



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:00 PM GMT

PDB ID : 4WK4  
Title : Metal Ion and Ligand Binding of Integrin  
Authors : Xia, W.; Springer, T.A.  
Deposited on : 2014-10-01  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

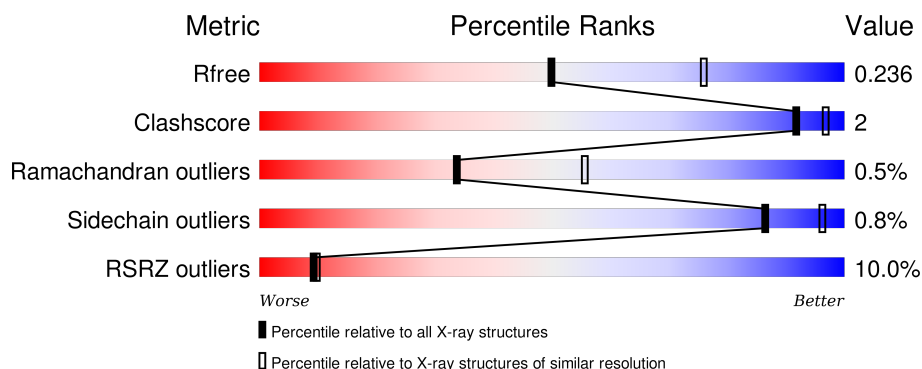
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

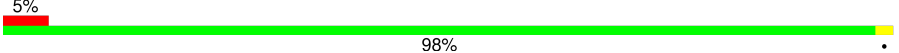


The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	450	 5% 98% .
2	B	445	 15% 91% 7% .
3	C	8	 88% 13%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14331 atoms, of which 6904 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	450	Total	C	H	N	O	S	0	0	0
			6567	2152	3180	555	672	8			

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	435	Total	C	H	N	O	S	0	0	0
			6694	2115	3310	573	671	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	THR	SER	conflict	UNP P05556

- Molecule 3 is a protein called ALA-CYS-ARG-GLY-ASP-GLY-TRP-CYS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	8	Total	C	H	N	O	S	0	0	0
			103	34	45	12	10	2			

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

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

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	6	Total	C	H	N	O	0	0
			136	40	64	2	30		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	4	Total	C	H	N	O	0	0
			95	28	45	2	20		
6	A	4	Total	C	H	N	O	0	0
			95	28	45	2	20		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	3	Total	C	H	N	O	0	0
			75	22	36	2	15		
7	B	3	Total	C	H	N	O	0	0
			75	22	36	2	15		

- Molecule 8 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	7	Total	C	H	N	O	0	0
			157	46	74	2	35		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
11	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
11	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

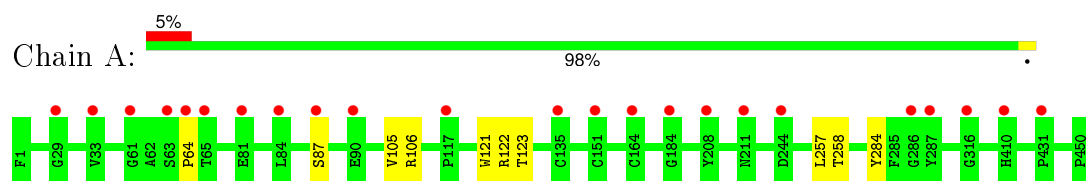
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	120	Total	O	0	0
			120	120		
12	B	64	Total	O	0	0
			64	64		
12	C	4	Total	O	0	0
			4	4		

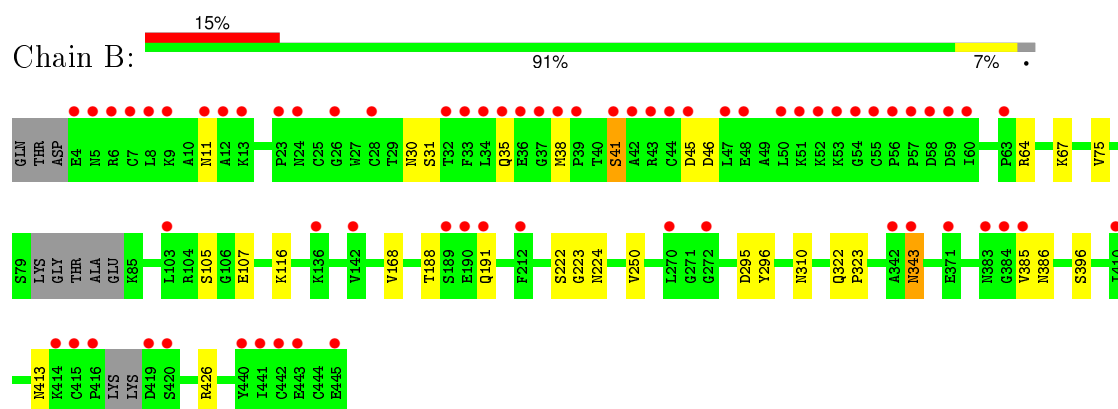
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

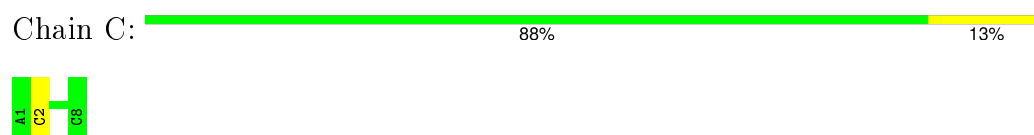
- Molecule 1: Integrin alpha-5



- Molecule 2: Integrin beta-1



- Molecule 3: ALA-CYS-ARG-GLY-ASP-GLY-TRP-CYS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.52Å 112.16Å 169.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.50 47.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.60-2.50) 99.3 (47.60-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.187 , 0.236 0.189 , 0.236	Depositor DCC
$R_{free}$ test set	1995 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 38535 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, BMA, CA, NAG, MAN

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	0.24	0/3482	0.42	1/4749 (0.0%)
2	B	0.23	0/3441	0.40	0/4645
3	C	0.19	0/59	0.29	0/78
All	All	0.24	0/6982	0.41	1/9472 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	SER	C-N-CA	7.27	139.88	121.70

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	A	3387	3180	3180	3	0
2	B	3384	3310	3318	27	0
3	C	58	45	48	0	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
5	A	72	64	61	0	0
6	A	100	90	86	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	39	36	34	0	0
7	B	39	36	34	0	0
8	A	83	74	70	0	0
9	B	1	0	0	0	0
10	B	28	27	25	4	0
11	B	42	42	39	6	0
12	A	120	0	0	0	0
12	B	64	0	0	1	0
12	C	4	0	0	0	0
All	All	7427	6904	6895	30	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 2.

The worst 5 of 30 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:B:30:ASN:ND2	11:B:511:NAG:C1	1.69	1.54
2:B:386:ASN:ND2	10:B:507:NAG:C1	1.73	1.50
2:B:386:ASN:HD21	10:B:507:NAG:C1	1.36	1.29
2:B:30:ASN:ND2	11:B:511:NAG:C2	2.09	1.14
2:B:30:ASN:CG	11:B:511:NAG:C1	2.33	0.96

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	A	448/450 (100%)	419 (94%)	28 (6%)	1 (0%)	52 75
2	B	429/445 (96%)	403 (94%)	24 (6%)	2 (0%)	34 55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
All	All	883/903 (98%)	827 (94%)	52 (6%)	4 (0%)	34	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	2	CYS
2	B	168	VAL
2	B	250	VAL
1	A	64	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	356/356 (100%)	354 (99%)	2 (1%)	90	97
2	B	387/395 (98%)	383 (99%)	4 (1%)	82	95
3	C	5/5 (100%)	5 (100%)	0	100	100
All	All	748/756 (99%)	742 (99%)	6 (1%)	86	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	41	SER
2	B	396	SER
2	B	224	ASN
1	A	284	TYR
2	B	343	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN

### 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 ⓘ

29 carbohydrates 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	$\# Z  > 2$
5	NAG	A	505	1,5	14,14,15	0.33	0	15,19,21	0.33	0
5	NAG	A	506	5	14,14,15	0.25	0	15,19,21	0.33	0
5	BMA	A	507	5	11,11,12	0.68	0	14,15,17	0.70	0
5	MAN	A	508	5	11,11,12	0.70	0	14,15,17	1.01	2 (14%)
5	MAN	A	509	5	11,11,12	0.58	0	14,15,17	1.00	1 (7%)
5	MAN	A	510	5	11,11,12	0.63	0	14,15,17	1.06	2 (14%)
6	NAG	A	511	1,6	14,14,15	0.33	0	15,19,21	0.33	0
6	NAG	A	512	6	14,14,15	0.30	0	15,19,21	0.27	0
6	BMA	A	513	6	11,11,12	0.64	0	14,15,17	0.71	0
6	MAN	A	514	6	11,11,12	0.90	1 (9%)	14,15,17	2.35	4 (28%)
6	NAG	A	515	6	14,14,15	0.31	0	15,19,21	0.78	0
6	NAG	A	516	6	14,14,15	0.29	0	15,19,21	0.72	0
6	BMA	A	517	6	11,11,12	0.25	0	14,15,17	1.60	1 (7%)
6	MAN	A	518	6	11,11,12	0.60	0	14,15,17	1.33	2 (14%)
7	NAG	A	519	1,7	14,14,15	0.35	0	15,19,21	0.83	0
7	NAG	A	520	7	14,14,15	0.29	0	15,19,21	0.85	0
7	BMA	A	521	7	11,11,12	0.60	0	14,15,17	0.74	0
8	NAG	A	522	1,8	14,14,15	0.27	0	15,19,21	0.26	0
8	NAG	A	523	8	14,14,15	0.32	0	15,19,21	0.22	0
8	BMA	A	524	8	11,11,12	0.79	0	14,15,17	0.81	0
8	MAN	A	525	8	11,11,12	0.67	0	14,15,17	1.09	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	A	526	8	11,11,12	0.76	0	14,15,17	0.96	1 (7%)
8	MAN	A	527	8	11,11,12	0.75	1 (9%)	14,15,17	1.10	2 (14%)
8	MAN	A	528	8	11,11,12	0.66	0	14,15,17	1.24	2 (14%)
7	NAG	B	504	2,7	14,14,15	0.79	1 (7%)	15,19,21	0.58	0
7	NAG	B	505	7	14,14,15	0.16	0	15,19,21	0.63	0
7	BMA	B	506	7	11,11,12	0.75	1 (9%)	14,15,17	0.63	0
10	NAG	B	507	10	14,14,15	0.30	0	15,19,21	0.73	0
10	NAG	B	508	10	14,14,15	0.26	0	15,19,21	0.69	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
5	NAG	A	505	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	506	5	-	0/6/23/26	0/1/1/1
5	BMA	A	507	5	-	0/2/19/22	0/1/1/1
5	MAN	A	508	5	-	0/2/19/22	0/1/1/1
5	MAN	A	509	5	-	0/2/19/22	0/1/1/1
5	MAN	A	510	5	-	0/2/19/22	0/1/1/1
6	NAG	A	511	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	512	6	-	0/6/23/26	0/1/1/1
6	BMA	A	513	6	-	0/2/19/22	0/1/1/1
6	MAN	A	514	6	-	0/2/19/22	0/1/1/1
6	NAG	A	515	6	-	0/6/23/26	0/1/1/1
6	NAG	A	516	6	-	0/6/23/26	0/1/1/1
6	BMA	A	517	6	-	0/2/19/22	0/1/1/1
6	MAN	A	518	6	-	0/2/19/22	0/1/1/1
7	NAG	A	519	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	520	7	-	0/6/23/26	0/1/1/1
7	BMA	A	521	7	-	0/2/19/22	0/1/1/1
8	NAG	A	522	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	523	8	-	0/6/23/26	0/1/1/1
8	BMA	A	524	8	-	0/2/19/22	0/1/1/1
8	MAN	A	525	8	-	0/2/19/22	0/1/1/1
8	MAN	A	526	8	-	0/2/19/22	0/1/1/1
8	MAN	A	527	8	-	0/2/19/22	0/1/1/1
8	MAN	A	528	8	-	0/2/19/22	0/1/1/1
7	NAG	B	504	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	505	7	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	B	506	7	-	0/2/19/22	0/1/1/1
10	NAG	B	507	10	-	0/6/23/26	0/1/1/1
10	NAG	B	508	10	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	504	NAG	O5-C1	-2.76	1.39	1.43
8	A	527	MAN	O5-C1	-2.11	1.40	1.43
7	B	506	BMA	O5-C1	-2.00	1.40	1.43
6	A	514	MAN	C1-C2	2.35	1.57	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	514	MAN	O2-C2-C3	-2.43	105.24	110.12
8	A	527	MAN	O2-C2-C3	-2.31	105.47	110.12
8	A	525	MAN	O2-C2-C3	-2.27	105.56	110.12
5	A	510	MAN	O2-C2-C3	-2.19	105.72	110.12
6	A	518	MAN	O2-C2-C3	-2.16	105.77	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	507	NAG	4	0

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 7 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
11	NAG	B	509	2	14,14,15	0.20	0	15,19,21	0.26	0
11	NAG	B	510	2	14,14,15	0.36	0	15,19,21	0.55	0
11	NAG	B	511	-	14,14,15	0.24	0	15,19,21	0.38	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
11	NAG	B	509	2	-	0/6/23/26	0/1/1/1
11	NAG	B	510	2	-	0/6/23/26	0/1/1/1
11	NAG	B	511	-	-	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.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	511	NAG	6	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	A	450/450 (100%)	0.43	23 (5%) 32 36	47, 78, 137, 224	0
2	B	435/445 (97%)	0.79	66 (15%) 3 3	49, 89, 162, 239	0
3	C	8/8 (100%)	0.27	0 100 100	75, 95, 147, 148	0
All	All	893/903 (98%)	0.60	89 (9%) 9 10	47, 82, 158, 239	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	12	ALA	8.1
2	B	33	PHE	6.8
2	B	38	MET	5.8
2	B	415	CYS	5.6
2	B	35	GLN	5.6

### 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](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	MAN	A	528	11/12	0.78	0.28	1.97	197,227,261,273	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	515	14/15	0.93	0.21	1.90	35,46,56,57	0
7	NAG	B	504	14/15	0.86	0.22	1.61	150,202,236,248	0
5	NAG	A	505	14/15	0.97	0.14	-0.82	44,63,76,82	0
5	NAG	A	506	14/15	0.95	0.12	-1.43	63,79,104,109	0
6	NAG	A	511	14/15	0.89	0.13	-1.60	79,99,119,128	0
7	NAG	A	519	14/15	0.91	0.10	-3.76	81,106,148,180	0
6	MAN	A	514	11/12	0.62	0.44	-	229,251,299,303	0
6	BMA	A	513	11/12	0.69	0.24	-	171,208,245,250	0
6	NAG	A	516	14/15	0.81	0.16	-	127,145,168,174	0
8	MAN	A	526	11/12	0.72	0.14	-	130,164,200,200	0
8	NAG	A	523	14/15	0.89	0.17	-	125,139,165,167	0
7	NAG	B	505	14/15	0.86	0.20	-	254,283,337,341	0
6	MAN	A	518	11/12	0.89	0.29	-	201,216,258,260	0
10	NAG	B	507	14/15	0.91	0.26	-	105,141,167,175	0
8	MAN	A	527	11/12	0.88	0.20	-	108,118,137,145	0
7	NAG	A	520	14/15	0.68	0.28	-	219,263,334,345	0
7	BMA	A	521	11/12	0.39	0.49	-	262,272,321,327	0
5	MAN	A	509	11/12	0.87	0.25	-	172,213,256,256	0
5	MAN	A	508	11/12	0.76	0.20	-	199,231,273,277	0
10	NAG	B	508	14/15	0.87	0.32	-	132,180,234,234	0
8	NAG	A	522	14/15	0.85	0.12	-	119,143,170,177	0
7	BMA	B	506	11/12	0.49	0.45	-	202,250,302,307	0
5	MAN	A	510	11/12	0.92	0.15	-	150,160,191,192	0
8	MAN	A	525	11/12	0.90	0.30	-	169,175,209,211	0
6	BMA	A	517	11/12	0.80	0.22	-	133,187,226,235	0
5	BMA	A	507	11/12	0.92	0.13	-	114,149,187,187	0
8	BMA	A	524	11/12	0.85	0.16	-	144,158,187,190	0
6	NAG	A	512	14/15	0.83	0.21	-	117,149,180,188	0

## 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MG	B	501	1/1	0.92	0.16	0.90	64,64,64,64	0
4	CA	B	503	1/1	0.96	0.20	0.46	65,65,65,65	0
11	NAG	B	511	14/15	0.83	0.31	-0.40	169,202,237,237	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	B	502	1/1	0.78	0.18	-0.44	127,127,127,127	0
4	CA	A	504	1/1	0.46	0.13	-0.96	149,149,149,149	0
4	CA	A	503	1/1	0.75	0.09	-1.67	100,100,100,100	0
4	CA	A	502	1/1	0.99	0.09	-2.12	67,67,67,67	0
4	CA	A	501	1/1	0.90	0.06	-2.25	68,68,68,68	0
11	NAG	B	510	14/15	0.73	0.41	-	138,172,207,207	0
11	NAG	B	509	14/15	0.57	0.38	-	248,315,379,387	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.