWD	C6-N1	3.87	1.44	1.37
3	C	903	NWD	C2-N1	3.80	1.43	1.37
3	D	902	NWD	C6-N1	3.77	1.44	1.37
3	B	903	NWD	C7-N1	-3.75	1.42	1.47
3	B	903	NWD	C2-N1	3.53	1.42	1.37
3	D	902	NWD	C7-N1	-3.42	1.43	1.47
3	B	903	NWD	C7-C8	-3.34	1.49	1.53
3	A	903	NWD	C7-N1	-3.33	1.43	1.47
3	C	903	NWD	C7-C8	-3.00	1.49	1.53
3	C	903	NWD	C7-N1	-2.95	1.43	1.47
3	D	902	NWD	C7-C8	-2.94	1.49	1.53
3	A	903	NWD	C7-C8	-2.93	1.49	1.53
3	D	902	NWD	C5-C4	2.28	1.50	1.47
3	A	903	NWD	C5-C4	2.22	1.49	1.47
3	B	903	NWD	C5-C4	2.22	1.49	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	903	NWD	C5-C4-N3	12.51	118.44	112.19
3	B	903	NWD	C5-C4-N3	12.35	118.35	112.19
3	C	903	NWD	C5-C4-N3	12.00	118.18	112.19
3	D	902	NWD	C5-C4-N3	11.86	118.11	112.19
3	A	903	NWD	C4-N3-C2	-3.40	122.95	127.35
3	D	902	NWD	C4-N3-C2	-3.37	122.99	127.35
3	B	903	NWD	C7-N1-C2	-3.21	115.26	118.53
3	B	903	NWD	C6-N1-C2	3.18	124.61	121.29
3	B	903	NWD	C4-N3-C2	-3.14	123.28	127.35
3	C	903	NWD	C4-N3-C2	-3.14	123.29	127.35
3	A	903	NWD	C6-N1-C2	2.96	124.38	121.29
3	B	903	NWD	C6-C5-N2	2.90	120.68	116.32
3	A	903	NWD	C6-C5-N2	2.72	120.42	116.32
3	D	902	NWD	O4-C4-C5	2.59	122.33	118.98
3	D	902	NWD	C6-N1-C2	2.56	123.97	121.29
3	B	903	NWD	O4-C4-C5	2.43	122.11	118.98
3	C	903	NWD	C6-C5-N2	2.40	119.94	116.32
3	C	903	NWD	O4-C4-C5	2.40	122.07	118.98
3	A	903	NWD	O4-C4-C5	2.35	122.01	118.98
3	D	902	NWD	C6-C5-N2	2.34	119.83	116.32
4	D	901	NAG	O5-C1-C2	2.24	114.83	111.29
3	A	903	NWD	C7-N1-C2	-2.23	116.26	118.53
3	C	903	NWD	C7-N1-C2	-2.15	116.34	118.53
4	D	901	NAG	O5-C5-C6	2.05	110.42	107.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	NWD	C4-C5-N2-O1
3	A	903	NWD	C6-C5-N2-O1
3	B	903	NWD	C6-C5-N2-O1
3	C	903	NWD	C8-C7-N1-C2
4	D	901	NAG	C8-C7-N2-C2
4	D	901	NAG	O7-C7-N2-C2
4	D	901	NAG	O5-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
3	D	902	NWD	C6-C5-N2-O1
3	B	903	NWD	C4-C5-N2-O1
3	D	902	NWD	C4-C5-N2-O1
3	C	903	NWD	C8-C7-N1-C6
3	C	903	NWD	C6-C5-N2-O1
3	C	903	NWD	C4-C5-N2-O1

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)

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

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

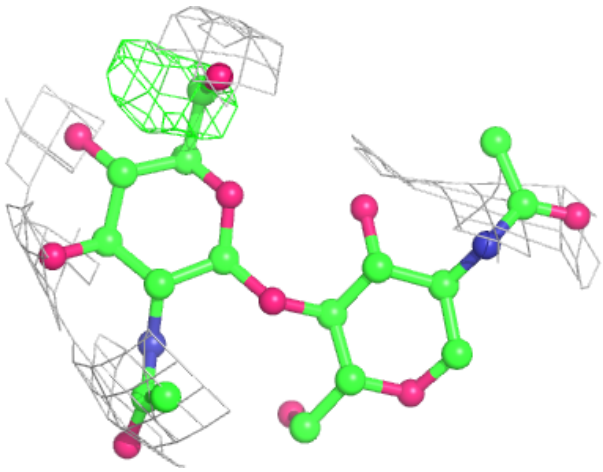
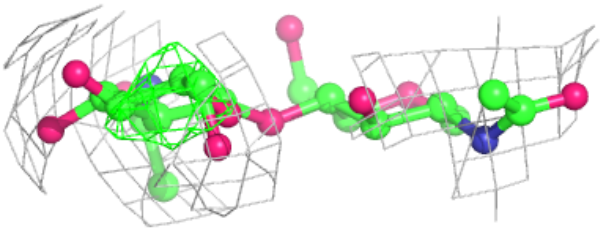
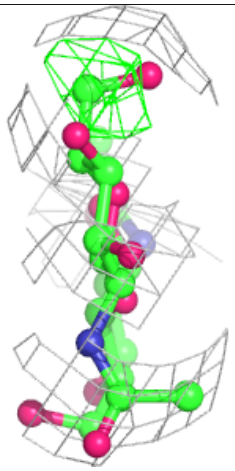
Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

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

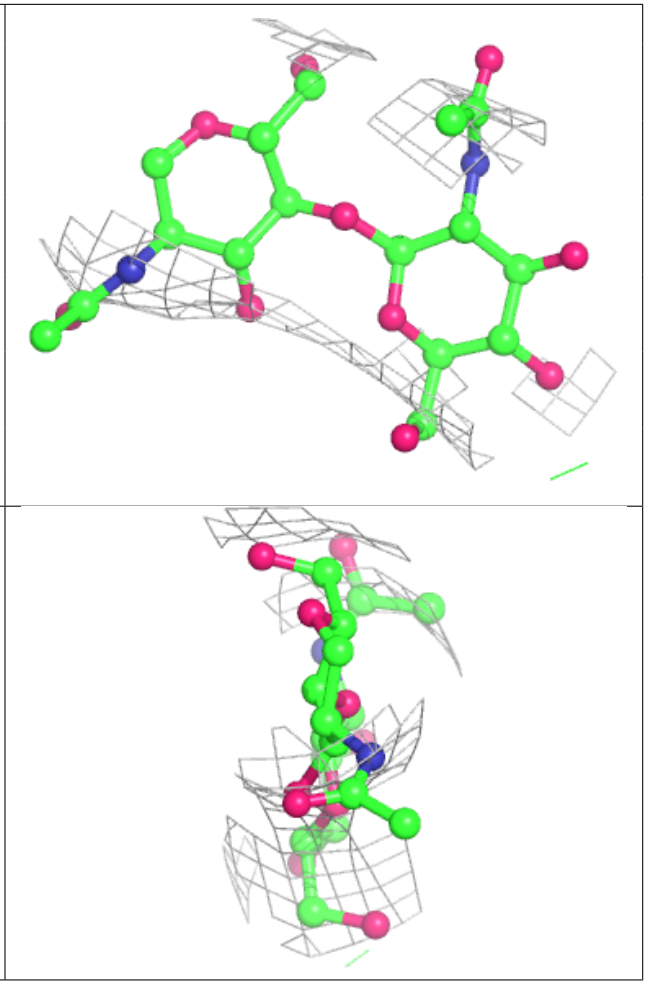
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

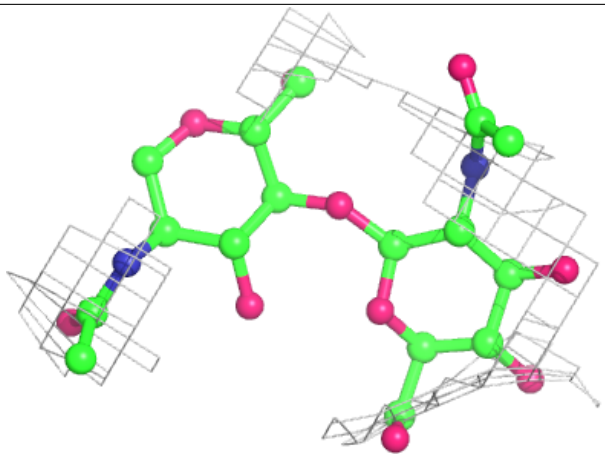
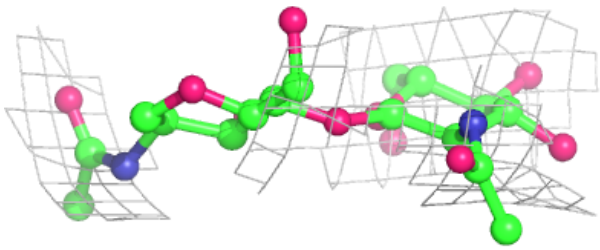
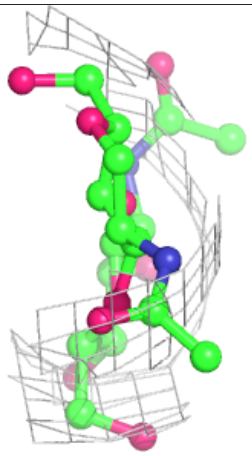
<table>
<tr><td>Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)</td><td>  </td></tr>
<tr><td>  </td><td>  </td></tr>
</table>

Electron density around Chain F:

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



Electron density around Chain G: $2mF_o$-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.