



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 08:33 PM JST

PDB ID : 5HZ3 / pdb\_00005hz3  
Title : Plant peptide hormone receptor RGFR1 in complex with RGFR5  
Authors : Song, W.; Han, Z.; Chai, J.  
Deposited on : 2016-02-02  
Resolution : 2.86 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

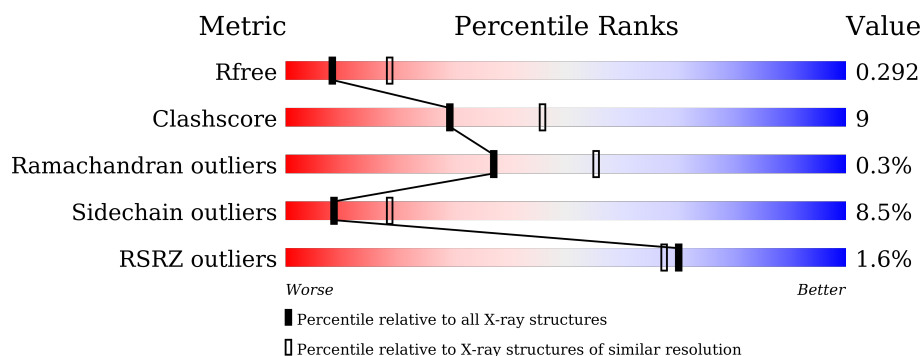
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.86 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))
$R_{free}$	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>..</div> </div> </div>
2	A	13	<div> <div>77%</div> <div>15%</div> <div>8%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4948 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
1	B	625	Total	C	N	O	S	0	0	0
			4776	3020	808	933	15			

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-PRO-LYS-PRO-SER-THR-ARG-PRO-HYP-ARG-HIS-ASN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	13	Total	C	N	O	P	0	0	0
			116	68	23	24	1			

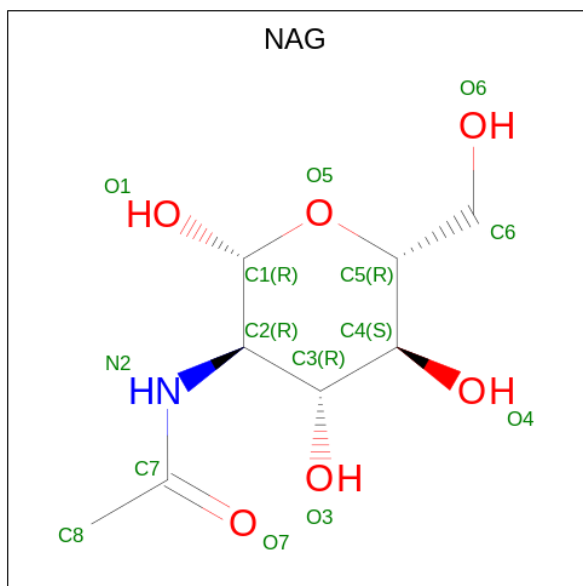
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

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

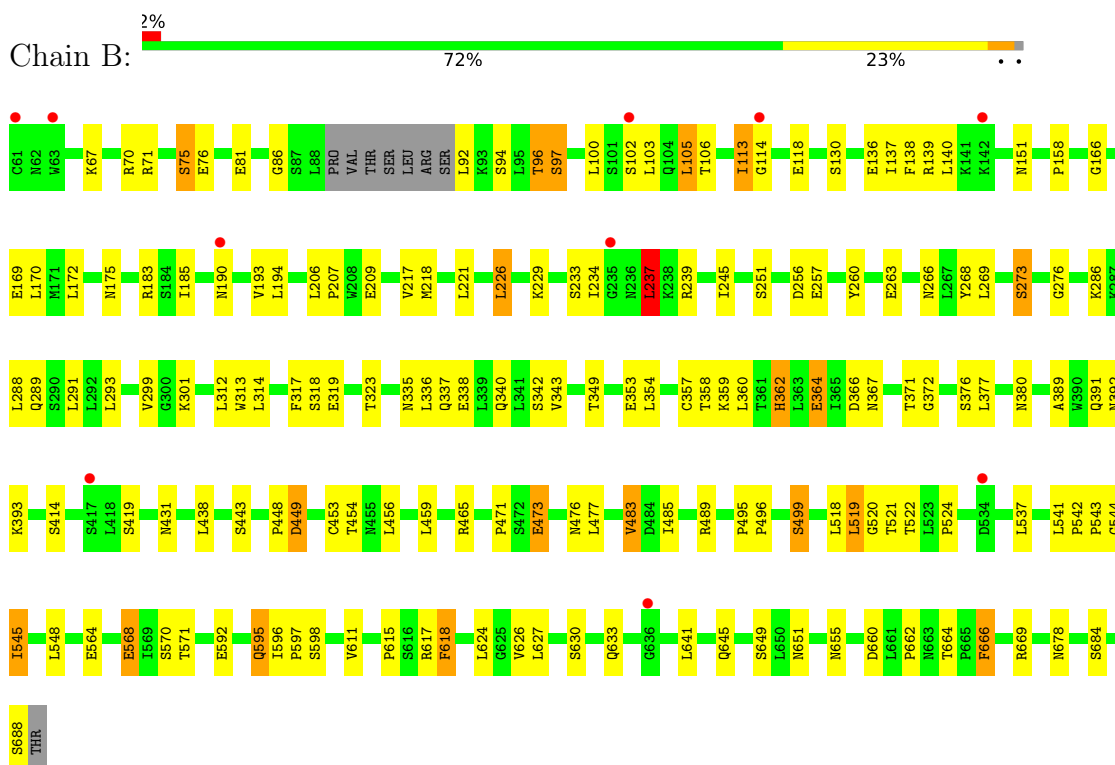


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

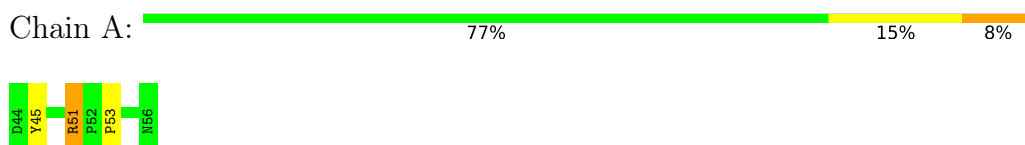
### 3 Residue-property plots

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



- Molecule 2: ASP-PTR-PRO-LYS-PRO-SER-THR-ARG-PRO-HYP-ARG-HIS-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, $\alpha$ , $\beta$ , $\gamma$	179.17Å 179.17Å 88.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.88 – 2.86 29.88 – 2.86	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.88-2.86) 93.1 (29.88-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 2.85Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, $R_{free}$	0.243 , (Not available) 0.234 , 0.292	Depositor DCC
$R_{free}$ test set	1243 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.2	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 22.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, PTR, HZP

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	0.39	0/4846	0.70	2/6575 (0.0%)
2	A	0.42	0/93	0.58	0/120
All	All	0.39	0/4939	0.69	2/6695 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	360	LEU	CA-CB-CG	5.27	127.41	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4776	0	4877	85	0
2	A	116	0	102	3	0
3	C	28	0	25	0	0
4	B	28	0	26	0	0
All	All	4948	0	5030	85	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 9.

All (85) 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:496:PRO:HA	1:B:522:THR:HG23	1.63	0.79
1:B:113:ILE:HG21	1:B:137:ILE:HG13	1.74	0.69
1:B:541:LEU:HD12	1:B:542:PRO:HD2	1.76	0.67
1:B:319:GLU:OE1	2:A:51:ARG:NH1	2.28	0.66
1:B:288:LEU:HD21	1:B:291:LEU:HD22	1.77	0.65
1:B:206:LEU:HD12	1:B:207:PRO:HD2	1.80	0.64
1:B:340:GLN:NE2	1:B:364:GLU:OE1	2.30	0.63
1:B:349:THR:HG22	1:B:372:GLY:HA3	1.80	0.63
1:B:371:THR:HA	1:B:393:LYS:O	1.99	0.62
1:B:138:PHE:CE2	1:B:158:PRO:HG2	2.34	0.62
1:B:499:SER:HA	1:B:524:PRO:HD3	1.84	0.60
1:B:76:GLU:HG2	1:B:97:SER:HB3	1.84	0.59
1:B:660:ASP:HB2	1:B:684:SER:HB3	1.83	0.59
1:B:251:SER:HA	1:B:273:SER:O	2.03	0.59
1:B:596:ILE:HG22	1:B:598:SER:HB3	1.84	0.58
1:B:615:PRO:HG2	1:B:618:PHE:CD1	2.40	0.57
1:B:234:ILE:HA	1:B:237:LEU:HD13	1.87	0.56
1:B:313:TRP:HB2	1:B:337:GLN:HG3	1.88	0.56
1:B:662:PRO:HB2	1:B:664:THR:HG23	1.88	0.55
1:B:448:PRO:O	1:B:473:GLU:HG3	2.07	0.55
1:B:209:GLU:OE1	1:B:209:GLU:N	2.32	0.55
1:B:314:LEU:HD13	1:B:338:GLU:HB3	1.89	0.54
1:B:289:GLN:HA	1:B:312:LEU:HA	1.89	0.54
1:B:520:GLY:HA3	1:B:544:GLY:HA3	1.90	0.54
1:B:114:GLY:HA2	1:B:140:LEU:HD21	1.89	0.54
1:B:473:GLU:O	1:B:476:ASN:HB2	2.07	0.54
1:B:301:LYS:HA	1:B:323:THR:O	2.08	0.53
1:B:465:ARG:HG2	1:B:489:ARG:NH1	2.23	0.53
1:B:624:LEU:HD21	1:B:627:LEU:HB2	1.92	0.52
1:B:221:LEU:HD13	1:B:226:LEU:HD13	1.91	0.52
1:B:136:GLU:HA	1:B:139:ARG:HG3	1.92	0.51
1:B:655:ASN:O	1:B:678:ASN:HA	2.11	0.51
1:B:166:GLY:HA2	1:B:190:ASN:HD21	1.75	0.51
1:B:313:TRP:HA	1:B:336:LEU:HA	1.92	0.50
1:B:568:GLU:O	1:B:571:THR:HG22	2.12	0.50
1:B:615:PRO:O	1:B:618:PHE:HB2	2.12	0.50
1:B:234:ILE:HA	1:B:237:LEU:CD1	2.42	0.49
1:B:193:VAL:HG22	1:B:218:MET:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:CYS:O	1:B:477:LEU:HD22	2.12	0.49
1:B:545:ILE:HD13	1:B:548:LEU:HD12	1.95	0.49
1:B:172:LEU:O	1:B:175:ASN:ND2	2.46	0.49
1:B:414:SER:OG	1:B:438:LEU:HG	2.12	0.49
1:B:335:ASN:HA	1:B:359:LYS:HD3	1.95	0.48
1:B:338:GLU:HG3	1:B:362:HIS:HB2	1.94	0.48
1:B:570:SER:HB3	1:B:592:GLU:HB3	1.95	0.48
1:B:518:LEU:HD13	1:B:537:LEU:HD13	1.95	0.47
1:B:630:SER:HB3	1:B:651:ASN:OD1	2.13	0.47
1:B:349:THR:HA	1:B:371:THR:O	2.15	0.47
1:B:318:SER:HB3	2:A:51:ARG:HD3	1.97	0.47
1:B:113:ILE:CG2	1:B:137:ILE:HG13	2.44	0.46
1:B:449:ASP:OD1	1:B:449:ASP:N	2.48	0.46
1:B:81:GLU:H	1:B:102:SER:HB2	1.81	0.46
1:B:151:ASN:O	1:B:175:ASN:HA	2.17	0.45
1:B:377:LEU:HD23	1:B:377:LEU:HA	1.72	0.44
1:B:518:LEU:O	1:B:519:LEU:HD13	2.18	0.44
1:B:86:GLY:O	1:B:106:THR:N	2.26	0.44
1:B:170:LEU:HD23	1:B:194:LEU:HD13	1.98	0.44
1:B:626:VAL:HG13	1:B:649:SER:HB3	1.98	0.44
1:B:75:SER:O	1:B:96:THR:N	2.50	0.43
1:B:595:GLN:O	1:B:597:PRO:HD3	2.18	0.43
1:B:289:GLN:O	1:B:312:LEU:HD12	2.18	0.43
1:B:67:LYS:HB2	1:B:76:GLU:HB2	2.00	0.43
1:B:367:ASN:HA	1:B:391:GLN:HB3	2.01	0.43
1:B:276:GLY:O	1:B:299:VAL:HG12	2.19	0.42
1:B:166:GLY:C	1:B:190:ASN:HD21	2.23	0.42
1:B:459:LEU:O	1:B:483:VAL:HA	2.19	0.41
1:B:543:PRO:HB3	1:B:568:GLU:OE1	2.20	0.41
1:B:245:ILE:O	1:B:269:LEU:HA	2.19	0.41
1:B:318:SER:CB	2:A:51:ARG:HD3	2.50	0.41
1:B:103:LEU:HB2	1:B:105:LEU:HD22	2.02	0.41
1:B:456:LEU:HD21	1:B:459:LEU:HD13	2.01	0.41
1:B:611:VAL:HG12	1:B:633:GLN:HB2	2.02	0.41
1:B:266:ASN:HB3	1:B:268:TYR:CZ	2.55	0.41
1:B:666:PHE:O	1:B:669:ARG:HB3	2.20	0.41
1:B:100:LEU:HB3	1:B:103:LEU:HD12	2.03	0.41
1:B:257:GLU:O	1:B:260:TYR:HB2	2.20	0.41
1:B:495:PRO:HA	1:B:496:PRO:HD3	1.93	0.41
1:B:183:ARG:H	1:B:183:ARG:HG2	1.69	0.40
1:B:357:CYS:O	1:B:359:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:SER:HA	1:B:366:ASP:O	2.21	0.40
1:B:239:ARG:HA	1:B:263:GLU:HG3	2.02	0.40
1:B:293:LEU:HD12	1:B:317:PHE:CE1	2.56	0.40
1:B:389:ALA:O	1:B:392:ASN:ND2	2.42	0.40
1:B:471:PRO:HB2	1:B:473:GLU:HG2	2.02	0.40
1:B:354:LEU:O	1:B:357:CYS:HB2	2.21	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	621/633 (98%)	587 (94%)	32 (5%)	2 (0%)	37	55
2	A	9/13 (69%)	9 (100%)	0	0	100	100
All	All	630/646 (98%)	596 (95%)	32 (5%)	2 (0%)	37	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	THR
1	B	343	VAL

### 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	553/568 (97%)	506 (92%)	47 (8%)	8	18
2	A	11/11 (100%)	10 (91%)	1 (9%)	7	15
All	All	564/579 (97%)	516 (92%)	48 (8%)	8	18

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	ARG
1	B	71	ARG
1	B	75	SER
1	B	92	LEU
1	B	94	SER
1	B	96	THR
1	B	97	SER
1	B	105	LEU
1	B	113	ILE
1	B	118	GLU
1	B	130	SER
1	B	169	GLU
1	B	185	ILE
1	B	217	VAL
1	B	226	LEU
1	B	229	LYS
1	B	233	SER
1	B	237	LEU
1	B	256	ASP
1	B	273	SER
1	B	286	LYS
1	B	353	GLU
1	B	362	HIS
1	B	364	GLU
1	B	376	SER
1	B	380	ASN
1	B	419	SER
1	B	431	ASN
1	B	443	SER
1	B	449	ASP
1	B	454	THR
1	B	473	GLU
1	B	483	VAL
1	B	485	ILE
1	B	499	SER

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Mol	Chain	Res	Type
1	B	519	LEU
1	B	521	THR
1	B	545	ILE
1	B	564	GLU
1	B	568	GLU
1	B	595	GLN
1	B	617	ARG
1	B	618	PHE
1	B	641	LEU
1	B	645	GLN
1	B	666	PHE
1	B	688	SER
2	A	51	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	53	2	6,8,9	1.01	0	5,10,12	1.69	1 (20%)
2	PTR	A	45	2	15,16,17	1.33	1 (6%)	19,22,24	0.81	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	53	2	-	0/0/11/13	0/1/1/1
2	PTR	A	45	2	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	45	PTR	OH-CZ	-4.45	1.30	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	53	HZP	CB-CG-CD	3.34	107.36	103.27

There are no chirality outliers.

There are no torsion outliers.

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	3,1	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
3	NAG	C	2	3	14,14,15	0.57	0	17,19,21	0.73	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	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	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	C	1	NAG	C1-O5-C5	2.55	115.65	112.19

There are no chirality outliers.

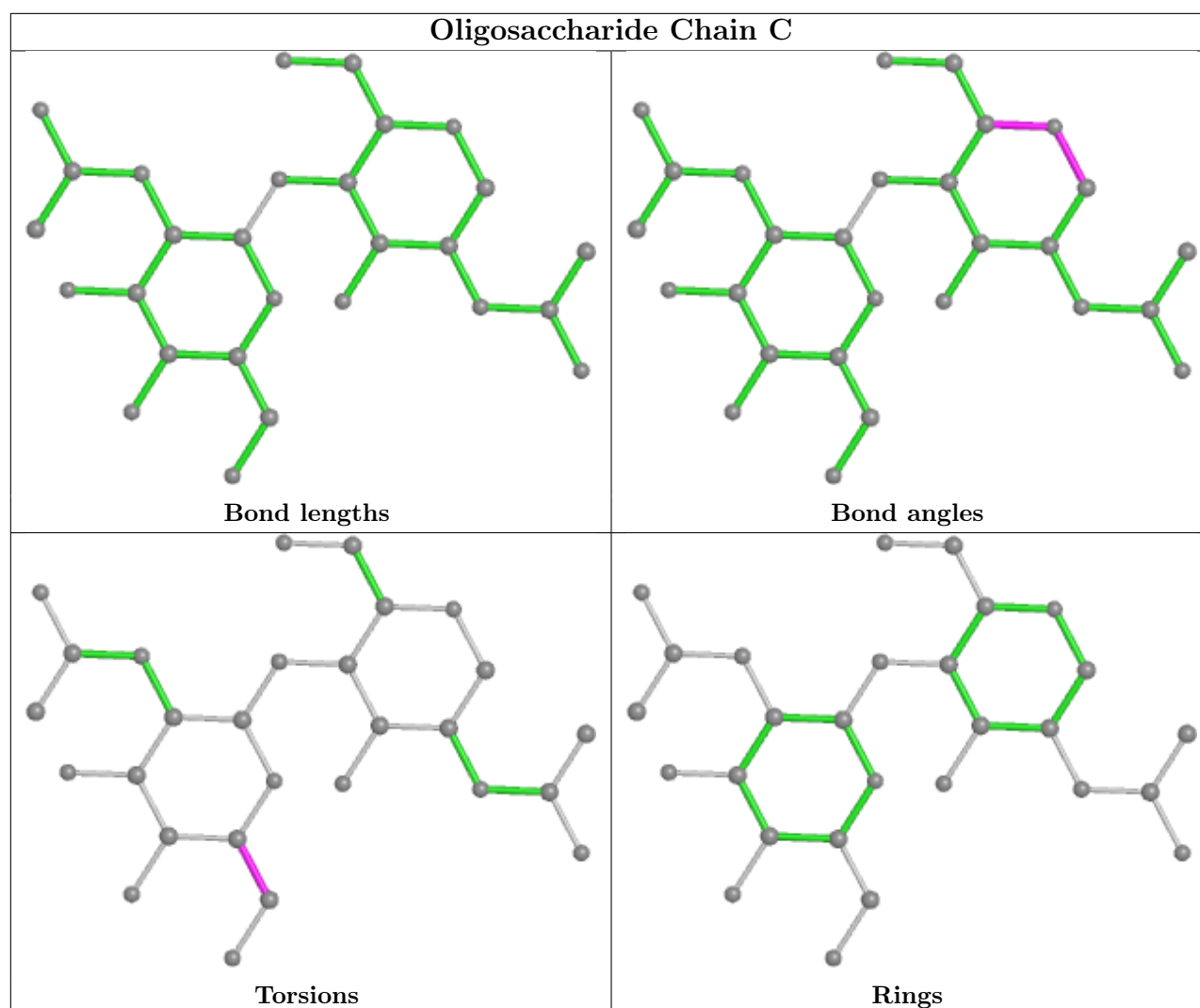
All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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	704	1	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
4	NAG	B	703	1	14,14,15	0.48	0	17,19,21	1.46	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	703	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NAG	C1-O5-C5	4.01	117.62	112.19
4	B	704	NAG	C1-O5-C5	3.04	116.32	112.19
4	B	703	NAG	O3-C3-C2	-2.17	104.97	109.47
4	B	703	NAG	O5-C5-C6	2.02	110.36	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	NAG	C8-C7-N2-C2
4	B	703	NAG	O7-C7-N2-C2

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	625/633 (98%)	-0.47	10 (1%) 70 67	3, 21, 64, 101	0
2	A	11/13 (84%)	-0.88	0 100 100	6, 11, 31, 70	0
All	All	636/646 (98%)	-0.47	10 (1%) 70 67	3, 21, 64, 101	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	GLY	3.4
1	B	114	GLY	3.1
1	B	61	CYS	2.9
1	B	417	SER	2.6
1	B	63	TRP	2.5
1	B	190	ASN	2.2
1	B	636	GLY	2.2
1	B	102	SER	2.1
1	B	142	LYS	2.1
1	B	534	ASP	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.

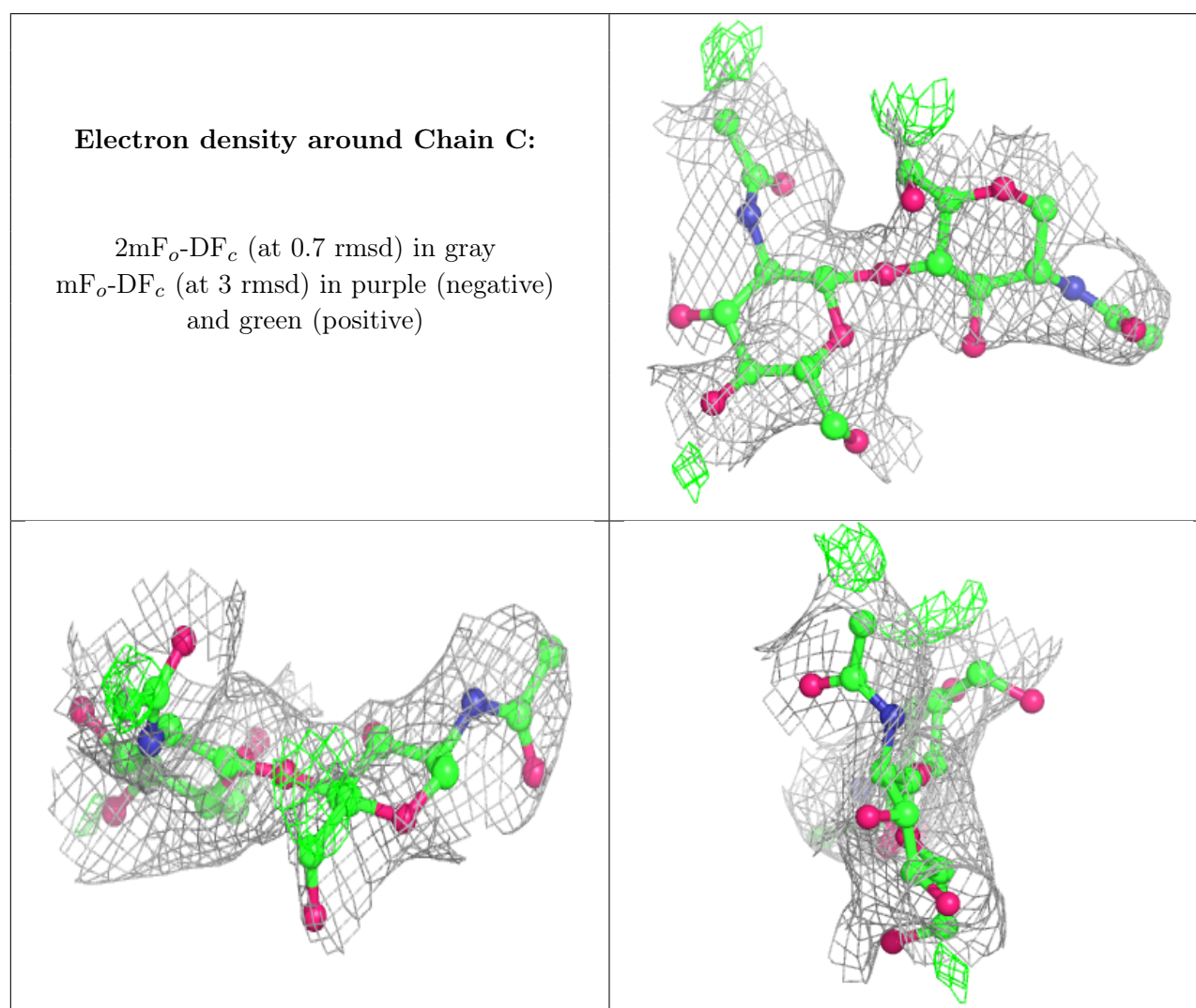
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HZP	A	53	8/9	0.89	0.09	2,8,22,42	0
2	PTR	A	45	16/17	0.96	0.08	10,16,36,48	0

### 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	2	14/15	0.78	0.10	34,55,67,71	0
3	NAG	C	1	14/15	0.92	0.07	16,29,47,55	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( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	703	14/15	0.82	0.10	6,7,32,38	0
4	NAG	B	704	14/15	0.84	0.09	7,11,25,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.