



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:22 PM GMT

PDB ID : 2V5O  
Title : STRUCTURE OF HUMAN IGF2R DOMAINS 11-14  
Authors : Brown, J.; Delaine, C.; Zaccheo, O.J.; Siebold, C.; Gilbert, R.J.; Van Boxel, G.; Denley, A.; Wallace, J.C.; Hassan, A.B.; Forbes, B.E.; Jones, E.Y.  
Deposited on : 2007-07-06  
Resolution : 2.91 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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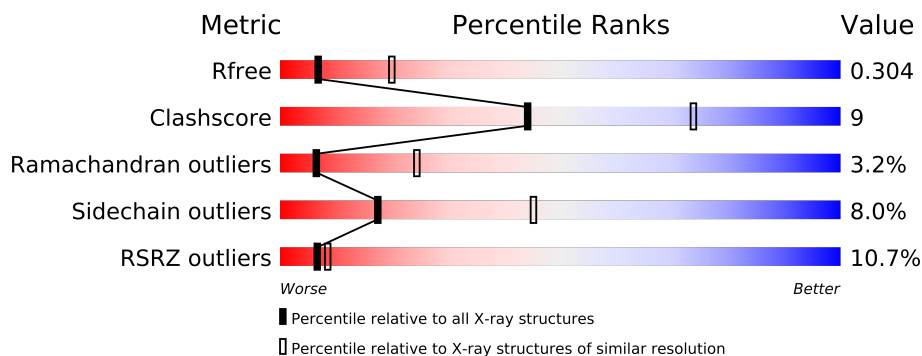
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.91 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))
$R_{free}$	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	627	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4686 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

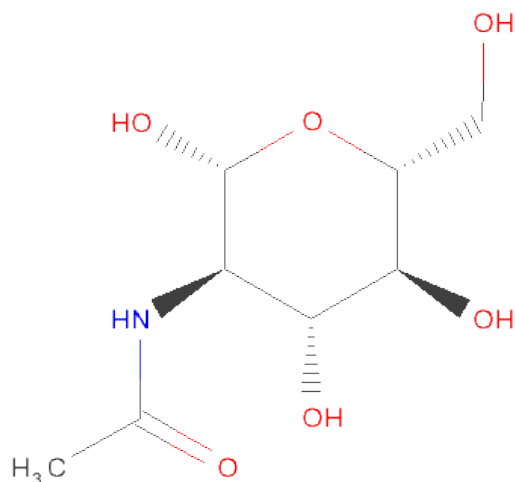
- Molecule 1 is a protein called CATION-INDEPENDENT MANNOSE-6-PHOSPHATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	0	0
			4642	2923	791	886	42			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1703	ALA	GLY	CONFLICT SEE REMARK 9	UNP P11717

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

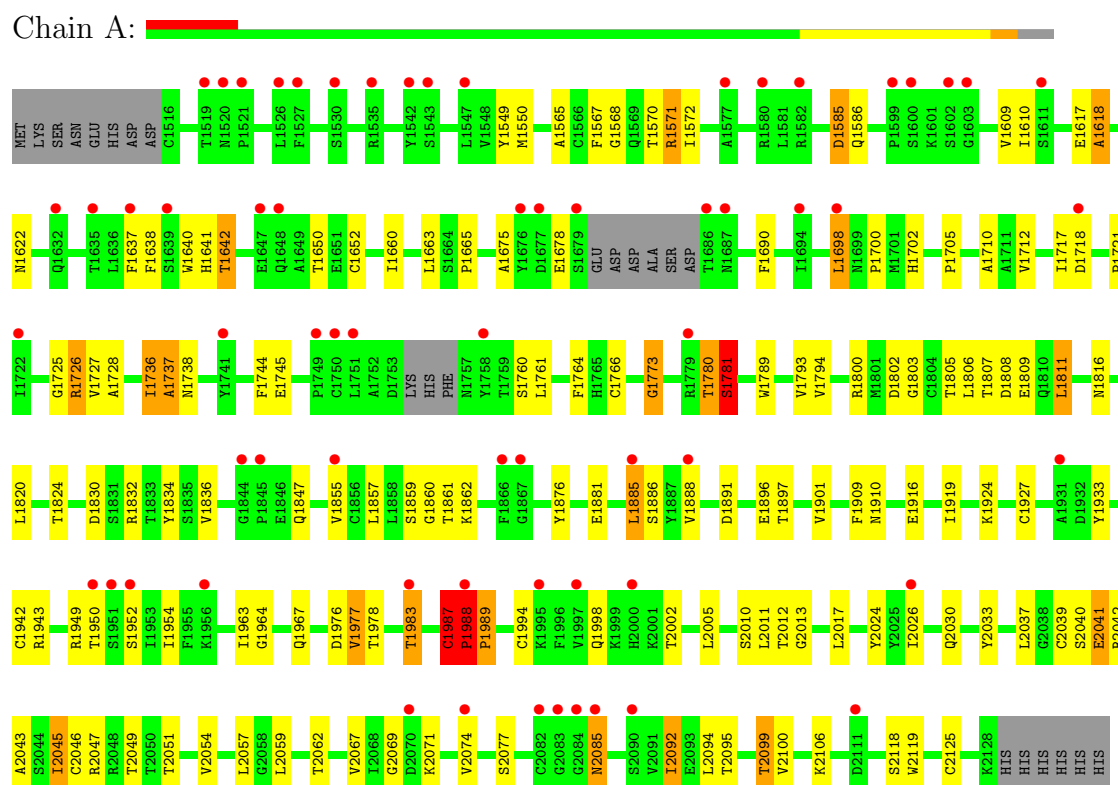
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: CATION-INDEPENDENT MANNOSE-6-PHOSPHATE RECEPTOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.55Å 69.25Å 98.01Å 90.00° 103.25° 90.00°	Depositor
Resolution (Å)	28.46 – 2.91 28.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.46-2.91) 98.6 (28.02-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.257 , 0.304 0.266 , 0.304	Depositor DCC
$R_{free}$ test set	1024 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 24.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19917 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	4686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL

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	0.39	0/4751	0.56	0/6447

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1781	SER	Peptide
1	A	1987	CYS	Peptide
1	A	1988	PRO	Peptide

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4642	0	4494	79	0
2	A	42	0	39	0	0
3	A	2	0	0	1	0
All	All	4686	0	4533	79	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (79) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1736:ILE:HG22	1:A:1737:ALA:H	0.96	1.11
1:A:1736:ILE:CG2	1:A:1737:ALA:H	1.76	0.98
1:A:1736:ILE:HG22	1:A:1737:ALA:N	1.78	0.97
1:A:1702:HIS:HB2	1:A:1924:LYS:HD3	1.54	0.89
1:A:1891:ASP:O	1:A:1949:ARG:HG3	1.71	0.88
1:A:1675:ALA:HB3	1:A:1690:PHE:HB2	1.60	0.83
1:A:1773:GLY:O	1:A:1789:TRP:NE1	2.13	0.81
1:A:1964:GLY:H	1:A:1983:THR:HG22	1.46	0.80
1:A:1885:LEU:HD12	1:A:1886:SER:N	2.02	0.74
1:A:1987:CYS:O	1:A:1989:PRO:HD3	1.88	0.72
1:A:1987:CYS:H	1:A:1988:PRO:HD3	1.54	0.71
1:A:1998:GLN:HG2	1:A:2067:VAL:HB	1.75	0.68
1:A:1808:ASP:HB3	1:A:1811:LEU:HD22	1.79	0.64
1:A:2041:GLU:O	1:A:2043:ALA:N	2.30	0.64
1:A:1964:GLY:H	1:A:1983:THR:CG2	2.11	0.64
1:A:1808:ASP:HB3	1:A:1811:LEU:CD2	2.31	0.61
1:A:2013:GLY:H	1:A:2033:TYR:HB2	1.63	0.60
1:A:1736:ILE:CG2	1:A:1737:ALA:N	2.46	0.60
1:A:1642:THR:HG22	3:A:3132:CL:CL	2.40	0.59
1:A:1806:LEU:HD11	1:A:1876:TYR:HB2	1.84	0.59
1:A:1744:PHE:HB2	1:A:1760:SER:HB3	1.86	0.57
1:A:1805:THR:HG22	1:A:1816:ASN:HA	1.88	0.56
1:A:1570:THR:O	1:A:1572:ILE:HG13	2.06	0.55
1:A:1994:CYS:HB3	1:A:2005:LEU:HB2	1.89	0.55
1:A:1954:ILE:O	1:A:1954:ILE:HG13	2.07	0.54
1:A:1927:CYS:HB3	1:A:1942:CYS:SG	2.49	0.52
1:A:1987:CYS:O	1:A:1989:PRO:CD	2.57	0.52
1:A:1820:LEU:HD23	1:A:1963:ILE:HG12	1.90	0.52
1:A:1964:GLY:N	1:A:1983:THR:HG22	2.21	0.52
1:A:1820:LEU:HD21	1:A:1983:THR:HG21	1.91	0.52
1:A:1764:PHE:HB3	1:A:1794:VAL:HG21	1.90	0.52
1:A:1705:PRO:HD2	1:A:1721:PRO:HG2	1.93	0.51
1:A:2045:ILE:HG13	1:A:2057:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1780:THR:O	1:A:1781:SER:C	2.50	0.50
1:A:1641:HIS:NE2	1:A:1700:PRO:HD3	2.28	0.49
1:A:1836:VAL:HG22	1:A:1855:VAL:HG13	1.94	0.49
1:A:2059:LEU:O	1:A:2062:THR:HG22	2.12	0.49
1:A:2074:VAL:HB	1:A:2092:ILE:HG23	1.94	0.48
1:A:2094:LEU:HA	1:A:2119:TRP:O	2.13	0.48
1:A:1859:SER:O	1:A:1861:THR:N	2.46	0.48
1:A:1570:THR:O	1:A:1571:ARG:C	2.52	0.48
1:A:2011:LEU:HD23	1:A:2030:GLN:HE22	1.78	0.47
1:A:2012:THR:O	1:A:2012:THR:HG23	2.14	0.47
1:A:1663:LEU:C	1:A:1665:PRO:HD2	2.35	0.47
1:A:1717:ILE:O	1:A:1718:ASP:HB2	2.14	0.47
1:A:1952:SER:O	1:A:1978:THR:HA	2.14	0.47
1:A:1896:GLU:OE1	1:A:1943:ARG:NH2	2.42	0.47
1:A:1549:TYR:O	1:A:1565:ALA:HA	2.15	0.46
1:A:1909:PHE:HD1	1:A:1933:TYR:CD2	2.34	0.46
1:A:1876:TYR:OH	1:A:1881:GLU:HA	2.15	0.46
1:A:2041:GLU:C	1:A:2043:ALA:H	2.18	0.46
1:A:2040:SER:C	1:A:2041:GLU:O	2.54	0.45
1:A:1618:ALA:HA	1:A:1622:ASN:HD21	1.80	0.45
1:A:2047:ARG:HB2	1:A:2057:LEU:HD11	1.98	0.45
1:A:1550:MET:HB3	1:A:1565:ALA:HB2	1.99	0.44
1:A:1830:ASP:HB2	1:A:1832:ARG:NH1	2.32	0.44
1:A:2017:LEU:HG	1:A:2024:TYR:HB2	2.00	0.44
1:A:1609:VAL:HG23	1:A:1637:PHE:HA	2.00	0.44
1:A:1567:PHE:HB2	1:A:1572:ILE:HB	2.00	0.43
1:A:1712:VAL:HB	1:A:1725:GLY:HA3	2.01	0.43
1:A:1610:ILE:HA	1:A:1638:PHE:HB2	2.00	0.43
1:A:2062:THR:HG23	1:A:2077:SER:H	1.83	0.43
1:A:2094:LEU:HG	1:A:2119:TRP:HB3	2.00	0.43
1:A:1987:CYS:N	1:A:1988:PRO:HD3	2.27	0.43
1:A:2100:VAL:O	1:A:2100:VAL:HG22	2.18	0.43
1:A:1698:LEU:HB2	1:A:1710:ALA:O	2.18	0.42
1:A:1702:HIS:HB2	1:A:1924:LYS:CD	2.39	0.42
1:A:1808:ASP:OD1	1:A:1809:GLU:N	2.52	0.42
1:A:1834:TYR:CZ	1:A:1977:VAL:HG11	2.54	0.42
1:A:1950:THR:O	1:A:1976:ASP:HA	2.19	0.42
1:A:1967:GLN:HA	1:A:1967:GLN:OE1	2.20	0.42
1:A:2071:LYS:HE3	1:A:2095:THR:HG23	2.02	0.41
1:A:1640:TRP:CD1	1:A:1642:THR:HG23	2.55	0.41
1:A:1726:ARG:N	1:A:1745:GLU:O	2.54	0.41
1:A:1710:ALA:HA	1:A:1726:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2099:THR:OG1	1:A:2100:VAL:N	2.54	0.40
1:A:1800:ARG:NH1	1:A:1803:GLY:O	2.43	0.40
1:A:2106:LYS:HE3	1:A:2118:SER:HB2	2.03	0.40
1:A:1897:THR:OG1	1:A:1901:VAL:HG12	2.21	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	598/627 (95%)	521 (87%)	58 (10%)	19 (3%)	6	24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1571	ARG
1	A	1618	ALA
1	A	1678	GLU
1	A	2041	GLU
1	A	2085	ASN
1	A	1568	GLY
1	A	1727	VAL
1	A	1736	ILE
1	A	1860	GLY
1	A	2042	ARG
1	A	2069	GLY
1	A	1728	ALA
1	A	1781	SER
1	A	1989	PRO
1	A	1585	ASP
1	A	1737	ALA
1	A	1987	CYS
1	A	1773	GLY
1	A	1988	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	524/549 (95%)	482 (92%)	42 (8%)	17	45

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1585	ASP
1	A	1586	GLN
1	A	1617	GLU
1	A	1642	THR
1	A	1650	THR
1	A	1652	CYS
1	A	1660	ILE
1	A	1698	LEU
1	A	1726	ARG
1	A	1738	ASN
1	A	1761	LEU
1	A	1766	CYS
1	A	1780	THR
1	A	1793	VAL
1	A	1802	ASP
1	A	1807	THR
1	A	1811	LEU
1	A	1824	THR
1	A	1847	GLN
1	A	1857	LEU
1	A	1862	LYS
1	A	1885	LEU
1	A	1888	VAL
1	A	1910	ASN
1	A	1916	GLU
1	A	1919	ILE
1	A	1977	VAL
1	A	1983	THR
1	A	2002	THR
1	A	2010	SER
1	A	2026	ILE

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Mol	Chain	Res	Type
1	A	2037	LEU
1	A	2039	CYS
1	A	2045	ILE
1	A	2046	CYS
1	A	2049	THR
1	A	2051	THR
1	A	2054	VAL
1	A	2085	ASN
1	A	2092	ILE
1	A	2099	THR
1	A	2125	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1525	HIS
1	A	1558	ASN
1	A	1586	GLN
1	A	1589	GLN
1	A	1696	GLN
1	A	1847	GLN
1	A	1889	ASN
1	A	1910	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	A	3129	1	12,14,15	0.64	0	15,19,21	1.85	2 (13%)
2	NAG	A	3130	1	12,14,15	0.55	0	15,19,21	0.92	1 (6%)
2	NAG	A	3131	1	12,14,15	0.57	0	15,19,21	1.04	1 (6%)

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	A	3129	1	-	0/6/23/26	0/1/1/1
2	NAG	A	3130	1	-	1/6/23/26	0/1/1/1
2	NAG	A	3131	1	-	1/6/23/26	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(°)
2	A	3129	NAG	O5-C5-C6	5.76	113.03	106.98
2	A	3129	NAG	C3-C2-N2	-2.81	107.49	111.76
2	A	3131	NAG	C2-N2-C7	2.61	127.48	123.09
2	A	3130	NAG	O5-C5-C6	2.37	109.47	106.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3130	NAG	C3-C2-N2-C7
2	A	3131	NAG	C1-C2-N2-C7

There are no ring outliers.

## 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 ⓘ

### 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, 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	604/627 (96%)	0.74	65 (10%) 6 8	66, 66, 66, 66	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1602	SER	5.0
1	A	2084	GLY	4.9
1	A	1679	SER	4.4
1	A	1676	TYR	4.3
1	A	1718	ASP	4.3
1	A	1845	PRO	4.3
1	A	1603	GLY	4.2
1	A	1580	ARG	4.2
1	A	1686	THR	3.4
1	A	1647	GLU	3.4
1	A	1988	PRO	3.4
1	A	1519	THR	3.2
1	A	1521	PRO	3.1
1	A	2083	GLY	3.1
1	A	2082	CYS	3.0
1	A	1751	LEU	2.8
1	A	1677	ASP	2.8
1	A	1520	ASN	2.7
1	A	1687	ASN	2.7
1	A	1542	TYR	2.7
1	A	1600	SER	2.7
1	A	1535	ARG	2.6
1	A	1582	ARG	2.6
1	A	1694	ILE	2.6
1	A	1611	SER	2.6
1	A	1855	VAL	2.6
1	A	1844	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1543	SER	2.5
1	A	1758	TYR	2.5
1	A	1527	PHE	2.5
1	A	1741	TYR	2.5
1	A	1722	ILE	2.4
1	A	1648	GLN	2.4
1	A	1951	SER	2.4
1	A	1637	PHE	2.4
1	A	2074	VAL	2.3
1	A	1950	THR	2.3
1	A	1931	ALA	2.3
1	A	1952	SER	2.3
1	A	1956	LYS	2.3
1	A	2085	ASN	2.2
1	A	1530	SER	2.2
1	A	1983	THR	2.2
1	A	2090	SER	2.2
1	A	1526	LEU	2.2
1	A	2000	HIS	2.2
1	A	2111	ASP	2.2
1	A	1577	ALA	2.2
1	A	2070	ASP	2.2
1	A	1867	GLY	2.1
1	A	1779	ARG	2.1
1	A	1632	GLN	2.1
1	A	1866	PHE	2.1
1	A	1749	PRO	2.1
1	A	1888	VAL	2.1
1	A	1639	SER	2.1
1	A	1885	LEU	2.1
1	A	1599	PRO	2.1
1	A	1547	LEU	2.1
1	A	1750	CYS	2.0
1	A	1997	VAL	2.0
1	A	1995	LYS	2.0
1	A	2026	ILE	2.0
1	A	1635	THR	2.0
1	A	1698	LEU	2.0

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

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



### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	3129	14/15	0.21	-	65,65,65,65	0
3	CL	A	3133	1/1	0.32	-	65,65,65,65	0
2	NAG	A	3130	14/15	0.33	-	65,65,65,65	0
2	NAG	A	3131	14/15	0.22	-	65,65,65,65	0
3	CL	A	3132	1/1	0.15	-	65,65,65,65	0

### 6.5 Other polymers

There are no such residues in this entry.