



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:49 PM BST

PDB ID : 3S94  
Title : Crystal structure of LRP6-E1E2  
Authors : Cheng, Z.; Xu, W.  
Deposited on : 2011-05-31  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

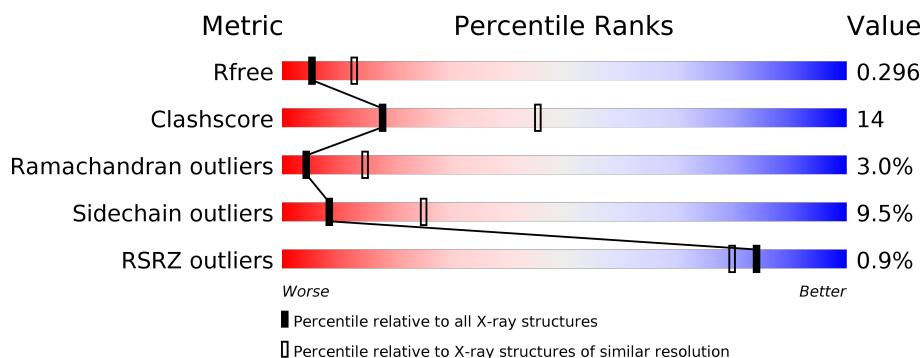
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	619	<div> <div></div> <div> <div></div> <div>62%</div> <div>28%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	619	<div> <div></div> <div> <div></div> <div>60%</div> <div>28%</div> <div>6%</div> <div>6%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9406 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.

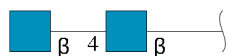
- Molecule 1 is a protein called Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4684	2973	799	888	24			
1	B	583	Total	C	N	O	S	0	0	0
			4652	2949	796	883	24			

There are 16 discrepancies between the modelled and reference sequences:

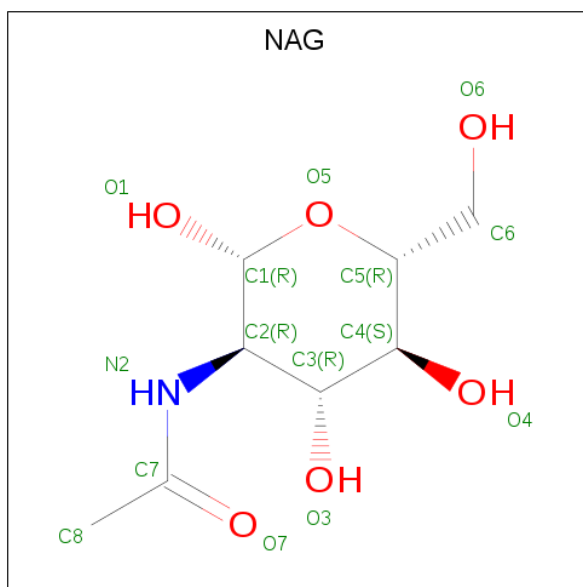
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	HIS	-	expression tag	UNP O75581
A	13	HIS	-	expression tag	UNP O75581
A	14	HIS	-	expression tag	UNP O75581
A	15	HIS	-	expression tag	UNP O75581
A	16	HIS	-	expression tag	UNP O75581
A	17	HIS	-	expression tag	UNP O75581
A	18	HIS	-	expression tag	UNP O75581
A	19	HIS	-	expression tag	UNP O75581
B	12	HIS	-	expression tag	UNP O75581
B	13	HIS	-	expression tag	UNP O75581
B	14	HIS	-	expression tag	UNP O75581
B	15	HIS	-	expression tag	UNP O75581
B	16	HIS	-	expression tag	UNP O75581
B	17	HIS	-	expression tag	UNP O75581
B	18	HIS	-	expression tag	UNP O75581
B	19	HIS	-	expression tag	UNP O75581

- 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			
2	D	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:  $C_8H_{15}NO_6$ ).

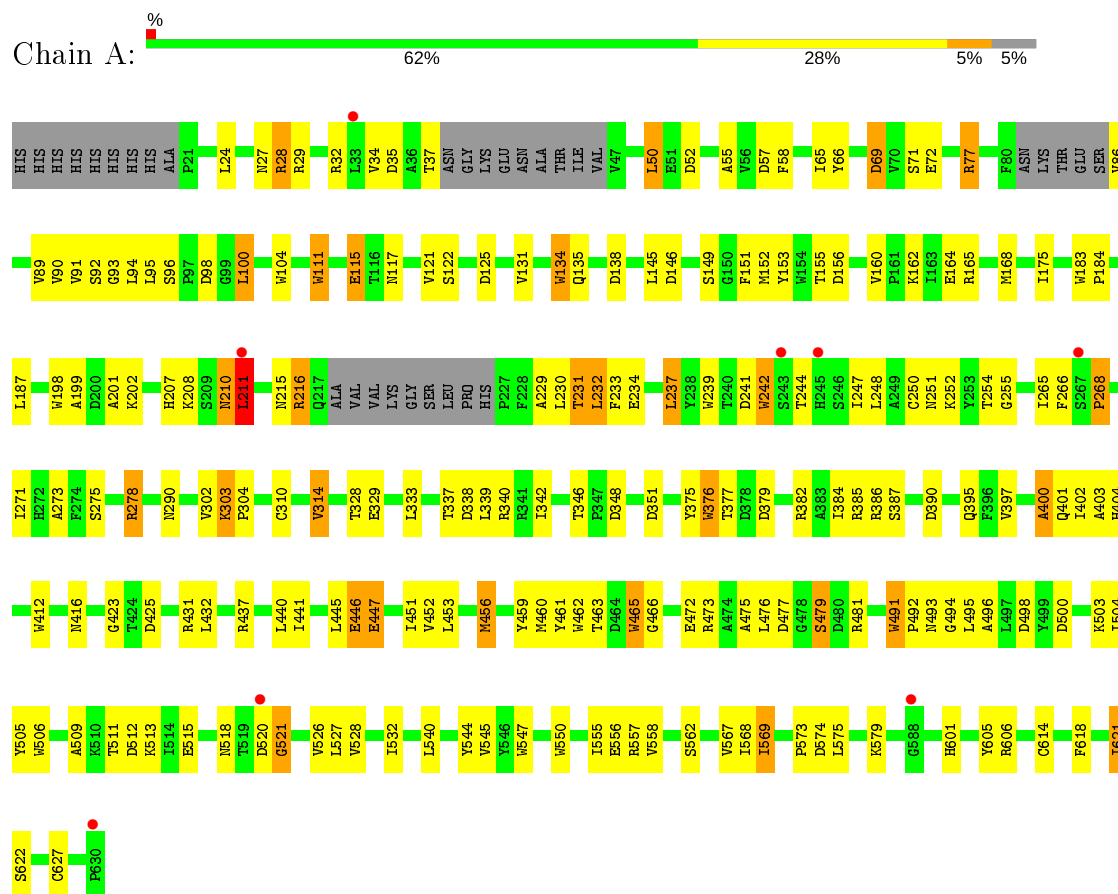


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

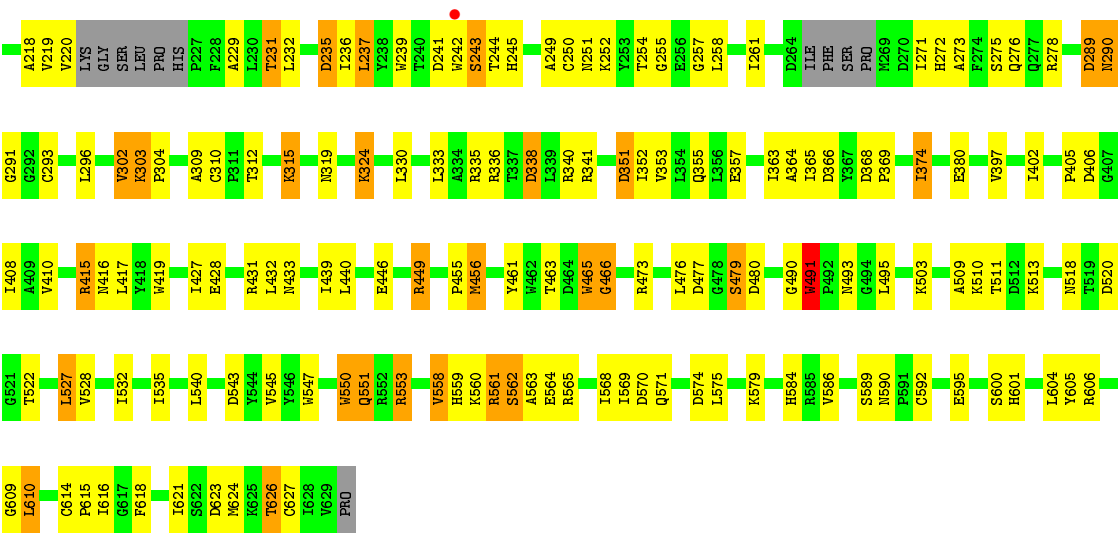
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Low-density lipoprotein receptor-related protein 6

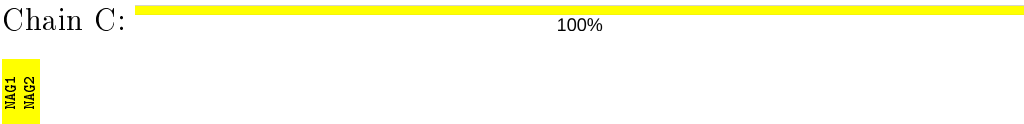


- Molecule 1: Low-density lipoprotein receptor-related protein 6





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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.54Å 144.51Å 70.76Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 70.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.80) 99.1 (70.37-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.237 , 0.296 0.237 , 0.296	Depositor DCC
$R_{free}$ test set	2179 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.287 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.58	12/4795 (0.3%)	0.66	2/6519 (0.0%)
1	B	0.58	7/4758 (0.1%)	0.65	0/6466
All	All	0.58	19/9553 (0.2%)	0.65	2/12985 (0.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	TRP	CD2-CE2	5.62	1.48	1.41
1	A	550	TRP	CD2-CE2	5.57	1.48	1.41
1	B	419	TRP	CD2-CE2	5.57	1.48	1.41
1	B	465	TRP	CD2-CE2	5.57	1.48	1.41
1	B	550	TRP	CD2-CE2	5.48	1.48	1.41
1	A	134	TRP	CD2-CE2	5.43	1.47	1.41
1	A	491	TRP	CD2-CE2	5.34	1.47	1.41
1	B	198	TRP	CD2-CE2	5.33	1.47	1.41
1	A	462	TRP	CD2-CE2	5.30	1.47	1.41
1	A	111	TRP	CD2-CE2	5.29	1.47	1.41
1	A	198	TRP	CD2-CE2	5.24	1.47	1.41
1	A	465	TRP	CD2-CE2	5.22	1.47	1.41
1	A	239	TRP	CD2-CE2	5.20	1.47	1.41
1	A	412	TRP	CD2-CE2	5.13	1.47	1.41
1	B	134	TRP	CD2-CE2	5.08	1.47	1.41
1	B	111	TRP	CD2-CE2	5.06	1.47	1.41
1	B	491	TRP	CD2-CE2	5.04	1.47	1.41
1	A	376	TRP	CD2-CE2	5.03	1.47	1.41
1	A	104	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	211	LEU	CA-CB-CG	5.35	127.60	115.30

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	4684	0	4536	123	0
1	B	4652	0	4506	127	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
3	A	14	0	13	0	0
All	All	9406	0	9105	251	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 14.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ILE:HD12	1:A:569:ILE:HD12	1.37	1.07
1:B:303:LYS:HB3	1:B:304:PRO:HD3	1.48	0.95
1:B:553:ARG:HH11	1:B:553:ARG:HG3	1.30	0.95
1:B:302:VAL:HG13	1:B:303:LYS:H	1.31	0.94
1:A:303:LYS:CB	1:A:304:PRO:HD2	1.99	0.92
1:A:210:ASN:O	1:A:211:LEU:HD13	1.72	0.91
1:B:364:ALA:HB2	1:B:406:ASP:O	1.72	0.90
1:B:231:THR:HG21	1:B:273:ALA:H	1.36	0.89
1:A:303:LYS:HB3	1:A:304:PRO:CD	2.05	0.87
1:A:621:ILE:HG12	1:A:622:SER:H	1.39	0.85
1:A:303:LYS:CB	1:A:304:PRO:CD	2.55	0.85
1:B:162:LYS:HD2	1:B:175:ILE:HD12	1.56	0.84
1:B:188:THR:HG21	1:B:231:THR:HA	1.58	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LYS:HB2	1:A:304:PRO:HD2	1.60	0.82
1:A:568:ILE:HG22	1:A:569:ILE:HG13	1.62	0.82
1:B:333:LEU:HD11	1:B:575:LEU:HD22	1.61	0.81
1:A:601:HIS:HD2	1:A:627:CYS:HB2	1.46	0.79
1:A:555:ILE:HD12	1:A:569:ILE:CD1	2.13	0.79
1:A:28:ARG:HG2	1:A:52:ASP:HA	1.66	0.77
1:B:553:ARG:HH11	1:B:553:ARG:CG	1.97	0.76
1:A:379:ASP:OD1	1:A:404:HIS:HD2	1.69	0.76
1:A:310:CYS:HB3	1:A:314:VAL:CG2	2.17	0.74
1:A:333:LEU:HD23	1:A:340:ARG:HB2	1.69	0.74
1:B:550:TRP:O	1:B:551:GLN:HB2	1.86	0.74
1:A:518:ASN:HB2	1:A:521:GLY:O	1.88	0.73
1:B:417:LEU:HB2	1:B:432:LEU:HD23	1.73	0.71
1:B:237:LEU:HD23	1:B:252:LYS:HA	1.73	0.71
1:B:364:ALA:CB	1:B:406:ASP:O	2.39	0.70
1:B:601:HIS:CD2	1:B:627:CYS:HB2	2.26	0.70
1:B:229:ALA:HB3	1:B:271:ILE:HG22	1.72	0.69
1:A:145:LEU:HB3	1:A:168:MET:CE	2.22	0.69
1:B:330:LEU:HD22	1:B:341:ARG:HG3	1.76	0.67
1:B:231:THR:HG21	1:B:273:ALA:N	2.09	0.67
1:B:249:ALA:HB2	1:B:261:ILE:HD11	1.76	0.66
1:A:303:LYS:HB3	1:A:304:PRO:HD2	1.66	0.66
1:B:547:TRP:CH2	1:B:558:VAL:HG11	2.30	0.66
1:A:386:ARG:HD3	1:A:397:VAL:HG22	1.78	0.66
1:A:152:MET:HE2	1:A:168:MET:HA	1.77	0.65
1:A:342:ILE:HD11	1:A:351:ASP:HB3	1.78	0.65
1:B:232:LEU:HD23	1:B:237:LEU:HB3	1.79	0.65
1:B:181:ILE:HD11	1:B:184:PRO:HB3	1.80	0.64
1:B:365:ILE:HD11	1:B:374:ILE:HD11	1.80	0.64
1:A:601:HIS:CD2	1:A:627:CYS:HB2	2.31	0.63
1:B:590:ASN:OD1	1:B:592:CYS:HB2	1.98	0.63
1:B:27:ASN:O	1:B:28:ARG:HB2	1.97	0.63
1:A:495:LEU:HD22	1:A:504:ILE:HD11	1.80	0.62
1:B:302:VAL:HG13	1:B:303:LYS:N	2.10	0.62
1:A:463:THR:HB	1:A:492:PRO:HB2	1.82	0.62
1:B:303:LYS:CB	1:B:304:PRO:HD3	2.28	0.61
1:B:568:ILE:HG13	1:B:569:ILE:H	1.66	0.61
1:B:101:ALA:HB2	1:B:143:ILE:HG23	1.83	0.61
1:A:494:GLY:O	1:A:506:TRP:HA	1.99	0.60
1:A:621:ILE:HG12	1:A:622:SER:N	2.14	0.60
1:B:415:ARG:HB3	1:B:431:ARG:HH21	1.67	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:THR:HG22	1:A:232:LEU:H	1.66	0.60
1:B:251:ASN:HB3	1:B:255:GLY:H	1.67	0.60
1:A:614:CYS:HB3	1:A:618:PHE:HB3	1.83	0.59
1:A:145:LEU:HB3	1:A:168:MET:HE2	1.83	0.59
1:B:219:VAL:O	1:B:220:VAL:HB	2.02	0.59
1:B:550:TRP:O	1:B:551:GLN:CB	2.51	0.58
1:B:235:ASP:HA	1:B:252:LYS:CE	2.34	0.58
1:A:145:LEU:HB3	1:A:168:MET:HE1	1.85	0.58
1:B:229:ALA:CB	1:B:271:ILE:HG22	2.34	0.57
1:A:310:CYS:HB3	1:A:314:VAL:HG22	1.87	0.57
1:B:558:VAL:HA	1:B:564:GLU:O	2.04	0.57
1:B:315:LYS:HB3	1:B:324:LYS:HE2	1.87	0.57
1:B:52:ASP:HB3	1:B:70:VAL:HG23	1.87	0.57
1:B:333:LEU:HD23	1:B:340:ARG:HB2	1.88	0.56
1:A:251:ASN:HD22	1:A:254:THR:H	1.52	0.56
1:A:233:PHE:CD2	1:A:234:GLU:HG2	2.41	0.55
1:A:199:ALA:HB2	1:A:230:LEU:HD23	1.88	0.55
1:A:89:VAL:HG12	1:A:90:VAL:HG23	1.89	0.55
1:A:95:LEU:HB3	1:A:115:GLU:HG2	1.89	0.54
1:B:553:ARG:NH1	1:B:553:ARG:HG3	2.11	0.54
1:B:275:SER:O	1:B:278:ARG:HB3	2.07	0.54
1:A:447:GLU:HB2	1:A:465:TRP:HB2	1.90	0.54
1:B:397:VAL:HG13	1:B:433:ASN:O	2.07	0.54
1:B:476:LEU:HD12	1:B:605:TYR:HB3	1.88	0.54
1:B:78:THR:HG22	1:B:86:VAL:HG22	1.89	0.54
1:A:416:ASN:HA	1:A:431:ARG:HA	1.90	0.54
1:A:302:VAL:HG22	1:A:303:LYS:H	1.73	0.53
1:B:152:MET:HG2	1:B:166:ALA:O	2.09	0.53
1:A:379:ASP:OD1	1:A:404:HIS:CD2	2.56	0.53
1:B:198:TRP:HZ3	1:B:209:SER:HB2	1.71	0.53
1:B:335:ARG:HB2	1:B:338:ASP:HB3	1.91	0.53
1:B:198:TRP:CZ3	1:B:209:SER:HB2	2.44	0.53
1:A:545:VAL:O	1:A:557:ARG:HA	2.08	0.53
1:A:556:GLU:HG2	1:A:567:VAL:HG22	1.89	0.53
1:A:377:THR:HG22	1:A:384:ILE:HG12	1.91	0.53
1:A:557:ARG:HD3	1:A:568:ILE:HD11	1.91	0.53
1:B:402:ILE:HD11	1:B:405:PRO:HG3	1.90	0.53
1:B:235:ASP:HA	1:B:252:LYS:HE3	1.90	0.53
1:B:621:ILE:HG13	1:B:623:ASP:OD1	2.09	0.52
1:A:303:LYS:HB3	1:A:304:PRO:HD3	1.90	0.52
1:B:559:HIS:CE1	1:B:561:ARG:HB3	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HD11	1:A:575:LEU:HD22	1.92	0.52
1:B:57:ASP:OD2	1:B:101:ALA:HA	2.09	0.52
1:B:490:GLY:HA3	1:B:510:LYS:HB3	1.92	0.52
1:B:503:LYS:NZ	1:B:518:ASN:OD1	2.34	0.52
1:A:382:ARG:HD2	1:A:402:ILE:O	2.10	0.52
1:B:449:ARG:NE	1:B:491:TRP:CH2	2.77	0.52
1:B:181:ILE:HG13	1:B:184:PRO:HD3	1.92	0.51
1:A:302:VAL:HG13	1:A:303:LYS:HG3	1.92	0.51
1:A:375:TYR:OH	1:A:432:LEU:HB3	2.09	0.51
1:B:167:GLY:C	1:B:169:ASP:H	2.14	0.51
1:A:491:TRP:HB2	1:A:509:ALA:HB3	1.93	0.51
1:A:568:ILE:HG22	1:A:569:ILE:CG1	2.37	0.51
1:A:229:ALA:CB	1:A:271:ILE:HG22	2.41	0.51
1:A:511:THR:HB	1:A:513:LYS:HE2	1.93	0.51
1:B:446:GLU:HB3	1:B:466:GLY:HA2	1.93	0.50
1:B:70:VAL:HG12	1:B:96:SER:HA	1.93	0.50
1:A:183:TRP:HB2	1:A:202:LYS:HB2	1.93	0.50
1:B:351:ASP:OD1	1:B:351:ASP:N	2.44	0.50
1:B:527:LEU:HG	1:B:528:VAL:HG23	1.93	0.50
1:B:553:ARG:NH1	1:B:553:ARG:CG	2.63	0.50
1:B:302:VAL:CG1	1:B:303:LYS:H	2.15	0.50
1:B:92:SER:HB2	1:B:353:VAL:HB	1.92	0.50
1:A:614:CYS:HB3	1:A:618:PHE:CB	2.42	0.50
1:B:615:PRO:O	1:B:618:PHE:HB2	2.11	0.50
1:B:100:LEU:HD22	1:B:109:LEU:HD11	1.92	0.50
1:A:459:TYR:CD1	1:A:473:ARG:HD2	2.47	0.49
1:B:545:VAL:CG1	1:B:558:VAL:HG13	2.43	0.49
1:B:427:ILE:O	1:B:440:LEU:HB3	2.12	0.49
1:A:208:LYS:HZ2	1:A:215:ASN:HD22	1.61	0.49
1:B:477:ASP:OD1	1:B:479:SER:HB2	2.13	0.49
1:A:121:VAL:HG22	1:A:122:SER:N	2.28	0.49
1:A:69:ASP:HB3	1:A:72:GLU:HB2	1.95	0.49
1:A:310:CYS:HB3	1:A:314:VAL:HG23	1.93	0.48
1:B:570:ASP:OD1	1:B:571:GLN:N	2.46	0.48
1:B:477:ASP:HA	1:B:604:LEU:HD13	1.95	0.48
1:A:131:VAL:HG13	1:A:131:VAL:O	2.12	0.48
1:A:208:LYS:NZ	1:A:215:ASN:HD22	2.11	0.48
1:A:498:ASP:HB3	1:A:503:LYS:HB2	1.95	0.48
1:A:511:THR:O	1:A:513:LYS:HG3	2.13	0.48
1:A:547:TRP:HZ3	1:A:558:VAL:HB	1.78	0.48
1:A:446:GLU:CG	1:A:466:GLY:HA3	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ASP:HB2	1:B:244:THR:OG1	2.13	0.48
1:B:415:ARG:HB3	1:B:431:ARG:NH2	2.27	0.48
1:B:251:ASN:HD22	1:B:254:THR:H	1.60	0.48
1:A:515:GLU:HG2	1:A:526:VAL:HG22	1.95	0.47
1:A:66:TYR:OH	1:A:77:ARG:NH1	2.48	0.47
1:B:198:TRP:HZ3	1:B:209:SER:CB	2.27	0.47
1:B:296:LEU:HB2	1:B:309:ALA:HB3	1.95	0.47
1:B:89:VAL:HG12	1:B:90:VAL:HG23	1.96	0.47
1:B:330:LEU:CD2	1:B:341:ARG:HG3	2.41	0.47
2:D:1:NAG:O3	2:D:2:NAG:C1	2.63	0.47
1:A:29:ARG:HA	1:A:50:LEU:O	2.15	0.47
1:B:363:ILE:HG21	1:B:406:ASP:HA	1.96	0.47
1:A:111:TRP:HZ3	1:A:122:SER:HB3	1.80	0.47
1:A:237:LEU:HD23	1:A:252:LYS:HA	1.97	0.47
1:A:231:THR:HG21	1:A:273:ALA:N	2.30	0.47
1:B:51:GLU:O	1:B:52:ASP:HB2	2.14	0.47
1:B:606:ARG:HB2	1:B:609:GLY:O	2.15	0.46
1:B:57:ASP:OD1	1:B:58:PHE:N	2.38	0.46
1:A:55:ALA:HB2	1:A:98:ASP:O	2.16	0.46
1:A:509:ALA:HA	1:A:532:ILE:HB	1.97	0.45
1:A:400:ALA:O	1:A:402:ILE:N	2.49	0.45
1:B:184:PRO:HA	1:B:199:ALA:O	2.16	0.45
1:B:75:ILE:O	1:B:89:VAL:O	2.33	0.45
1:A:456:MET:N	1:A:456:MET:SD	2.81	0.45
1:B:237:LEU:CD2	1:B:252:LYS:HA	2.43	0.45
1:A:156:ASP:HB2	1:A:162:LYS:HG2	1.98	0.45
1:A:233:PHE:HE1	1:A:275:SER:CB	2.30	0.45
1:B:290:ASN:HB3	1:B:293:CYS:HB2	1.98	0.45
1:A:555:ILE:CD1	1:A:569:ILE:HD12	2.26	0.45
1:B:415:ARG:HA	1:B:415:ARG:HD2	1.69	0.45
1:A:153:TYR:CD1	1:A:165:ARG:HB3	2.52	0.45
1:B:130:LYS:HG3	1:B:310:CYS:O	2.17	0.45
1:B:428:GLU:OE2	1:B:439:ILE:HG12	2.17	0.45
1:A:459:TYR:CG	1:A:473:ARG:HD2	2.51	0.45
1:B:543:ASP:HA	1:B:560:LYS:HD3	1.98	0.45
1:B:439:ILE:H	1:B:616:ILE:HD11	1.81	0.45
1:B:416:ASN:HD22	1:B:431:ARG:HA	1.81	0.45
1:A:207:HIS:NE2	1:A:216:ARG:HG3	2.32	0.44
1:A:302:VAL:HG22	1:A:303:LYS:N	2.32	0.44
1:B:235:ASP:HA	1:B:252:LYS:HE2	1.98	0.44
1:B:476:LEU:HB2	1:B:605:TYR:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLU:HB3	1:A:175:ILE:HA	1.97	0.44
1:A:231:THR:HG21	1:A:273:ALA:H	1.82	0.44
1:B:114:SER:HA	1:B:140:PRO:HD2	1.98	0.44
1:B:105:LEU:HB3	1:B:147:PRO:HB3	1.98	0.44
1:B:623:ASP:OD2	1:B:626:THR:HG23	2.18	0.44
1:A:241:ASP:HB2	1:A:248:LEU:HD12	2.00	0.44
1:A:241:ASP:HB3	1:A:244:THR:OG1	2.18	0.44
1:B:60:PHE:CD2	1:B:276:GLN:HB2	2.53	0.44
1:A:251:ASN:ND2	1:A:254:THR:H	2.13	0.44
1:A:465:TRP:CD1	1:A:492:PRO:HD2	2.53	0.44
1:B:509:ALA:HA	1:B:532:ILE:HB	2.00	0.44
1:A:117:ASN:ND2	1:A:138:ASP:O	2.51	0.44
1:A:183:TRP:N	1:A:184:PRO:HD3	2.33	0.44
1:A:34:VAL:HG12	1:A:35:ASP:H	1.83	0.44
1:B:324:LYS:HG2	1:B:324:LYS:H	1.56	0.44
1:A:475:ALA:HB1	1:A:606:ARG:HG2	2.00	0.44
1:A:451:ILE:HD11	1:A:460:MET:HG3	2.00	0.43
1:A:207:HIS:CD2	1:A:216:ARG:HG3	2.53	0.43
1:A:513:LYS:HD2	1:A:526:VAL:HG21	1.99	0.43
1:B:366:ASP:OD1	1:B:579:LYS:HE3	2.18	0.43
1:A:250:CYS:HB2	1:A:255:GLY:O	2.19	0.43
1:B:239:TRP:HZ3	1:B:250:CYS:HG	1.64	0.43
1:A:403:ALA:HB3	1:A:423:GLY:HA3	2.01	0.43
1:B:23:LEU:HD22	1:B:271:ILE:HD11	2.00	0.43
1:A:155:THR:HG23	1:A:187:LEU:HD13	1.99	0.43
1:B:203:LEU:HB3	1:B:205:PHE:CD2	2.54	0.43
1:B:520:ASP:HB2	1:B:522:THR:HG22	2.00	0.43
1:A:91:VAL:O	1:A:93:GLY:N	2.52	0.43
1:B:336:ARG:NH1	1:B:574:ASP:OD1	2.52	0.43
1:A:247:ILE:HG13	1:A:265:ILE:HG12	2.00	0.42
1:A:461:TYR:CE1	1:A:473:ARG:HD3	2.54	0.42
1:A:146:ASP:H	1:A:168:MET:CE	2.32	0.42
1:A:266:PHE:O	1:A:268:PRO:HD3	2.19	0.42
1:A:376:TRP:CE2	1:A:385:ARG:HB2	2.55	0.42
1:B:600:SER:OG	1:B:601:HIS:HD2	2.01	0.42
1:B:545:VAL:HG13	1:B:558:VAL:HG13	2.00	0.42
1:A:496:ALA:HB1	1:A:540:LEU:HB3	2.00	0.42
1:B:239:TRP:HZ3	1:B:250:CYS:SG	2.42	0.42
1:A:57:ASP:OD2	1:A:58:PHE:N	2.40	0.42
1:A:621:ILE:CG1	1:A:622:SER:H	2.21	0.42
1:B:95:LEU:HB2	1:B:115:GLU:HB3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD23	1:A:441:ILE:HG13	2.02	0.42
1:B:207:HIS:CD2	1:B:218:ALA:HA	2.55	0.42
1:A:445:LEU:HB2	1:A:481:ARG:NH2	2.36	0.41
1:A:544:TYR:CD1	1:A:557:ARG:HD2	2.55	0.41
1:B:559:HIS:HB3	1:B:562:SER:HB2	2.01	0.41
1:B:610:LEU:H	1:B:610:LEU:HD23	1.85	0.41
1:B:249:ALA:CB	1:B:261:ILE:HD11	2.47	0.41
1:A:65:ILE:O	1:A:77:ARG:HA	2.21	0.41
1:A:210:ASN:N	1:A:210:ASN:OD1	2.52	0.41
1:A:400:ALA:HB3	1:A:437:ARG:HH12	1.85	0.41
1:A:346:THR:HB	1:A:348:ASP:OD1	2.21	0.41
1:A:495:LEU:HA	1:A:505:TYR:O	2.19	0.41
1:B:408:ILE:O	1:B:408:ILE:HG23	2.20	0.41
1:A:229:ALA:HB3	1:A:271:ILE:HG22	2.02	0.41
1:A:446:GLU:HG3	1:A:466:GLY:HA3	2.03	0.41
1:B:289:ASP:C	1:B:291:GLY:H	2.25	0.41
1:B:463:THR:HG23	1:B:495:LEU:HG	2.01	0.41
1:B:511:THR:HB	1:B:513:LYS:HE2	2.03	0.41
1:A:278:ARG:HA	1:A:278:ARG:HH11	1.86	0.41
1:A:477:ASP:OD1	1:A:479:SER:HB2	2.20	0.41
1:B:185:ASN:OD1	1:B:186:GLY:N	2.52	0.41
1:B:455:PRO:HD2	1:B:456:MET:HE1	2.03	0.41
1:A:149:SER:HB3	1:A:151:PHE:CD2	2.56	0.40
1:A:518:ASN:CB	1:A:521:GLY:O	2.65	0.40
1:B:95:LEU:HD12	1:B:116:THR:HG23	2.02	0.40
1:B:528:VAL:HG11	1:B:565:ARG:HD2	2.03	0.40
1:B:614:CYS:HB3	1:B:618:PHE:CB	2.51	0.40
1:A:125:ASP:OD1	1:A:125:ASP:N	2.54	0.40
1:B:368:ASP:HA	1:B:369:PRO:HD2	1.96	0.40
1:B:465:TRP:O	1:B:465:TRP:CG	2.74	0.40
1:B:461:TYR:CD1	1:B:473:ARG:HB2	2.55	0.40
1:A:476:LEU:HB2	1:A:605:TYR:O	2.22	0.40
1:B:231:THR:HG21	1:B:272:HIS:HA	2.04	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	579/619 (94%)	504 (87%)	61 (10%)	14 (2%)	6	20
1	B	573/619 (93%)	499 (87%)	53 (9%)	21 (4%)	3	11
All	All	1152/1238 (93%)	1003 (87%)	114 (10%)	35 (3%)	4	15

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	PRO
1	A	303	LYS
1	A	562	SER
1	B	28	ARG
1	B	479	SER
1	B	562	SER
1	B	563	ALA
1	A	28	ARG
1	A	201	ALA
1	A	521	GLY
1	B	290	ASN
1	B	302	VAL
1	B	352	ILE
1	B	480	ASP
1	B	551	GLN
1	A	92	SER
1	A	400	ALA
1	A	401	GLN
1	A	520	ASP
1	B	52	ASP
1	B	338	ASP
1	B	527	LEU
1	A	27	ASN
1	A	211	LEU
1	A	290	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	90	VAL
1	B	168	MET
1	B	210	ASN
1	A	134	TRP
1	B	257	GLY
1	B	586	VAL
1	B	243	SER
1	B	303	LYS
1	B	535	ILE
1	B	466	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	508/535 (95%)	460 (91%)	48 (9%)	8	26
1	B	504/535 (94%)	456 (90%)	48 (10%)	8	25
All	All	1012/1070 (95%)	916 (90%)	96 (10%)	8	25

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	32	ARG
1	A	37	THR
1	A	50	LEU
1	A	69	ASP
1	A	71	SER
1	A	77	ARG
1	A	86	VAL
1	A	94	LEU
1	A	96	SER
1	A	100	LEU
1	A	115	GLU
1	A	135	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	160	VAL
1	A	210	ASN
1	A	216	ARG
1	A	231	THR
1	A	232	LEU
1	A	237	LEU
1	A	242	TRP
1	A	278	ARG
1	A	314	VAL
1	A	328	THR
1	A	329	GLU
1	A	337	THR
1	A	338	ASP
1	A	339	LEU
1	A	387	SER
1	A	390	ASP
1	A	395	GLN
1	A	425	ASP
1	A	446	GLU
1	A	447	GLU
1	A	452	VAL
1	A	453	LEU
1	A	456	MET
1	A	472	GLU
1	A	479	SER
1	A	493	ASN
1	A	500	ASP
1	A	512	ASP
1	A	527	LEU
1	A	528	VAL
1	A	569	ILE
1	A	573	PRO
1	A	574	ASP
1	A	579	LYS
1	A	621	ILE
1	B	50	LEU
1	B	52	ASP
1	B	76	LYS
1	B	78	THR
1	B	79	GLU
1	B	100	LEU
1	B	115	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	128	LEU
1	B	129	ARG
1	B	130	LYS
1	B	180	GLU
1	B	188	THR
1	B	189	LEU
1	B	203	LEU
1	B	231	THR
1	B	235	ASP
1	B	236	ILE
1	B	237	LEU
1	B	242	TRP
1	B	243	SER
1	B	245	HIS
1	B	258	LEU
1	B	289	ASP
1	B	312	THR
1	B	315	LYS
1	B	319	ASN
1	B	324	LYS
1	B	351	ASP
1	B	355	GLN
1	B	357	GLU
1	B	374	ILE
1	B	380	GLU
1	B	410	VAL
1	B	415	ARG
1	B	449	ARG
1	B	456	MET
1	B	491	TRP
1	B	493	ASN
1	B	540	LEU
1	B	553	ARG
1	B	558	VAL
1	B	561	ARG
1	B	584	HIS
1	B	589	SER
1	B	595	GLU
1	B	610	LEU
1	B	624	MET
1	B	626	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	135	GLN
1	A	139	GLN
1	A	215	ASN
1	A	251	ASN
1	A	272	HIS
1	A	290	ASN
1	A	319	ASN
1	A	404	HIS
1	A	493	ASN
1	B	81	ASN
1	B	117	ASN
1	B	204	ASN
1	B	207	HIS
1	B	215	ASN
1	B	251	ASN
1	B	295	HIS
1	B	355	GLN
1	B	416	ASN
1	B	493	ASN
1	B	601	HIS

### 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 ⓘ

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	1,2	14,14,15	0.67	0	17,19,21	1.55	3 (17%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.75	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.62	0	17,19,21	1.83	5 (29%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	0.80	0

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	6.24	120.65	112.19
2	C	1	NAG	C1-O5-C5	3.54	116.99	112.19
2	D	1	NAG	C3-C4-C5	-3.53	103.95	110.24
2	C	1	NAG	C4-C3-C2	3.19	115.69	111.02
2	D	1	NAG	O5-C5-C6	3.17	112.18	107.20
2	D	1	NAG	C1-O5-C5	2.92	116.16	112.19
2	D	1	NAG	O4-C4-C3	2.62	116.41	110.35
2	C	1	NAG	O5-C1-C2	2.49	115.22	111.29
2	D	1	NAG	C4-C3-C2	-2.26	107.70	111.02
2	C	2	NAG	O5-C1-C2	2.16	114.69	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

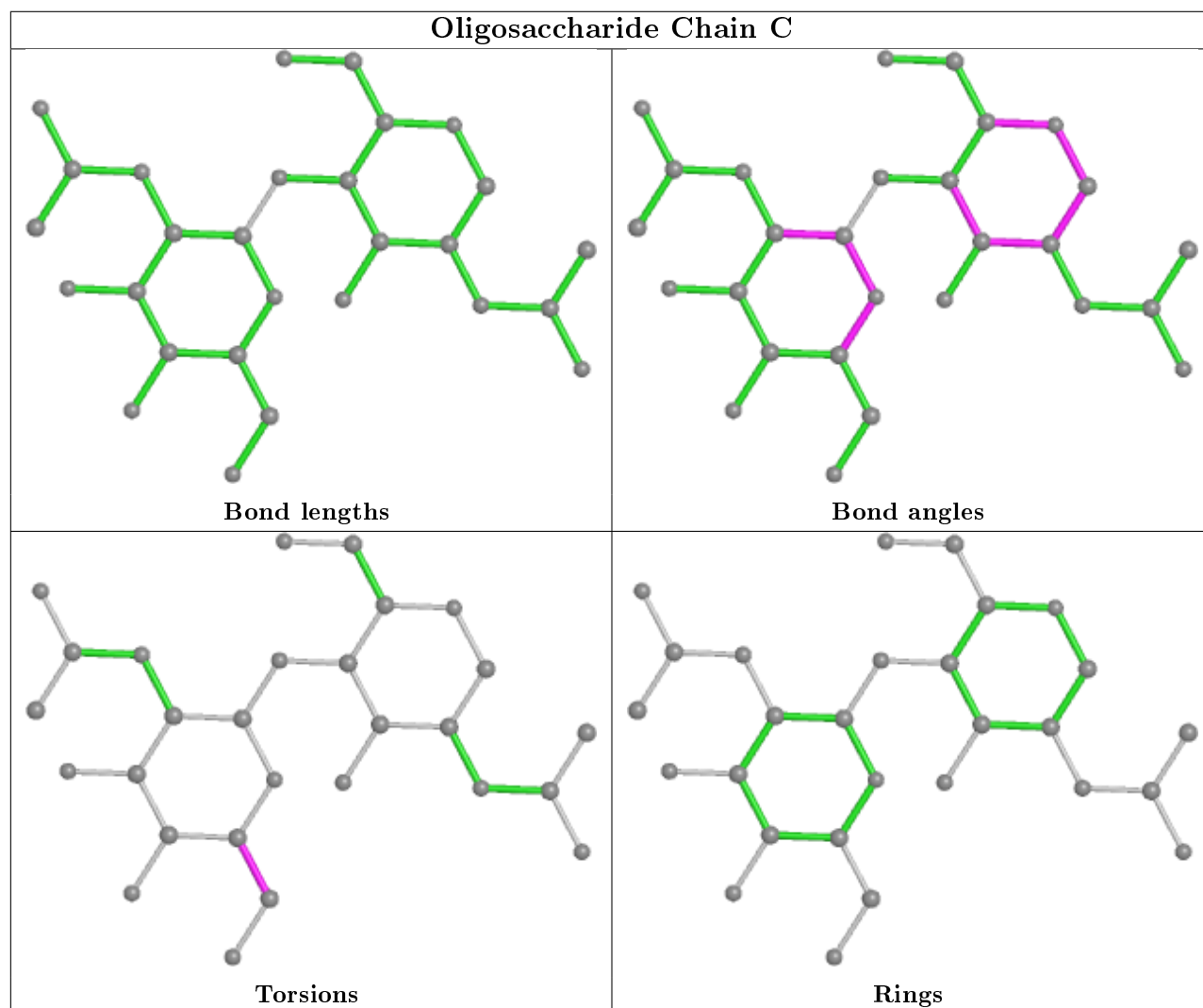
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

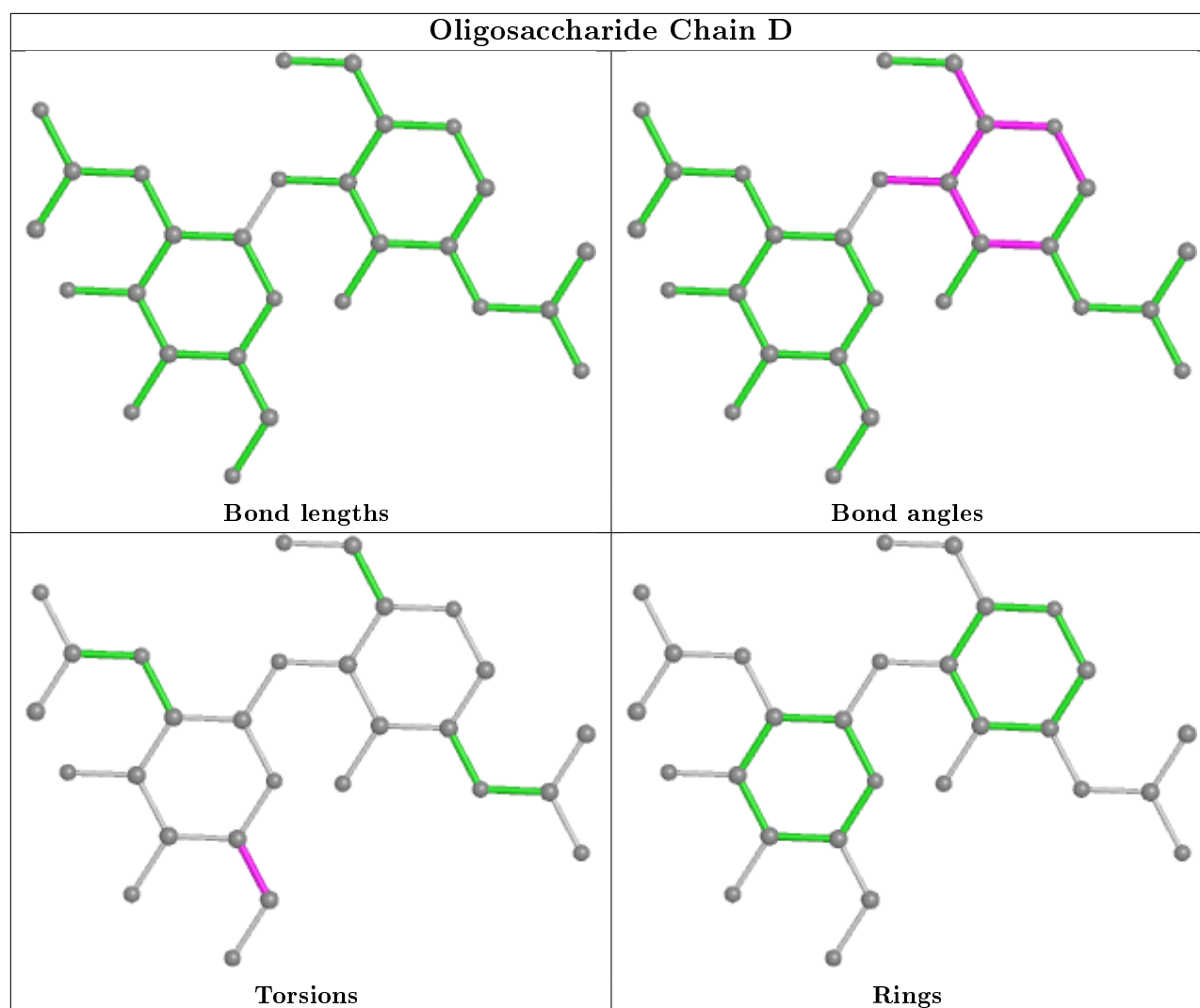
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	D	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 [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	635	1	14,14,15	0.56	0	17,19,21	0.91	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
3	NAG	A	635	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	587/619 (94%)	-0.21	8 (1%) 75 70	33, 69, 107, 140	0
1	B	583/619 (94%)	-0.34	3 (0%) 91 88	33, 65, 101, 122	0
All	All	1170/1238 (94%)	-0.27	11 (0%) 84 80	33, 67, 105, 140	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	HIS	3.8
1	A	630	PRO	3.2
1	A	211	LEU	2.7
1	B	242	TRP	2.6
1	B	29	ARG	2.5
1	A	267	SER	2.5
1	A	33	LEU	2.5
1	A	520	ASP	2.3
1	B	34	VAL	2.2
1	A	243	SER	2.1
1	A	588	GLY	2.1

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

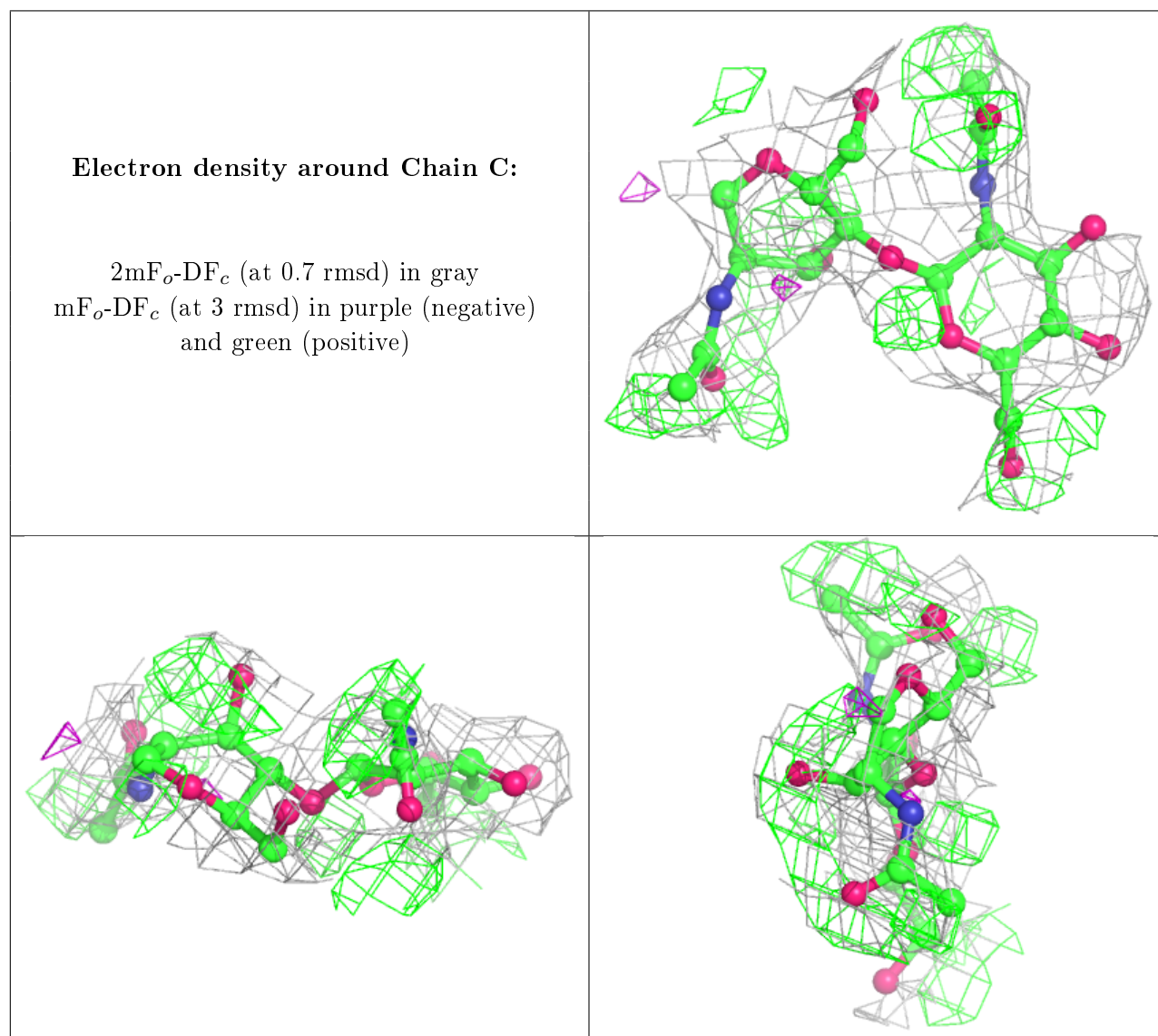
There are no non-standard protein/DNA/RNA residues in this entry.

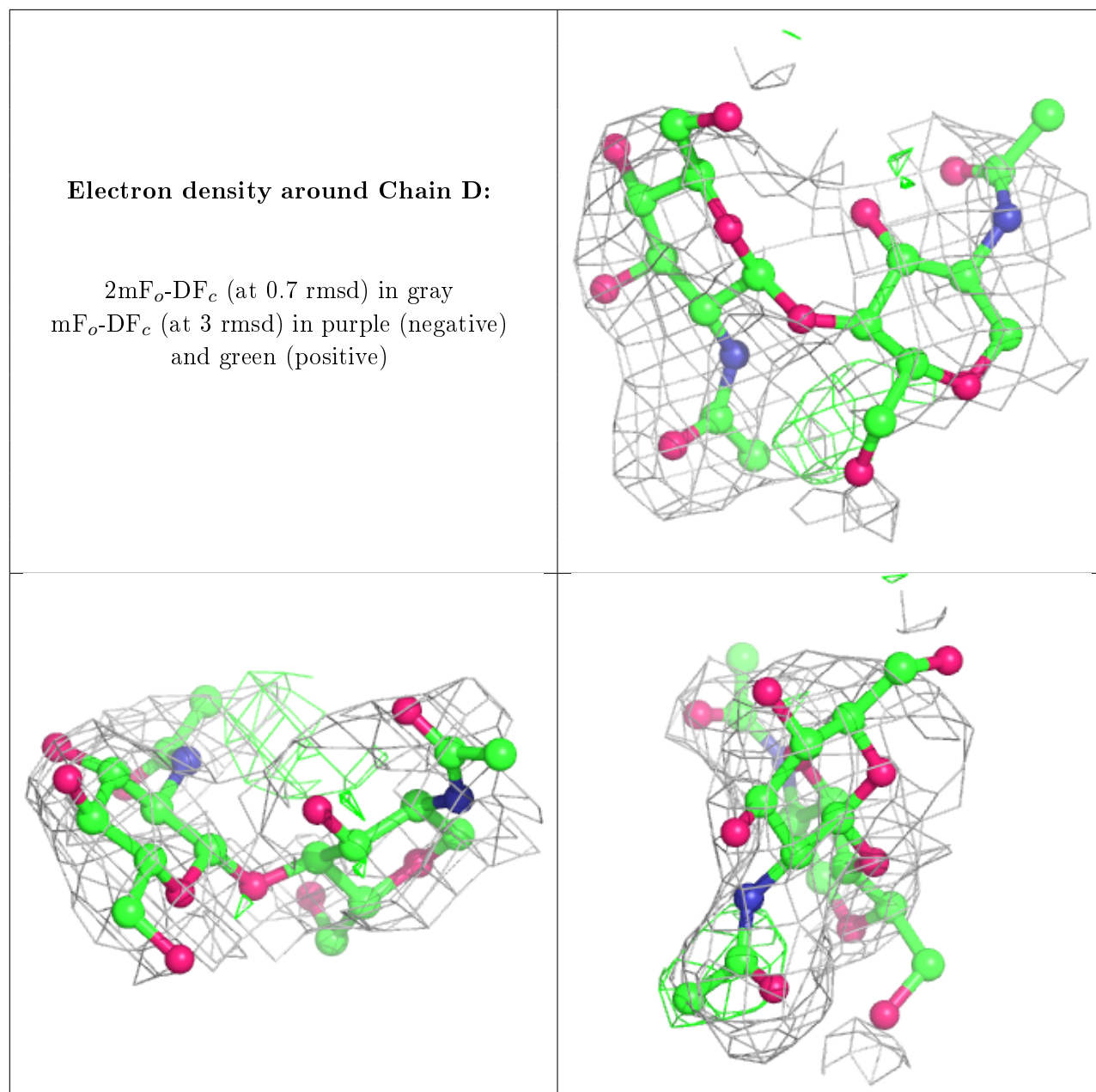
### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	1	14/15	0.56	0.27	136,136,136,136	0
2	NAG	C	2	14/15	0.65	0.24	136,136,136,136	0
2	NAG	D	1	14/15	0.72	0.21	130,130,130,130	0
2	NAG	D	2	14/15	0.83	0.14	130,130,130,130	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	635	14/15	0.84	0.16	130,130,130,130	0

## 6.5 Other polymers

There are no such residues in this entry.