



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:12 PM BST

PDB ID : 5HZ0  
Title : Plant peptide hormone receptor RGFR1 in complex with RGF2  
Authors : Song, W.; Han, Z.; Chai, J.  
Deposited on : 2016-02-02  
Resolution : 2.56 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

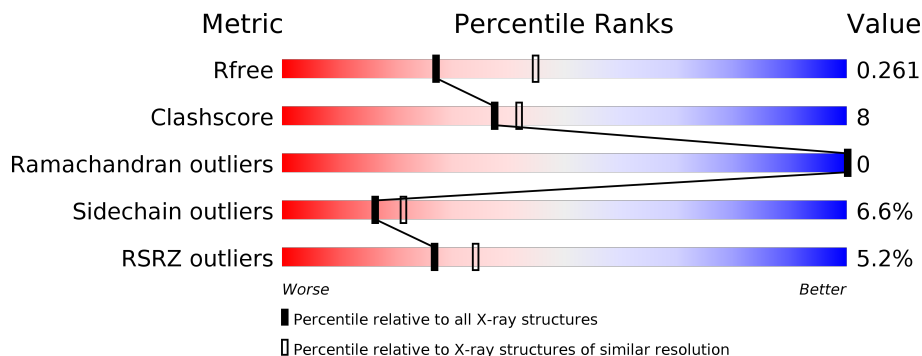
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	B	633	
2	A	13	
3	C	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	2	X	-	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4954 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 Probable LRR receptor-like serine/threonine-protein kinase At4g26540.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	624	4770	3017	807	931	15	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	64	THR	VAL	engineered mutation	UNP C0LGR3
B	81	GLU	GLY	engineered mutation	UNP C0LGR3
B	82	LYS	MET	engineered mutation	UNP C0LGR3
B	83	GLN	ASP	engineered mutation	UNP C0LGR3
B	104	GLN	ASN	engineered mutation	UNP C0LGR3

- Molecule 2 is a protein called ASP-PTR-TRP-LYS-PRO-ARG-HIS-HIS-PRO-HYP-ARG-A SN-ASN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	A	13	128	77	27	23	1	0	0	0

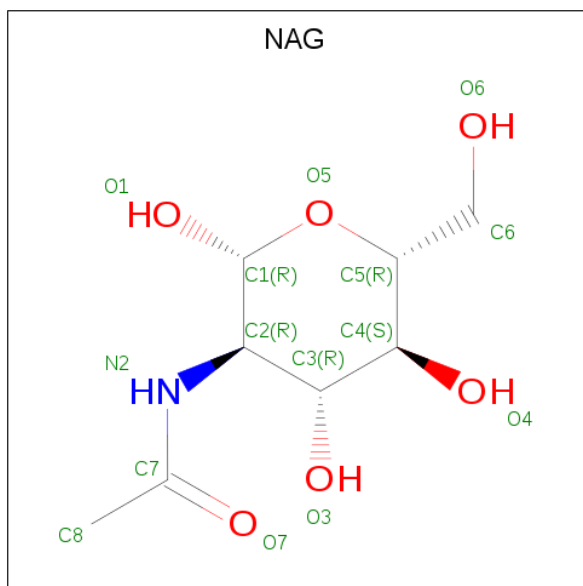
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

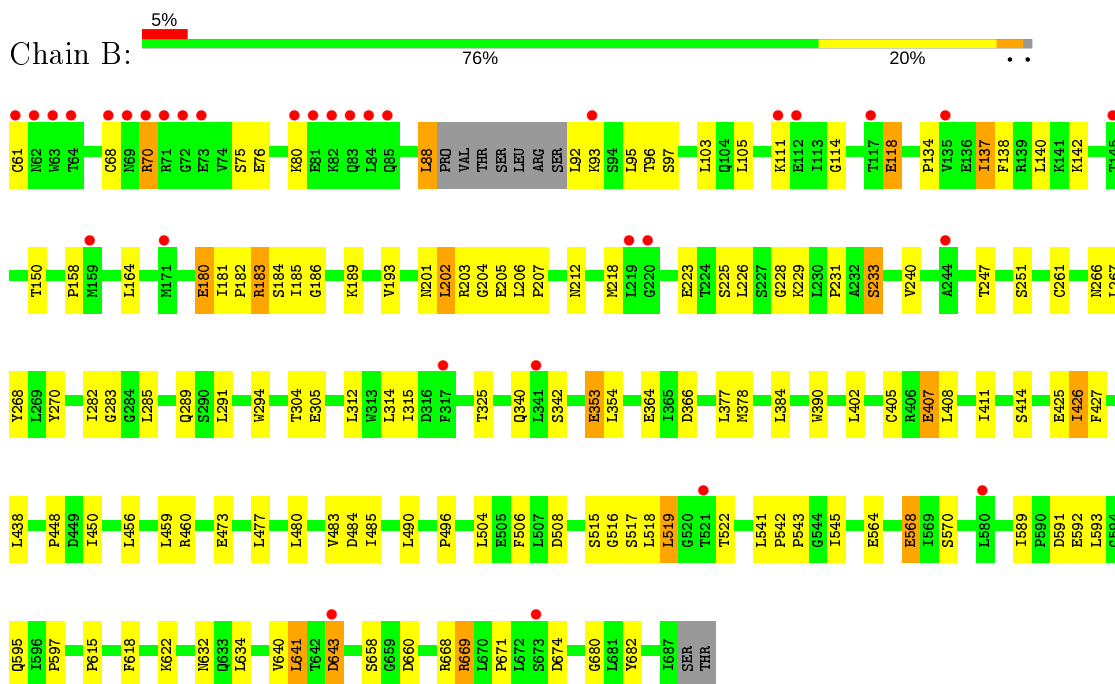


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

### 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 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: Probable LRR receptor-like serine/threonine-protein kinase At4g26540



- Molecule 2: ASP-PTR-TRP-LYS-PRO-ARG-HIS-HIS-PRO-HYP-ARG-ASN-ASN



- Molecule 3: 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	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.00 Å 181.00 Å 87.97 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.94 – 2.56 30.92 – 2.56	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.94-2.56) 96.9 (30.92-2.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.26 (at 2.54 Å)	Xtrriage
Refinement program	PHENIX, REFMAC	Depositor
R, $R_{free}$	0.232 , (Not available) 0.222 , 0.261	Depositor DCC
$R_{free}$ test set	1702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtrriage
Anisotropy	0.662	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: PTR, HZP, 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	B	0.45	0/4840	0.70	0/6567
2	A	0.44	0/107	0.70	0/140
All	All	0.45	0/4947	0.70	0/6707

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	B	4770	0	4872	77	0
2	A	128	0	109	2	0
3	C	28	0	25	1	0
4	B	28	0	26	0	0
All	All	4954	0	5032	77	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 (77) 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:407:GLU:N	1:B:407:GLU:OE1	2.10	0.83
1:B:118:GLU:OE2	1:B:142:LYS:NZ	2.19	0.71
1:B:180:GLU:HG2	1:B:204:GLY:HA3	1.77	0.66
1:B:541:LEU:HD12	1:B:542:PRO:HD2	1.77	0.66
1:B:496:PRO:HA	1:B:522:THR:HG23	1.77	0.65
1:B:340:GLN:NE2	1:B:364:GLU:OE1	2.22	0.62
1:B:483:VAL:HG12	1:B:504:LEU:HD11	1.82	0.62
1:B:384:LEU:N	1:B:407:GLU:OE2	2.33	0.61
1:B:660:ASP:HB3	1:B:682:TYR:CZ	2.36	0.60
1:B:622:LYS:NZ	1:B:643:ASP:OD1	2.34	0.57
1:B:203:ARG:HG2	1:B:225:SER:HB2	1.86	0.56
1:B:595:GLN:O	1:B:597:PRO:HD3	2.07	0.55
1:B:61:CYS:N	1:B:68:CYS:HG	2.04	0.55
1:B:138:PHE:HE2	1:B:158:PRO:HG2	1.72	0.55
1:B:201:ASN:O	1:B:203:ARG:HG3	2.07	0.54
1:B:180:GLU:CD	1:B:181:ILE:H	2.11	0.54
1:B:193:VAL:HG22	1:B:218:MET:HB3	1.90	0.54
1:B:138:PHE:HA	1:B:164:LEU:HD21	1.91	0.53
1:B:570:SER:HB3	1:B:592:GLU:HB3	1.91	0.53
1:B:669:ARG:HH21	1:B:669:ARG:HG2	1.73	0.52
1:B:658:SER:HB2	1:B:680:GLY:HA3	1.92	0.51
1:B:402:LEU:HB3	1:B:426:ILE:HD11	1.93	0.51
1:B:75:SER:O	1:B:95:LEU:HD12	2.12	0.50
1:B:519:LEU:HB2	1:B:522:THR:OG1	2.11	0.50
1:B:185:ILE:HD12	1:B:186:GLY:N	2.28	0.49
1:B:289:GLN:O	1:B:312:LEU:HD12	2.13	0.49
1:B:506:PHE:CE1	1:B:508:ASP:HB2	2.47	0.49
1:B:408:LEU:HD13	1:B:411:ILE:HD11	1.94	0.48
1:B:477:LEU:HD12	1:B:480:LEU:HD22	1.94	0.48
1:B:206:LEU:HD12	1:B:207:PRO:HD2	1.95	0.48
1:B:640:VAL:HG13	1:B:641:LEU:HD13	1.96	0.48
1:B:342:SER:OG	1:B:366:ASP:OD1	2.26	0.47
1:B:70:ARG:HG2	1:B:70:ARG:HH11	1.79	0.47
1:B:231:PRO:HB2	1:B:233:SER:HB2	1.97	0.47
1:B:111:LYS:HG3	1:B:134:PRO:HB3	1.96	0.47
1:B:515:SER:OG	1:B:516:GLY:N	2.49	0.46
1:B:267:LEU:HB3	1:B:291:LEU:HD12	1.98	0.46
1:B:543:PRO:HA	1:B:568:GLU:HG3	1.97	0.46
1:B:134:PRO:O	1:B:137:ILE:HB	2.14	0.45
1:B:181:ILE:HG13	1:B:202:LEU:HD11	1.97	0.45
1:B:485:ILE:O	1:B:485:ILE:HG22	2.18	0.44
1:B:390:TRP:CZ2	2:A:11:ARG:HG2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:PRO:HG2	1:B:674:ASP:CG	2.38	0.44
1:B:671:PRO:O	1:B:674:ASP:HB2	2.18	0.44
1:B:615:PRO:HG2	1:B:618:PHE:CD1	2.53	0.44
1:B:448:PRO:O	1:B:473:GLU:HG3	2.18	0.44
1:B:485:ILE:CG2	1:B:490:LEU:HD11	2.48	0.44
1:B:88:LEU:H	1:B:88:LEU:HD12	1.83	0.44
1:B:283:GLY:HA3	1:B:305:GLU:HB3	1.99	0.44
1:B:270:TYR:HB2	1:B:294:TRP:O	2.18	0.44
1:B:427:PHE:CE1	1:B:450:ILE:HG13	2.53	0.43
1:B:76:GLU:HG2	1:B:97:SER:HB3	1.99	0.43
1:B:353:GLU:H	1:B:353:GLU:HG2	1.38	0.43
1:B:615:PRO:O	1:B:618:PHE:HB2	2.18	0.43
1:B:103:LEU:HB2	1:B:105:LEU:HG	2.01	0.43
1:B:189:LYS:HE3	1:B:212:ASN:O	2.19	0.43
1:B:485:ILE:HG21	1:B:490:LEU:HD11	2.01	0.43
1:B:414:SER:OG	1:B:438:LEU:HG	2.19	0.43
1:B:456:LEU:HD21	1:B:459:LEU:HD13	2.01	0.43
1:B:114:GLY:HA2	1:B:140:LEU:HD21	2.00	0.43
1:B:377:LEU:HD23	1:B:377:LEU:HA	1.86	0.42
1:B:182:PRO:O	1:B:185:ILE:HG13	2.19	0.42
1:B:589:ILE:HG23	1:B:593:LEU:HD12	2.00	0.42
1:B:405:CYS:C	1:B:407:GLU:OE1	2.58	0.41
1:B:460:ARG:NH2	1:B:484:ASP:OD2	2.44	0.41
1:B:390:TRP:HZ2	2:A:11:ARG:HG2	1.85	0.41
1:B:266:ASN:HB3	1:B:268:TYR:CZ	2.55	0.41
1:B:517:SER:OG	1:B:518:LEU:N	2.53	0.41
1:B:202:LEU:HA	1:B:202:LEU:HD22	1.96	0.41
1:B:632:ASN:HB3	1:B:634:LEU:HD13	2.03	0.41
1:B:205:GLU:HG2	1:B:228:GLY:HA3	2.03	0.41
1:B:223:GLU:HA	1:B:247:THR:O	2.21	0.41
1:B:314:LEU:HD12	1:B:315:ILE:N	2.37	0.40
1:B:425:GLU:HA	3:C:1:NAG:H81	2.03	0.40
1:B:183:ARG:H	1:B:183:ARG:HG2	1.67	0.40
1:B:261:CYS:O	1:B:285:LEU:HD22	2.21	0.40
1:B:543:PRO:CA	1:B:568:GLU:HG3	2.51	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	B	620/633 (98%)	592 (96%)	28 (4%)	0	100	100
2	A	9/13 (69%)	9 (100%)	0	0	100	100
All	All	629/646 (97%)	601 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	552/568 (97%)	517 (94%)	35 (6%)	18	23
2	A	11/11 (100%)	9 (82%)	2 (18%)	1	1
All	All	563/579 (97%)	526 (93%)	37 (7%)	16	21

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	ARG
1	B	80	LYS
1	B	88	LEU
1	B	92	LEU
1	B	93	LYS
1	B	96	THR
1	B	118	GLU
1	B	137	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	150	THR
1	B	180	GLU
1	B	183	ARG
1	B	184	SER
1	B	202	LEU
1	B	226	LEU
1	B	229	LYS
1	B	233	SER
1	B	240	VAL
1	B	251	SER
1	B	282	ILE
1	B	304	THR
1	B	325	THR
1	B	353	GLU
1	B	354	LEU
1	B	378	MET
1	B	407	GLU
1	B	426	ILE
1	B	519	LEU
1	B	545	ILE
1	B	564	GLU
1	B	568	GLU
1	B	591	ASP
1	B	641	LEU
1	B	643	ASP
1	B	668	ARG
1	B	669	ARG
2	A	1	ASP
2	A	7	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	HZP	A	10	2	6,8,9	0.91	0	5,10,12	2.27	2 (40%)
2	PTR	A	2	2	15,16,17	1.35	1 (6%)	19,22,24	0.66	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	HZP	A	10	2	-	0/0/11/13	0/1/1/1
2	PTR	A	2	2	-	1/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	PTR	OH-CZ	-4.42	1.30	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	10	HZP	CB-CG-CD	4.37	108.63	103.27
2	A	10	HZP	CG-CB-CA	2.18	106.71	103.96

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	PTR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates i

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
3	NAG	C	1	1,3	14,14,15	0.50	0	17,19,21	0.95	1 (5%)
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	1.02	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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O5-C5-C6	2.43	111.02	107.20
3	C	2	NAG	C4-C3-C2	2.07	114.05	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	NAG	C1

All (2) torsion outliers are listed below:

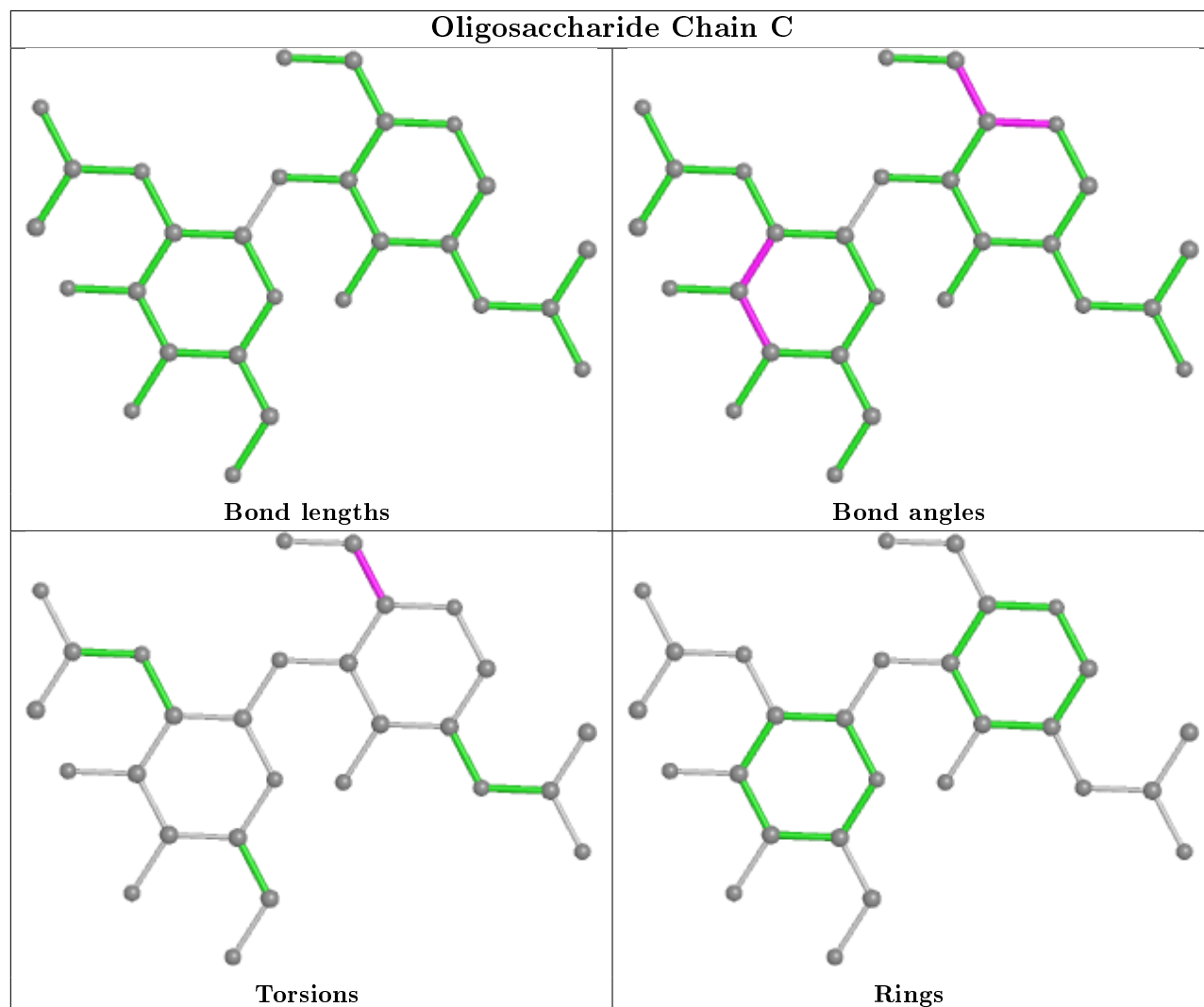
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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 [i](#)

2 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	B	703	1	14,14,15	0.59	0	17,19,21	1.62	5 (29%)
4	NAG	B	704	1	14,14,15	0.68	0	17,19,21	0.94	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. '1' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	703	1	-	0/6/23/26	0/1/1/1
4	NAG	B	704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NAG	C1-O5-C5	3.61	117.08	112.19
4	B	703	NAG	C2-N2-C7	2.65	126.67	122.90
4	B	703	NAG	C1-C2-N2	-2.49	106.24	110.49
4	B	703	NAG	C3-C4-C5	-2.29	106.16	110.24
4	B	703	NAG	O4-C4-C3	2.16	115.35	110.35

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 [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](#)

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	B	624/633 (98%)	0.05	33 (5%) 26 33	3, 16, 56, 115	0
2	A	11/13 (84%)	-0.03	0 100 100	7, 12, 27, 38	0
All	All	635/646 (98%)	0.05	33 (5%) 27 34	3, 16, 56, 115	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	ARG	5.9
1	B	63	TRP	5.8
1	B	72	GLY	5.2
1	B	83	GLN	5.1
1	B	68	CYS	5.1
1	B	71	ARG	4.8
1	B	64	THR	4.3
1	B	521	THR	4.0
1	B	61	CYS	3.8
1	B	85	GLN	3.7
1	B	62	ASN	3.5
1	B	81	GLU	3.4
1	B	84	LEU	3.4
1	B	82	LYS	3.2
1	B	135	VAL	3.1
1	B	159	MET	2.8
1	B	145	THR	2.8
1	B	69	ASN	2.7
1	B	111	LYS	2.5
1	B	643	ASP	2.4
1	B	220	GLY	2.4
1	B	117	THR	2.4
1	B	341	LEU	2.4
1	B	112	GLU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	673	SER	2.4
1	B	80	LYS	2.3
1	B	219	LEU	2.3
1	B	171	MET	2.3
1	B	317	PHE	2.2
1	B	73	GLU	2.1
1	B	93	LYS	2.0
1	B	244	ALA	2.0
1	B	580	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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.

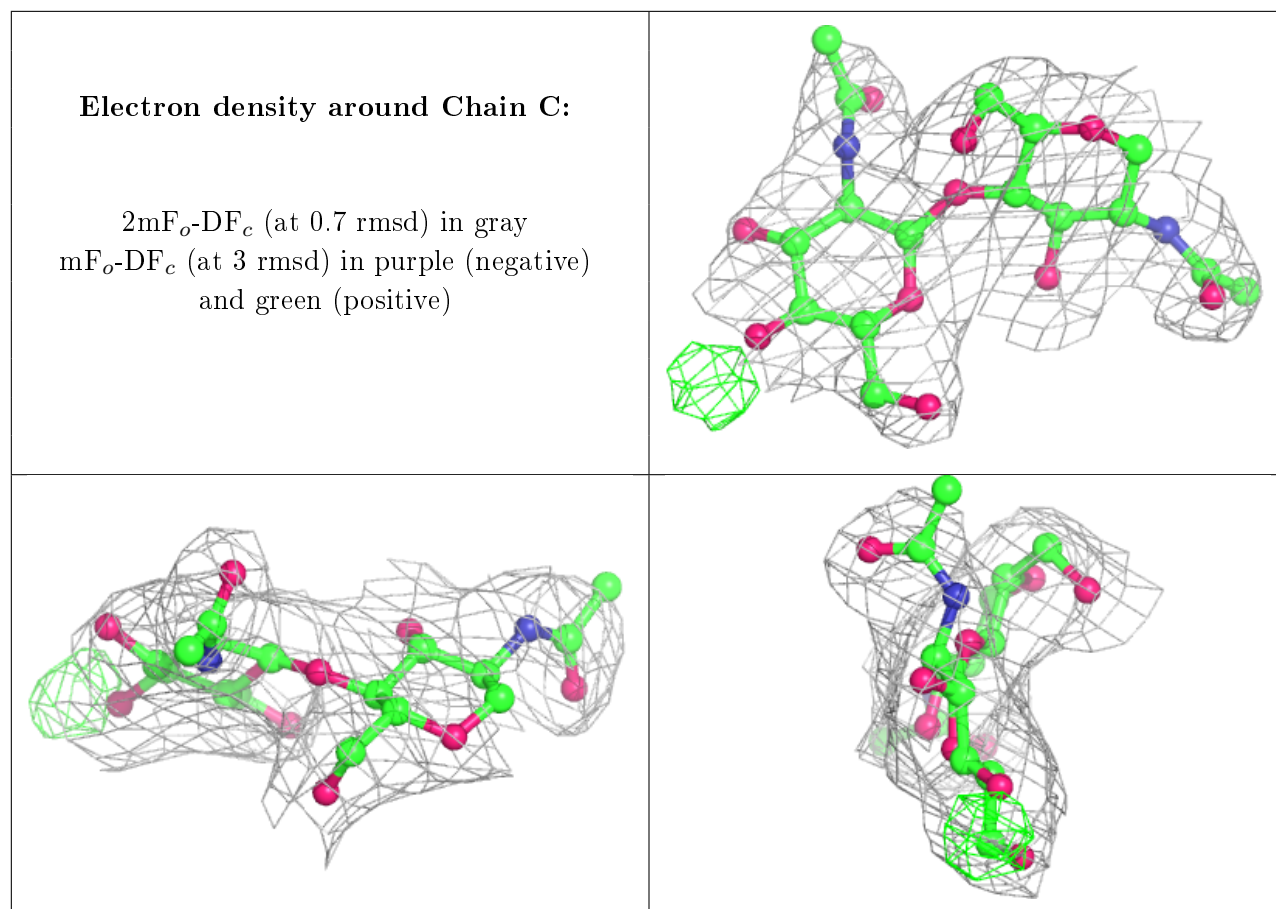
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HZP	A	10	8/9	0.94	0.12	16,17,26,37	0
2	PTR	A	2	16/17	0.96	0.15	9,11,20,20	0

## 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(Å <sup>2</sup> )	Q<0.9
3	NAG	C	2	14/15	0.87	0.34	30,41,46,50	0
3	NAG	C	1	14/15	0.94	0.16	16,21,31,36	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
4	NAG	B	703	14/15	0.94	0.10	4,6,10,11	0
4	NAG	B	704	14/15	0.95	0.11	5,11,16,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.