



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 10:09 AM EDT

PDB ID : 3V64  
Title : Crystal Structure of agrin and LRP4  
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Deposited on : 2011-12-18  
Resolution : 2.85 Å (reported)

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<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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

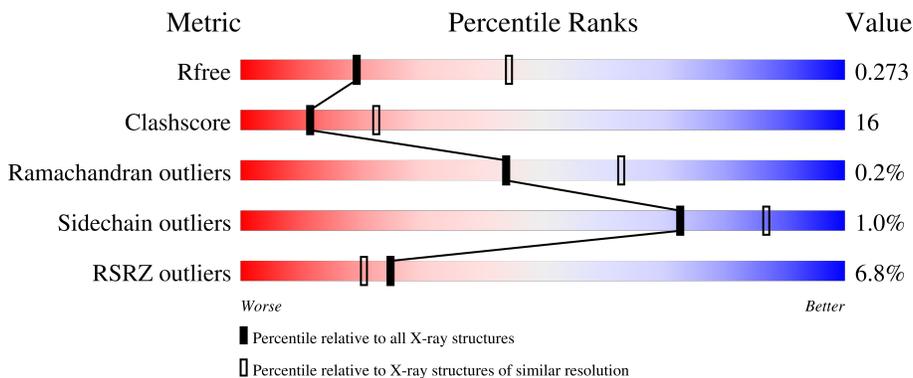
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	C	349	 5% 67% 30% ..
1	D	349	 6% 69% 26% ..
2	A	191	 2% 80% 19% .
2	B	191	 16% 63% 36% ..

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8471 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	338	2700	1697	498	490	15	0	0	0
1	D	334	2673	1683	492	483	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	738	LEU	-	expression tag	UNP Q9QYP1
C	739	GLU	-	expression tag	UNP Q9QYP1
C	740	VAL	-	expression tag	UNP Q9QYP1
C	741	LEU	-	expression tag	UNP Q9QYP1
C	742	PHE	-	expression tag	UNP Q9QYP1
C	743	GLN	-	expression tag	UNP Q9QYP1
C	744	GLY	-	expression tag	UNP Q9QYP1
D	738	LEU	-	expression tag	UNP Q9QYP1
D	739	GLU	-	expression tag	UNP Q9QYP1
D	740	VAL	-	expression tag	UNP Q9QYP1
D	741	LEU	-	expression tag	UNP Q9QYP1
D	742	PHE	-	expression tag	UNP Q9QYP1
D	743	GLN	-	expression tag	UNP Q9QYP1
D	744	GLY	-	expression tag	UNP Q9QYP1

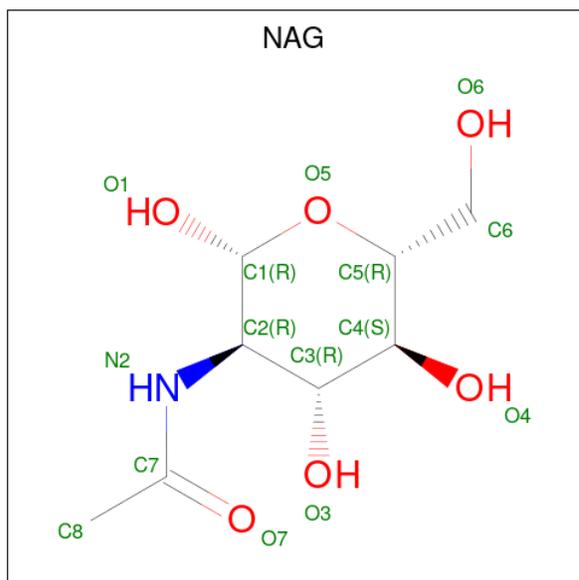
- Molecule 2 is a protein called agrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	191	1470	927	263	277	3	0	0	0
2	B	190	1465	924	262	276	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1758	ALA	-	expression tag	UNP P25304
B	1758	ALA	-	expression tag	UNP P25304

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

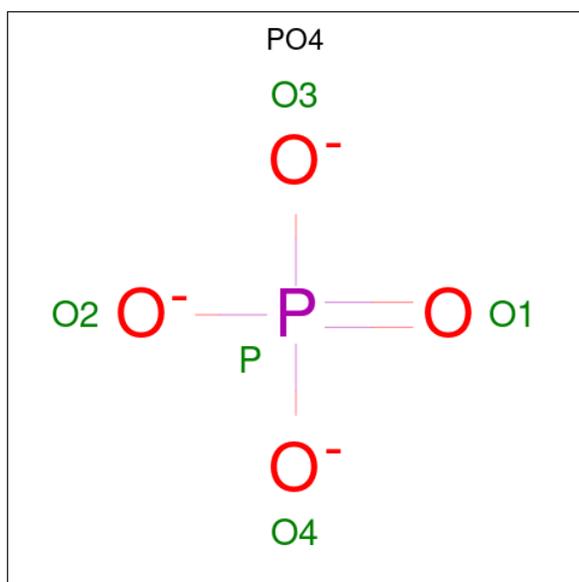


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	C	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	D	2	Total	Ca	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

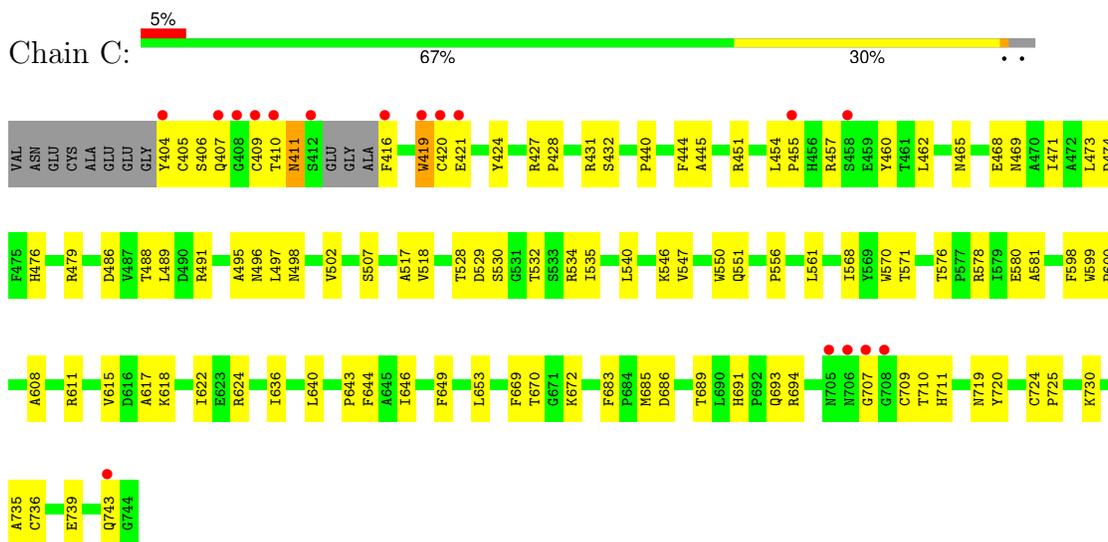
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	39	Total O 39 39	0	0
6	A	25	Total O 25 25	0	0
6	B	18	Total O 18 18	0	0
6	D	28	Total O 28 28	0	0

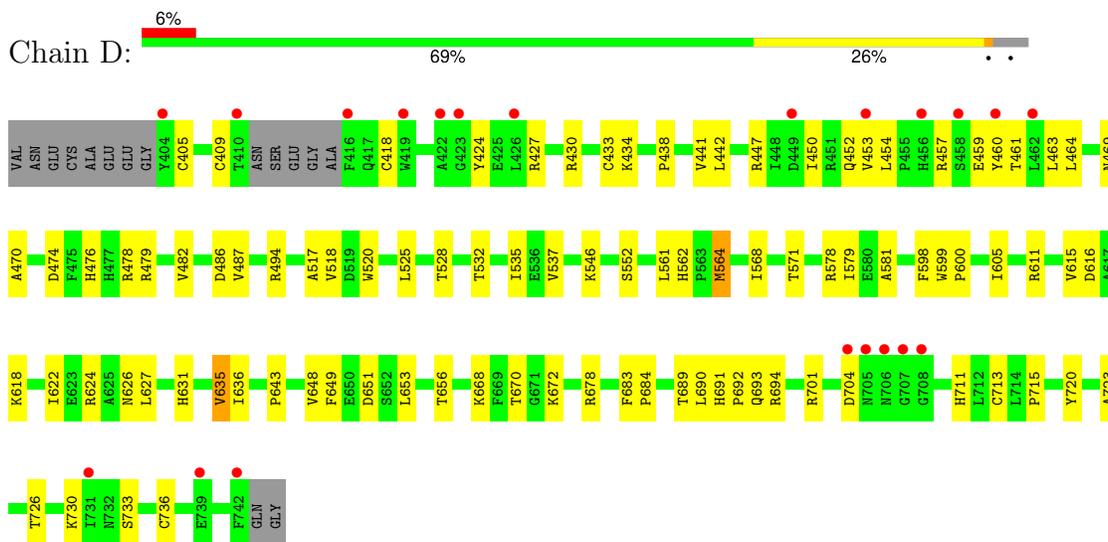
### 3 Residue-property plots [i](#)

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: Low-density lipoprotein receptor-related protein 4



- Molecule 1: Low-density lipoprotein receptor-related protein 4

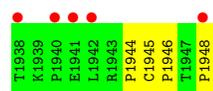
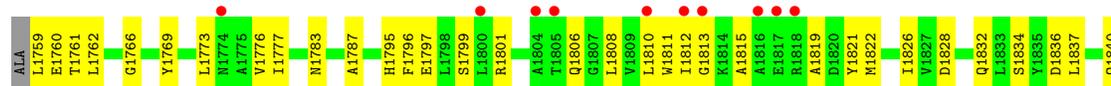


- Molecule 2: agrin





• Molecule 2: agrin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.46Å 106.07Å 112.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.85) 98.2 (50.00-2.85)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.203 , 0.273 0.226 , 0.273	Depositor DCC
$R_{free}$ test set	1383 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtrriage
Anisotropy	0.382	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, CA, PO4

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	C	0.50	0/2773	0.50	0/3768
1	D	0.49	0/2746	0.51	0/3732
2	A	0.40	0/1499	0.51	0/2041
2	B	0.41	0/1494	0.57	0/2034
All	All	0.46	0/8512	0.52	0/11575

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	C	2700	0	2595	87	0
1	D	2673	0	2574	70	0
2	A	1470	0	1474	34	0
2	B	1465	0	1469	73	0
3	C	28	0	26	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
6	A	25	0	0	0	0
6	B	18	0	0	2	0
6	C	39	0	0	0	0
6	D	28	0	0	0	0
All	All	8471	0	8138	260	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 16.

The worst 5 of 260 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)
2:A:1817:GLU:HG2	2:A:1904:VAL:HB	1.29	1.09
1:C:498:ASN:HB3	3:C:801:NAG:HN2	1.24	1.00
1:D:711:HIS:CD2	1:D:736:CYS:HB2	1.97	1.00
1:D:454:LEU:HD12	1:D:457:ARG:HH21	1.29	0.96
1:D:611:ARG:HD3	1:D:624:ARG:HD2	1.50	0.93

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	C	334/349 (96%)	308 (92%)	25 (8%)	1 (0%)	37	55
1	D	330/349 (95%)	300 (91%)	30 (9%)	0	100	100
2	A	189/191 (99%)	179 (95%)	10 (5%)	0	100	100
2	B	188/191 (98%)	179 (95%)	8 (4%)	1 (0%)	25	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1041/1080 (96%)	966 (93%)	73 (7%)	2 (0%)	44 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	411	ASN
2	B	1900	GLN

### 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	C	290/297 (98%)	285 (98%)	5 (2%)	56 78
1	D	287/297 (97%)	284 (99%)	3 (1%)	73 87
2	A	156/156 (100%)	155 (99%)	1 (1%)	84 92
2	B	156/156 (100%)	156 (100%)	0	100 100
All	All	889/906 (98%)	880 (99%)	9 (1%)	73 87

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	635	VAL
1	D	683	PHE
1	C	669	PHE
1	C	683	PHE
2	A	1792	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	706	ASN
1	D	691	HIS
2	B	1861	HIS

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Mol	Chain	Res	Type
1	D	688	HIS
2	B	1832	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z  > 2$
3	NAG	C	801	1	14,14,15	0.59	0	17,19,21	0.83	0
5	PO4	C	805	-	4,4,4	0.94	0	6,6,6	0.49	0
5	PO4	B	2002	-	4,4,4	0.97	0	6,6,6	0.44	0
5	PO4	C	804	-	4,4,4	0.94	0	6,6,6	0.42	0
3	NAG	C	802	-	14,14,15	0.54	0	17,19,21	0.84	0
5	PO4	A	2002	-	4,4,4	1.08	0	6,6,6	0.45	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	802	-	-	2/6/23/26	0/1/1/1
3	NAG	C	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802	NAG	O5-C5-C6-O6
3	C	802	NAG	C4-C5-C6-O6
3	C	801	NAG	C4-C5-C6-O6
3	C	801	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	NAG	4	0
3	C	802	NAG	4	0
5	A	2002	PO4	1	0

## 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	C	338/349 (96%)	0.04	17 (5%) 35 30	15, 37, 85, 157	0
1	D	334/349 (95%)	0.30	21 (6%) 27 23	18, 50, 109, 139	0
2	A	191/191 (100%)	-0.02	4 (2%) 63 60	20, 39, 93, 137	0
2	B	190/191 (99%)	0.93	30 (15%) 6 6	19, 76, 123, 148	0
All	All	1053/1080 (97%)	0.27	72 (6%) 25 20	15, 47, 108, 157	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1818	ARG	5.6
1	C	407	GLN	5.3
2	B	1817	GLU	5.3
1	D	419	TRP	4.7
1	C	416	PHE	4.6

### 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](#)

There are no monosaccharides in this entry.

### 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
3	NAG	C	802	14/15	0.53	0.18	120,139,147,148	0
3	NAG	C	801	14/15	0.60	0.15	90,97,100,100	0
4	CA	C	803	1/1	0.67	0.17	66,66,66,66	0
5	PO4	B	2002	5/5	0.75	0.21	96,106,114,115	0
5	PO4	C	805	5/5	0.78	0.22	79,88,110,111	0
4	CA	D	802	1/1	0.82	0.09	76,76,76,76	0
5	PO4	C	804	5/5	0.88	0.20	75,87,88,90	0
4	CA	D	801	1/1	0.91	0.08	85,85,85,85	0
4	CA	B	2001	1/1	0.93	0.07	77,77,77,77	0
5	PO4	A	2002	5/5	0.95	0.10	44,44,47,48	0
4	CA	A	2001	1/1	0.95	0.08	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.