



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:41 AM BST

PDB ID : 6GRS
Title : Paired immunoglobulin-like receptor B (PirB) or Leukocyte immunoglobulin-like receptor subfamily B member 3 (LILRB3) full extracellular domain
Authors : Vlieg, H.C.; Huizinga, E.G.; Janssen, B.J.C.
Deposited on : 2018-06-12
Resolution : 3.40 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

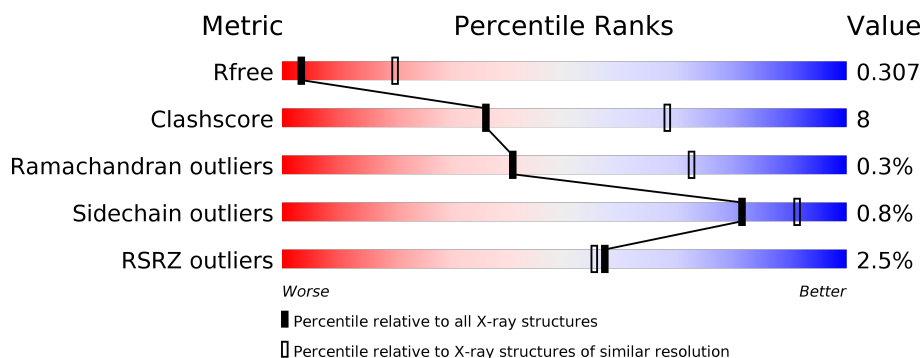
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on 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 $\leq 5\%$. 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	606	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>5%</div> </div> </div>
1	B	606	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>•</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9209 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.

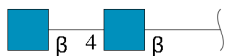
- Molecule 1 is a protein called Paired immunoglobulin-like receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4557	2886	775	875	21			
1	B	587	Total	C	N	O	S	0	0	0
			4610	2917	783	889	21			

There are 22 discrepancies between the modelled and reference sequences:

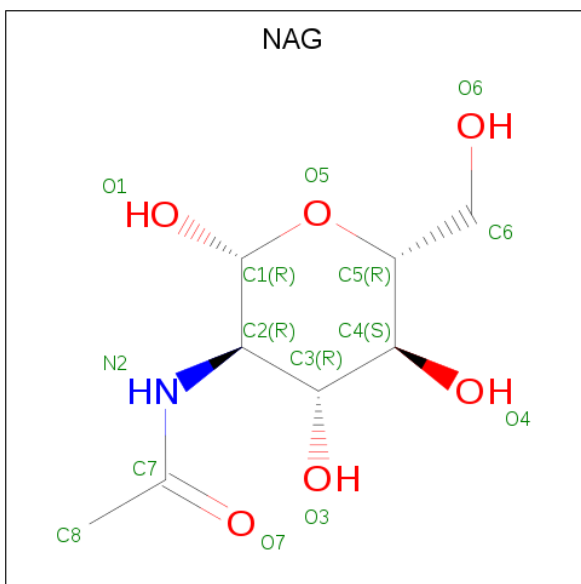
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP Q8K4V6
A	24	SER	-	expression tag	UNP Q8K4V6
A	620	ALA	-	expression tag	UNP Q8K4V6
A	621	ALA	-	expression tag	UNP Q8K4V6
A	622	ALA	-	expression tag	UNP Q8K4V6
A	623	HIS	-	expression tag	UNP Q8K4V6
A	624	HIS	-	expression tag	UNP Q8K4V6
A	625	HIS	-	expression tag	UNP Q8K4V6
A	626	HIS	-	expression tag	UNP Q8K4V6
A	627	HIS	-	expression tag	UNP Q8K4V6
A	628	HIS	-	expression tag	UNP Q8K4V6
B	23	GLY	-	expression tag	UNP Q8K4V6
B	24	SER	-	expression tag	UNP Q8K4V6
B	620	ALA	-	expression tag	UNP Q8K4V6
B	621	ALA	-	expression tag	UNP Q8K4V6
B	622	ALA	-	expression tag	UNP Q8K4V6
B	623	HIS	-	expression tag	UNP Q8K4V6
B	624	HIS	-	expression tag	UNP Q8K4V6
B	625	HIS	-	expression tag	UNP Q8K4V6
B	626	HIS	-	expression tag	UNP Q8K4V6
B	627	HIS	-	expression tag	UNP Q8K4V6
B	628	HIS	-	expression tag	UNP Q8K4V6

- 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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.

- Chain A:
-
- 4% 76% 19% 5%
- GLY SER SER LEU PRQ LYS P29 R32 V38 Y39 S40 V117 V33 Y121 Y122 T123 V134 K44 F48 E51 N56 E57 Y58 R59 L60 Y61 K62 D63 GLY LYS L66 K72 N73 K74 Q75 K76 P77 P77 A78 N79 K80 A81 E82 S86 N87 V88 D89 L90 S91 N92 A93 Y96 E97 C98 S99 Y100 Y103
- T102 Q103 G108 Y109 S110 D111 V177 V293 Y296 W303 P306 S307 D308 L312 V313 V314 T315 P323 L341 P347 D350 K351 L354 T355 K356 E357 D366 S372 T388 P393 P399 W406 S410 Q414 L420 T421 K422 K423 P424 D435 P436 L442 Y446
- S446 D451 L455 Q465 F475 S476 V477 F480 H499 N500 I501 S502 L520 L523 P524 S525 L526 S527 V528 K529 P530 N531 H535 SER GLY GLU THR V540 S541 S542 L543 C544 W545 S546 M547 I554 L555 S556 K557 E558 GLY SER SER ALA Q562 L565 R566 L567 O575

- Chain B:
-
- | Amino Acid | Count | Percentage |
|------------|-------|------------|
| GLY | 1 | 0.25% |
| SER | 1 | 0.25% |
| SER | 1 | 0.25% |
| L26 | 1 | 0.25% |
| P29 | 1 | 0.25% |
| Q34 | 1 | 0.25% |
| S40 | 1 | 0.25% |
| T43 | 1 | 0.25% |
| F47 | 1 | 0.25% |
| F48 | 1 | 0.25% |
| C49 | 1 | 0.25% |
| E50 | 1 | 0.25% |
| A55 | 1 | 0.25% |
| Y58 | 1 | 0.25% |
| R59 | 1 | 0.25% |
| H73 | 1 | 0.25% |
| LYS | 1 | 0.25% |
| GLN | 1 | 0.25% |
| LYS | 1 | 0.25% |
| PRO | 1 | 0.25% |
| ALA | 1 | 0.25% |
| H79 | 1 | 0.25% |
| R80 | 1 | 0.25% |
| F83 | 1 | 0.25% |
| N87 | 1 | 0.25% |
| V88 | 1 | 0.25% |
| D89 | 1 | 0.25% |
| L90 | 1 | 0.25% |
| S91 | 1 | 0.25% |
| N92 | 1 | 0.25% |
| A93 | 1 | 0.25% |
| S101 | 1 | 0.25% |
| S107 | 1 | 0.25% |
| S110 | 1 | 0.25% |
| V117 | 1 | 0.25% |
| W122 | 1 | 0.25% |
| L142 | 1 | 0.25% |
| Q143 | 1 | 0.25% |
| C144 | 1 | 0.25% |
| E145 | 1 | 0.25% |
| H148 | 1 | 0.25% |
| M149 | 1 | 0.25% |
| D150 | 1 | 0.25% |

ALA
HIS
HIS
HIS
HIS
HIS
HIS

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

Chain C:



NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.69Å 185.29Å 99.08Å 90.00° 105.56° 90.00°	Depositor
Resolution (Å)	52.69 – 3.40 52.69 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (52.69-3.40) 98.5 (52.69-3.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.256 , 0.307 0.256 , 0.307	Depositor DCC
R_{free} test set	1268 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	108.8	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9209	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.25	0/4680	0.45	0/6362
1	B	0.25	0/4735	0.46	0/6441
All	All	0.25	0/9415	0.46	0/12803

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	4557	0	4400	71	0
1	B	4610	0	4450	77	0
2	C	28	0	25	1	0
3	B	14	0	13	0	0
All	All	9209	0	8888	145	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 8.

All (145) 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:150:ASP:OD1	1:B:206:TYR:OH	1.98	0.81
1:A:523:THR:HG22	1:A:608:SER:HB2	1.69	0.75
1:B:442:LEU:HD12	1:B:455:LEU:HD21	1.73	0.70
1:A:442:LEU:HD12	1:A:455:LEU:HD21	1.78	0.66
1:A:58:TYR:OH	1:A:79:ASN:O	2.12	0.66
1:A:56:ASN:HD22	1:A:103:GLN:HG3	1.62	0.65
1:B:520:LEU:HB2	1:B:607:SER:HA	1.79	0.65
1:A:543:LEU:HD11	1:A:577:GLN:HB2	1.80	0.64
1:A:555:LEU:HB3	1:A:565:LEU:HB2	1.79	0.63
1:A:567:LEU:HD11	1:A:580:PHE:HB2	1.81	0.61
1:A:134:VAL:HG22	1:A:140:VAL:HG21	1.82	0.61
1:B:535:HIS:H	1:B:538:GLU:HG3	1.64	0.60
1:A:38:VAL:O	1:A:176:ARG:NH2	2.34	0.60
1:B:428:THR:HG22	1:B:442:LEU:HD22	1.84	0.60
1:B:143:GLN:NE2	1:B:145:GLU:OE2	2.35	0.60
1:B:271:LEU:HD11	1:B:279:LYS:HE3	1.82	0.59
1:B:493:TYR:HB2	1:B:512:LEU:HD23	1.85	0.59
1:A:356:LYS:HG2	1:A:357:GLU:HG2	1.85	0.58
1:B:142:LEU:HD12	1:B:155:LEU:HD21	1.84	0.58
1:A:142:LEU:HD12	1:A:155:LEU:HD21	1.84	0.58
1:B:87:ASN:OD1	1:B:176:ARG:NH1	2.36	0.58
1:B:356:LYS:HG2	1:B:357:GLU:HG2	1.86	0.57
1:B:93:ALA:HB2	1:B:117:VAL:HG23	1.87	0.57
1:B:529:LYS:HB3	1:B:530:PRO:HD3	1.87	0.56
1:A:244:ILE:HD11	1:A:312:LEU:HD11	1.87	0.56
1:A:123:THR:HG22	1:A:210:PRO:HG2	1.88	0.55
1:B:50:GLU:HA	1:B:80:LYS:HG2	1.88	0.55
1:A:424:PRO:HB3	1:A:446:SER:HB2	1.88	0.55
1:B:594:ARG:HD3	1:B:609:ALA:HB1	1.88	0.54
1:A:32:ARG:HB2	1:A:48:PHE:HB2	1.87	0.54
1:B:341:LEU:HD13	1:B:354:LEU:HD21	1.89	0.54
1:A:341:LEU:HD13	1:A:354:LEU:HD21	1.90	0.54
1:B:350:ASP:HB2	1:B:399:PHE:HA	1.89	0.54
1:B:247:GLN:HG2	1:B:277:LYS:HG2	1.89	0.53
1:B:440:LEU:HD11	1:B:482:LEU:HD12	1.91	0.53
1:A:76:LYS:HG3	1:A:77:PRO:HD2	1.89	0.53
1:B:573:ASP:HB2	1:B:575:GLN:HG2	1.91	0.53
1:B:216:GLU:O	1:B:264:LYS:NZ	2.42	0.53
1:A:414:GLN:NE2	1:A:465:GLN:OE1	2.42	0.53
1:B:59:ARG:HH12	1:B:101:SER:HB2	1.72	0.53
1:B:434:LEU:HD12	1:B:440:LEU:HD23	1.90	0.53
1:B:244:ILE:HD11	1:B:312:LEU:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD11	1:A:279:LYS:HE3	1.90	0.52
1:B:542:LEU:HD21	1:B:555:LEU:HD21	1.91	0.52
1:A:351:LYS:HD2	1:B:224:GLN:HE22	1.75	0.51
1:B:40:SER:O	1:B:43:THR:OG1	2.29	0.51
1:A:442:LEU:HB2	1:A:480:PHE:HB2	1.93	0.51
1:B:148:HIS:ND1	1:B:150:ASP:OD2	2.44	0.51
1:B:554:ILE:HD12	1:B:606:LEU:HD21	1.93	0.51
1:A:350:ASP:HB2	1:A:399:PHE:HA	1.93	0.51
1:A:40:SER:O	1:A:43:THR:OG1	2.29	0.50
1:B:554:ILE:HG12	1:B:566:ARG:HG2	1.93	0.50
1:A:313:VAL:HG11	1:A:406:TRP:CD2	2.47	0.49
1:B:225:LYS:HG2	1:B:305:GLN:HB2	1.94	0.49
1:B:259:ASN:HB3	1:B:263:GLN:HB2	1.93	0.49
1:A:201:ASP:OD1	1:A:202:ARG:N	2.45	0.49
1:B:534:VAL:HB	1:B:538:GLU:HB2	1.94	0.49
1:A:347:PHE:HE2	1:A:399:PHE:HZ	1.60	0.49
1:A:445:TYR:HB3	1:A:477:VAL:HG22	1.95	0.49
1:A:530:PRO:HG2	1:A:540:VAL:HG22	1.95	0.49
1:A:89:ASP:OD1	1:A:90:LEU:N	2.44	0.49
1:B:515:LEU:HD13	1:B:606:LEU:HD11	1.93	0.49
1:B:149:ASN:OD1	1:B:204:ARG:NH1	2.44	0.48
1:A:356:LYS:NZ	1:A:388:THR:O	2.42	0.48
1:A:420:LEU:HD11	1:B:501:LEU:HB2	1.96	0.48
1:B:47:PHE:HB2	1:B:83:PHE:HB2	1.95	0.48
1:A:134:VAL:HG13	1:A:140:VAL:HG23	1.96	0.48
1:A:351:LYS:HG2	1:A:366:ASP:HA	1.95	0.47
1:A:88:VAL:HG13	1:A:92:ASN:HB2	1.96	0.47
1:B:201:ASP:OD1	1:B:202:ARG:N	2.46	0.47
1:B:351:LYS:HG2	1:B:366:ASP:HA	1.96	0.47
1:B:325:LEU:HD13	1:B:343:CYS:HB2	1.96	0.47
1:A:56:ASN:O	1:A:72:LYS:N	2.34	0.47
1:B:201:ASP:OD2	1:B:204:ARG:NE	2.47	0.47
1:B:89:ASP:OD1	1:B:90:LEU:N	2.41	0.47
1:B:530:PRO:HG2	1:B:540:VAL:HG22	1.97	0.47
1:B:533:THR:HA	1:B:616:THR:O	2.15	0.47
1:B:88:VAL:HG13	1:B:92:ASN:HB2	1.96	0.46
1:A:323:PRO:HG2	1:A:410:SER:HB3	1.97	0.46
1:A:557:LYS:NZ	1:A:591:GLY:HA3	2.30	0.46
1:B:434:LEU:O	1:B:517:THR:HG22	2.15	0.46
1:A:451:ASP:OD2	1:A:500:ASN:HB2	2.15	0.46
1:B:122:TRP:HZ3	1:B:148:HIS:HA	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASN:HD22	1:B:149:ASN:H	1.63	0.46
1:A:520:LEU:HB2	1:A:607:SER:HA	1.97	0.46
1:B:29:PRO:HG2	1:B:110:SER:HB2	1.97	0.45
1:A:51:GLU:HG2	1:A:100:TYR:CD2	2.52	0.45
1:B:122:TRP:O	1:B:148:HIS:NE2	2.40	0.45
1:A:198:TYR:CZ	1:A:211:PRO:HB3	2.52	0.44
1:A:225:LYS:HG3	1:A:307:SER:HA	1.99	0.44
1:A:90:LEU:HD11	1:A:121:TYR:HE2	1.81	0.44
1:B:219:VAL:HB	1:B:303:TRP:CG	2.52	0.44
1:A:198:TYR:CE2	1:A:211:PRO:HB3	2.53	0.44
1:A:38:VAL:HB	1:A:176:ARG:HH21	1.82	0.44
1:A:555:LEU:HD23	1:A:565:LEU:HD12	2.00	0.44
1:A:73:ASN:C	1:A:75:GLN:H	2.21	0.44
1:A:44:LYS:HG3	1:A:86:SER:HA	2.00	0.44
1:B:347:PHE:HE2	1:B:399:PHE:HZ	1.65	0.44
1:B:254:VAL:HG22	1:B:268:THR:HG22	1.99	0.44
1:B:315:THR:HG22	1:B:406:TRP:HB2	2.00	0.44
1:A:446:SER:O	1:A:475:PHE:HB2	2.17	0.44
1:A:547:MET:SD	1:A:575:GLN:NE2	2.91	0.44
1:B:323:PRO:HG2	1:B:410:SER:HB3	2.00	0.44
1:A:219:VAL:HB	1:A:303:TRP:CG	2.53	0.43
1:B:34:GLN:HB2	1:B:48:PHE:HE2	1.83	0.43
1:B:332:VAL:HG11	1:B:496:TYR:CZ	2.53	0.43
1:B:439:THR:HG22	1:B:484:TYR:HD1	1.82	0.43
1:B:55:ALA:HB3	1:B:58:TYR:CZ	2.53	0.43
1:A:232:PRO:HG2	1:A:242:MET:HA	2.01	0.43
1:A:72:LYS:O	1:A:74:LYS:N	2.42	0.43
1:B:473:THR:HB	1:B:475:PHE:CE2	2.53	0.43
1:B:523:THR:HG22	1:B:608:SER:HB2	2.00	0.43
1:A:526:LEU:HD11	1:A:542:LEU:HB2	2.00	0.43
1:B:26:LEU:HB2	1:B:107:SER:HB3	2.00	0.43
1:A:499:HIS:HB2	1:A:502:SER:HB3	2.00	0.43
1:B:223:LEU:HD21	1:B:301:ALA:HB3	1.99	0.43
1:A:545:TRP:HE1	1:A:575:GLN:CD	2.23	0.42
1:A:308:ASP:OD1	1:B:309:THR:OG1	2.36	0.42
1:A:435:ASP:CG	1:A:436:PRO:HD2	2.39	0.42
1:A:93:ALA:HB2	1:A:117:VAL:HG23	2.01	0.42
1:B:567:LEU:HD23	1:B:580:PHE:CE2	2.53	0.42
1:B:149:ASN:ND2	1:B:149:ASN:H	2.17	0.42
1:B:529:LYS:HB2	1:B:541:SER:O	2.19	0.42
1:B:529:LYS:HD2	1:B:541:SER:OG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HD13	1:A:580:PHE:CZ	2.54	0.42
1:B:273:GLN:HA	1:B:274:PRO:HA	1.77	0.42
1:B:313:VAL:HG11	1:B:406:TRP:CD2	2.54	0.42
1:B:434:LEU:CD1	1:B:440:LEU:HB3	2.50	0.42
1:B:468:SER:HB2	1:B:476:SER:HB3	2.00	0.42
1:A:56:ASN:ND2	1:A:103:GLN:HG3	2.32	0.42
1:A:247:GLN:HG2	1:A:277:LYS:HG2	2.01	0.42
1:A:545:TRP:CZ2	1:A:547:MET:HG2	2.54	0.42
1:A:296:TYR:CE2	1:A:306:PRO:HB3	2.56	0.41
1:B:545:TRP:HA	1:B:576:SER:O	2.21	0.41
1:A:193:TRP:O	1:A:216:GLU:HG3	2.20	0.41
1:A:315:THR:HG22	1:A:406:TRP:HB2	2.02	0.41
1:A:134:VAL:HG11	1:A:187:VAL:HG21	2.02	0.41
1:B:317:ILE:HD12	1:B:405:LEU:HB3	2.02	0.41
1:A:259:ASN:HB2	1:A:293:TYR:CE2	2.55	0.41
1:B:424:PRO:HB3	1:B:446:SER:HB2	2.03	0.40
1:A:524:PRO:HB2	1:A:544:CYS:SG	2.60	0.40
1:B:479:ASN:OD1	2:C:1:NAG:H2	2.20	0.40
1:A:555:LEU:HD12	1:A:594:ARG:O	2.21	0.40
1:B:434:LEU:HD11	1:B:440:LEU:HB3	2.04	0.40
1:A:205:PRO:HG2	1:A:206:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	570/606 (94%)	543 (95%)	25 (4%)	2 (0%)	34	67
1	B	583/606 (96%)	559 (96%)	22 (4%)	2 (0%)	41	72
All	All	1153/1212 (95%)	1102 (96%)	47 (4%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	PRO
1	B	530	PRO
1	B	207	VAL
1	A	205	PRO

5.3.2 Protein sidechains ⓘ

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	515/534 (96%)	511 (99%)	4 (1%)	81	91
1	B	521/534 (98%)	517 (99%)	4 (1%)	81	91
All	All	1036/1068 (97%)	1028 (99%)	8 (1%)	81	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	A	200	TYR
1	A	246	CYS
1	A	545	TRP
1	B	246	CYS
1	B	543	LEU
1	B	544	CYS
1	B	615	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	148	HIS
1	B	143	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	1.53	2 (11%)
2	NAG	C	2	2	14,14,15	0.35	0	17,19,21	0.64	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	3.02	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	1	NAG	C1-O5-C5	4.45	118.22	112.19
2	C	1	NAG	O4-C4-C5	3.60	118.25	109.30
2	C	2	NAG	C1-O5-C5	2.21	115.18	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

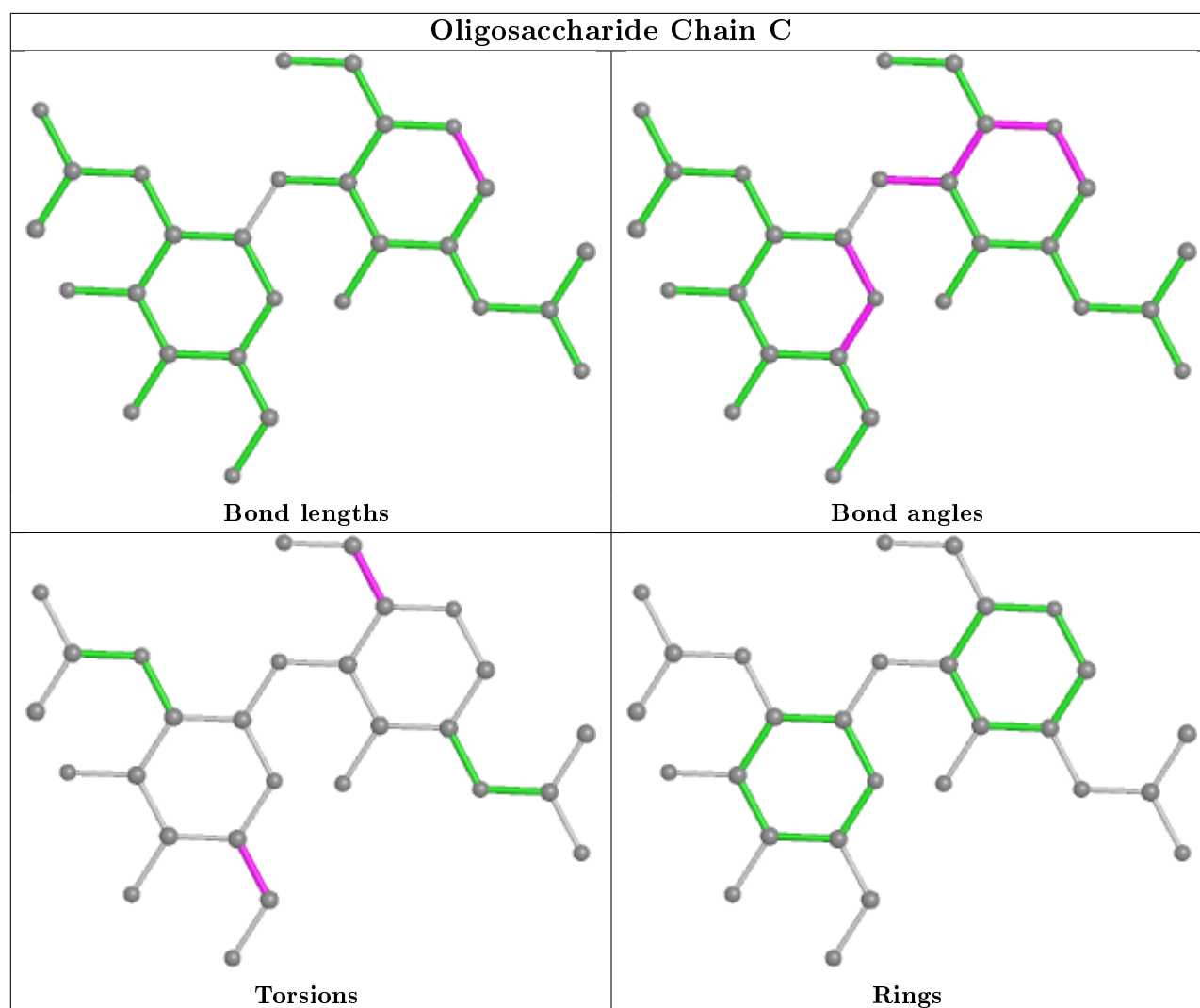
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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.



5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	703	1	14,14,15	0.47	0	17,19,21	0.88	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
3	NAG	B	703	1	-	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(°)	Ideal(°)
3	B	703	NAG	C1-O5-C5	3.24	116.58	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	NAG	O5-C5-C6-O6
3	B	703	NAG	C4-C5-C6-O6

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	578/606 (95%)	0.18	23 (3%) 38 37	57, 142, 220, 272	0
1	B	587/606 (96%)	-0.02	6 (1%) 82 81	68, 123, 192, 273	0
All	All	1165/1212 (96%)	0.08	29 (2%) 57 55	57, 132, 212, 273	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	592	THR	6.2
1	A	372	SER	4.6
1	A	422	LYS	3.8
1	A	566	ARG	3.7
1	B	339	MET	3.5
1	A	615	LEU	3.5
1	A	108	GLY	3.4
1	A	97	GLU	3.2
1	A	528	VAL	2.9
1	A	96	TYR	2.7
1	A	535	HIS	2.7
1	A	61	TYR	2.7
1	A	60	LEU	2.6
1	A	587	SER	2.6
1	B	176	ARG	2.5
1	A	82	GLU	2.5
1	A	109	TYR	2.4
1	A	393	PHE	2.4
1	A	99	SER	2.4
1	B	591	GLY	2.3
1	A	81	ALA	2.3
1	A	103	GLN	2.3
1	A	531	ASN	2.3
1	B	615	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	107	SER	2.2
1	A	111	ASP	2.2
1	A	580	PHE	2.2
1	A	554	ILE	2.2
1	A	312	LEU	2.1

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

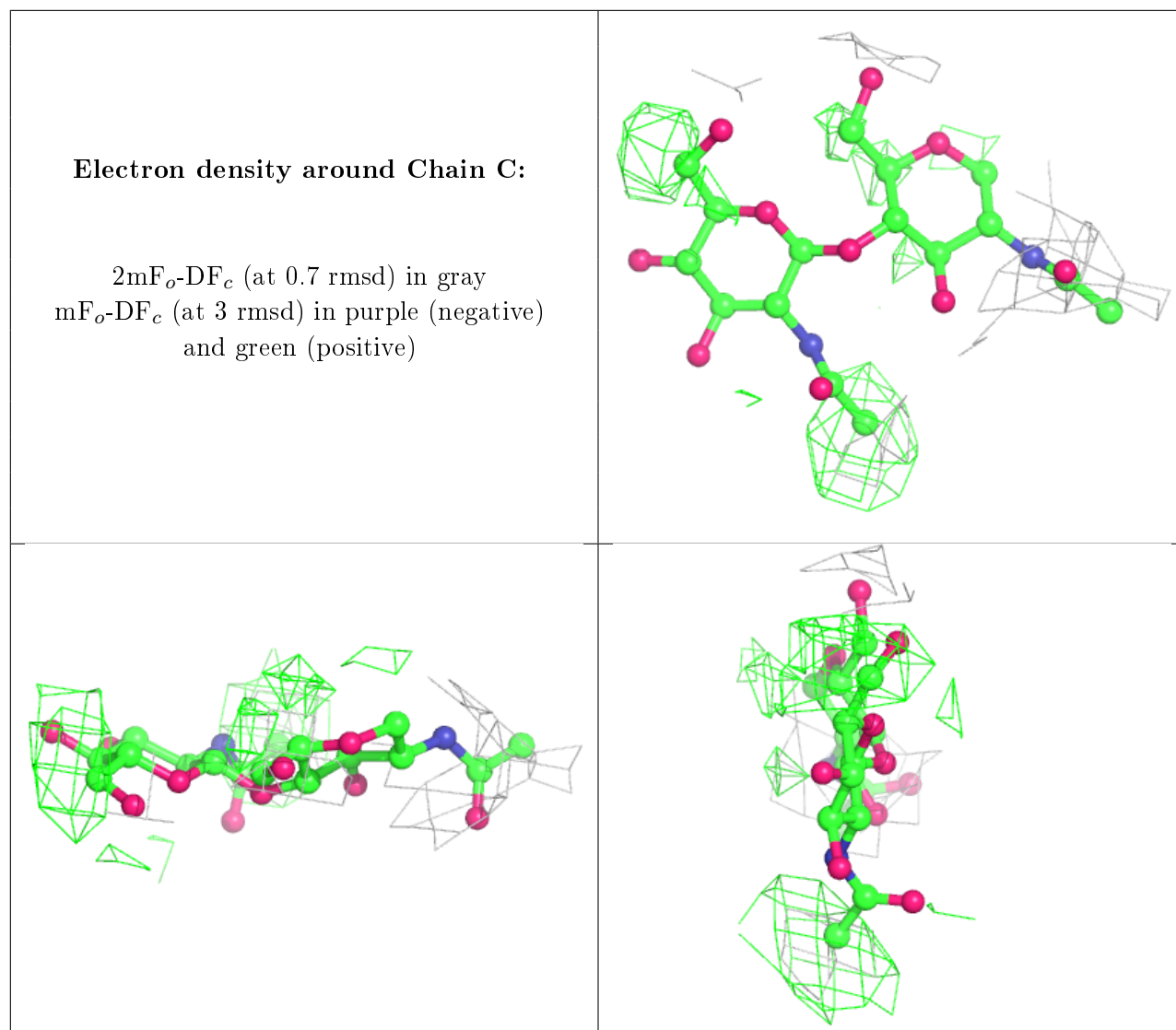
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.83	0.21	164,200,208,210	0
2	NAG	C	1	14/15	0.85	0.14	164,186,210,214	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.



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	703	14/15	0.70	0.25	163,248,261,261	0

6.5 Other polymers [i](#)

There are no such residues in this entry.