



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2021 – 04:55 AM EDT

PDB ID : 3INB  
Title : Structure of the measles virus hemagglutinin bound to the CD46 receptor  
Authors : Santiago, C.; Celma, M.L.; Stehle, T.; Casasnovas, J.M.  
Deposited on : 2009-08-12  
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

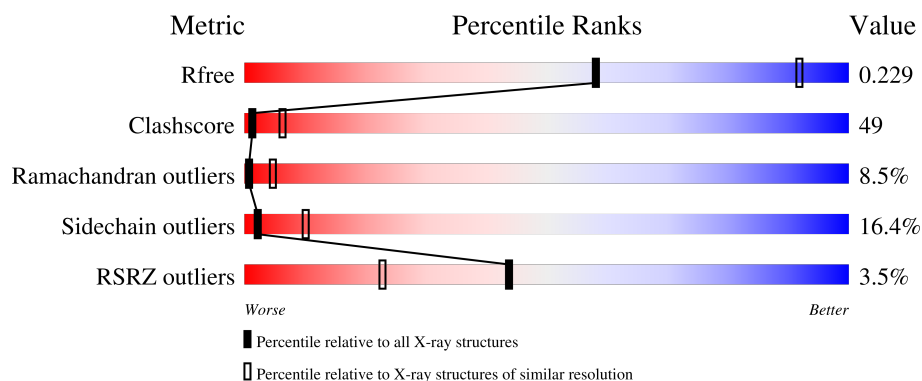
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

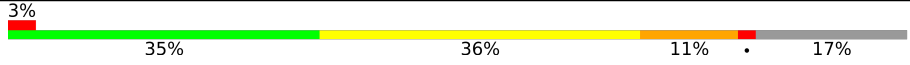
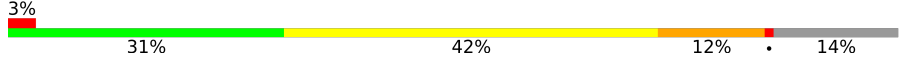
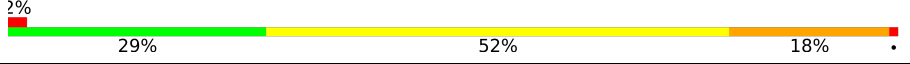
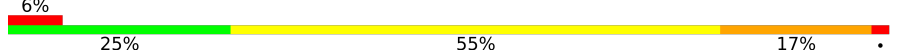
The reported resolution of this entry is 3.10 Å.

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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	466	
1	B	466	
2	C	126	
2	D	126	

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	A	1200	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8350 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 Hemagglutinin glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3047	1963	503	560	21			
1	B	403	Total	C	N	O	S	0	1	0
			3158	2030	522	583	23			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	TYR	-	expression tag	UNP P08362
A	153	PRO	-	expression tag	UNP P08362
A	154	TYR	-	expression tag	UNP P08362
A	155	ASP	-	expression tag	UNP P08362
A	156	VAL	-	expression tag	UNP P08362
A	157	PRO	-	expression tag	UNP P08362
A	158	ASP	-	expression tag	UNP P08362
A	159	TYR	-	expression tag	UNP P08362
A	160	ALA	-	expression tag	UNP P08362
A	161	GLY	-	expression tag	UNP P08362
A	162	ALA	-	expression tag	UNP P08362
A	163	GLN	-	expression tag	UNP P08362
A	164	PRO	-	expression tag	UNP P08362
A	165	ALA	-	expression tag	UNP P08362
A	166	ARG	-	expression tag	UNP P08362
A	167	SER	-	expression tag	UNP P08362
A	168	PRO	-	expression tag	UNP P08362
A	169	GLY	-	expression tag	UNP P08362
A	170	ILE	-	expression tag	UNP P08362
A	171	ARG	-	expression tag	UNP P08362
A	172	GLY	-	expression tag	UNP P08362
A	173	LEU	-	expression tag	UNP P08362
A	174	VAL	-	expression tag	UNP P08362
A	175	PRO	-	expression tag	UNP P08362
A	176	ARG	-	expression tag	UNP P08362

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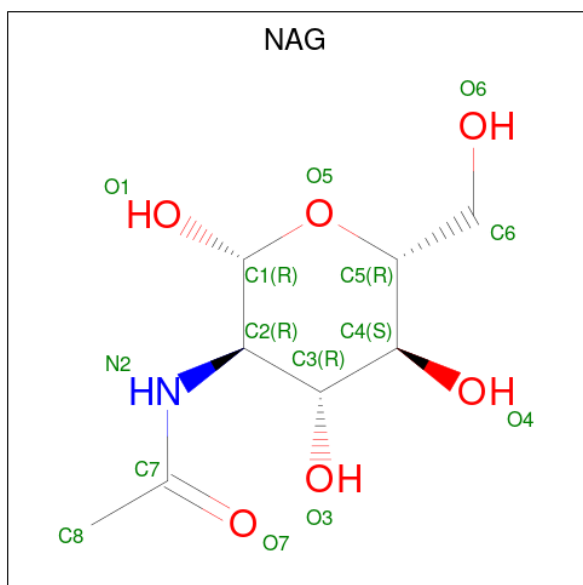
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Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	-	expression tag	UNP P08362
A	178	SER	-	expression tag	UNP P08362
A	331	ALA	THR	engineered mutation	UNP P08362
A	392	THR	ALA	engineered mutation	UNP P08362
A	484	THR	ASN	engineered mutation	UNP P08362
A	546	GLY	SER	engineered mutation	UNP P08362
A	600	VAL	GLU	engineered mutation	UNP P08362
B	152	TYR	-	expression tag	UNP P08362
B	153	PRO	-	expression tag	UNP P08362
B	154	TYR	-	expression tag	UNP P08362
B	155	ASP	-	expression tag	UNP P08362
B	156	VAL	-	expression tag	UNP P08362
B	157	PRO	-	expression tag	UNP P08362
B	158	ASP	-	expression tag	UNP P08362
B	159	TYR	-	expression tag	UNP P08362
B	160	ALA	-	expression tag	UNP P08362
B	161	GLY	-	expression tag	UNP P08362
B	162	ALA	-	expression tag	UNP P08362
B	163	GLN	-	expression tag	UNP P08362
B	164	PRO	-	expression tag	UNP P08362
B	165	ALA	-	expression tag	UNP P08362
B	166	ARG	-	expression tag	UNP P08362
B	167	SER	-	expression tag	UNP P08362
B	168	PRO	-	expression tag	UNP P08362
B	169	GLY	-	expression tag	UNP P08362
B	170	ILE	-	expression tag	UNP P08362
B	171	ARG	-	expression tag	UNP P08362
B	172	GLY	-	expression tag	UNP P08362
B	173	LEU	-	expression tag	UNP P08362
B	174	VAL	-	expression tag	UNP P08362
B	175	PRO	-	expression tag	UNP P08362
B	176	ARG	-	expression tag	UNP P08362
B	177	GLY	-	expression tag	UNP P08362
B	178	SER	-	expression tag	UNP P08362
B	331	ALA	THR	engineered mutation	UNP P08362
B	392	THR	ALA	engineered mutation	UNP P08362
B	484	THR	ASN	engineered mutation	UNP P08362
B	546	GLY	SER	engineered mutation	UNP P08362
B	600	VAL	GLU	engineered mutation	UNP P08362

- Molecule 2 is a protein called Membrane cofactor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	126	Total	C	N	O	S	0	0	0
			1019	659	160	190	10			
2	D	126	Total	C	N	O	S	0	0	0
			1019	659	160	190	10			

- 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
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



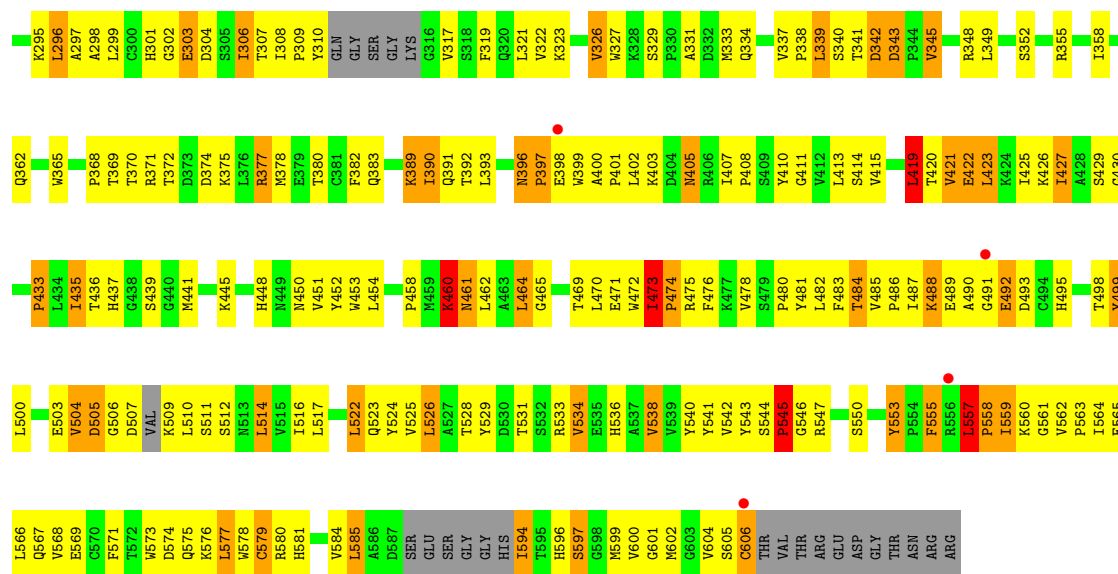
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

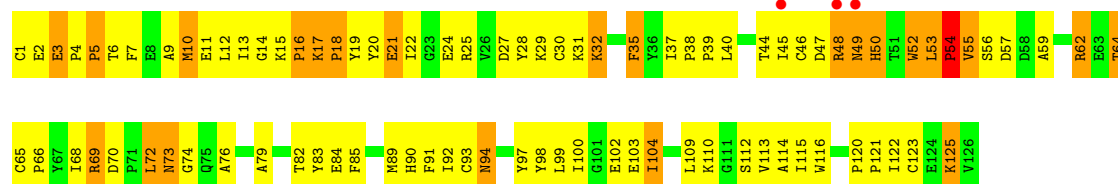
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	3	Total	O	0	0
			3	3		
5	C	1	Total	O	0	0
			1	1		



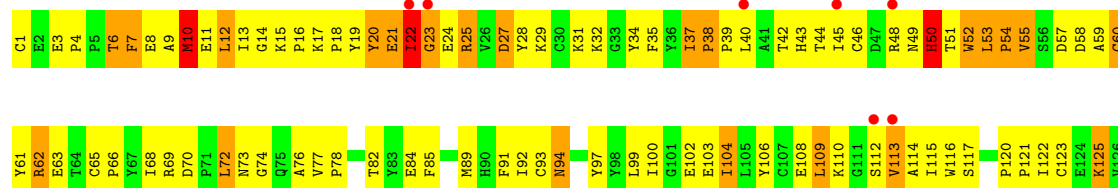




• Molecule 2: Membrane cofactor protein



• Molecule 2: Membrane cofactor protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.36Å 105.83Å 208.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.10 19.88 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.0 (14.98-3.10) 96.1 (19.88-3.01)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.227 , 0.259 0.227 , 0.229	Depositor DCC
$R_{free}$ test set	1752 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 96.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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, SO4

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	0.41	0/3125	0.71	1/4254 (0.0%)
1	B	0.41	0/3237	0.69	1/4404 (0.0%)
2	C	0.41	0/1053	0.72	2/1432 (0.1%)
2	D	0.44	0/1053	0.89	3/1432 (0.2%)
All	All	0.41	0/8468	0.73	7/11522 (0.1%)

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	5
1	B	0	3
2	C	0	2
2	D	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	LEU	CA-CB-CG	8.95	135.88	115.30
2	D	69	ARG	NE-CZ-NH2	8.50	124.55	120.30
2	D	69	ARG	NE-CZ-NH1	-8.27	116.17	120.30
2	C	69	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	B	343	ASP	N-CA-C	-7.07	91.90	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	THR	Peptide
1	A	342	ASP	Peptide
1	A	473	ILE	Peptide
1	A	529	TYR	Peptide
1	A	557	LEU	Peptide

## 5.2 Too-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 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	3047	0	3010	286	0
1	B	3158	0	3125	288	0
2	C	1019	0	962	136	0
2	D	1019	0	962	125	0
3	A	28	0	26	2	0
3	B	28	0	26	1	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
All	All	8350	0	8137	814	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 49.

The worst 5 of 814 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:C:85:PHE:HB2	2:C:109:LEU:HD11	1.34	1.09
1:B:555:PHE:HB2	1:B:557:LEU:HB2	1.35	1.06
2:C:52:TRP:C	2:C:54:PRO:HD2	1.72	1.06
1:A:460:LYS:HE2	1:A:460:LYS:CA	1.83	1.06
2:C:11:GLU:HB2	2:C:31:LYS:HG2	1.37	1.06

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	379/466 (81%)	293 (77%)	58 (15%)	28 (7%)	1	6
1	B	394/466 (84%)	309 (78%)	58 (15%)	27 (7%)	1	7
2	C	124/126 (98%)	84 (68%)	24 (19%)	16 (13%)	0	1
2	D	124/126 (98%)	81 (65%)	27 (22%)	16 (13%)	0	1
All	All	1021/1184 (86%)	767 (75%)	167 (16%)	87 (8%)	1	5

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ILE
1	A	224	SER
1	A	390	ILE
1	A	391	GLN
1	A	397	PRO

### 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	A	340/404 (84%)	288 (85%)	52 (15%)	2	12
1	B	355/404 (88%)	291 (82%)	64 (18%)	1	7
2	C	110/110 (100%)	94 (86%)	16 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	110/110 (100%)	91 (83%)	19 (17%)	2	9
All	All	915/1028 (89%)	764 (84%)	151 (16%)	2	10

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	606	CYS
2	D	52	TRP
2	C	35	PHE
2	C	112	SER
2	D	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	575	GLN
2	D	50	HIS
2	C	43	HIS
1	B	271	HIS
1	B	523	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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
3	NAG	B	1215	1	14,14,15	0.57	0	17,19,21	1.14	1 (5%)
3	NAG	C	1080	2	14,14,15	0.49	0	17,19,21	0.89	1 (5%)
3	NAG	A	1200	1	14,14,15	0.44	0	17,19,21	1.08	1 (5%)
3	NAG	B	1200	1	14,14,15	0.45	0	17,19,21	2.23	2 (11%)
4	SO4	B	1	-	4,4,4	0.15	0	6,6,6	0.09	0
3	NAG	A	1215	1	14,14,15	0.49	0	17,19,21	0.88	0
4	SO4	A	3	-	4,4,4	0.18	0	6,6,6	0.21	0
4	SO4	B	2	-	4,4,4	0.12	0	6,6,6	0.14	0
3	NAG	D	1080	2	14,14,15	0.50	0	17,19,21	0.91	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	B	1215	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1080	2	-	4/6/23/26	0/1/1/1
3	NAG	A	1200	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1200	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1215	1	-	1/6/23/26	0/1/1/1
3	NAG	D	1080	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1200	NAG	C1-O5-C5	7.05	121.74	112.19
3	B	1200	NAG	O5-C1-C2	5.01	119.21	111.29
3	A	1200	NAG	C1-O5-C5	4.14	117.81	112.19
3	B	1215	NAG	C1-O5-C5	3.33	116.71	112.19
3	C	1080	NAG	C1-O5-C5	2.61	115.73	112.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1200	NAG	C8-C7-N2-C2
3	A	1200	NAG	O7-C7-N2-C2
3	B	1200	NAG	C8-C7-N2-C2
3	B	1200	NAG	O7-C7-N2-C2
3	C	1080	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1215	NAG	1	0
3	A	1200	NAG	2	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	389/466 (83%)	-0.15	12 (3%) 49 26	78, 146, 256, 336	0
1	B	403/466 (86%)	-0.14	15 (3%) 41 21	89, 146, 229, 269	0
2	C	126/126 (100%)	-0.08	3 (2%) 59 37	120, 159, 237, 249	0
2	D	126/126 (100%)	0.21	7 (5%) 24 11	118, 161, 236, 257	0
All	All	1044/1184 (88%)	-0.09	37 (3%) 44 23	78, 151, 240, 336	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	ASN	4.9
1	A	193	THR	4.6
1	B	186	GLY	3.7
1	B	184	SER	3.7
2	D	45	ILE	3.7

### 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	1080	14/15	0.74	0.33	169,219,234,238	0
3	NAG	A	1200	14/15	0.79	0.48	243,269,290,293	0
3	NAG	A	1215	14/15	0.83	0.26	184,209,220,224	0
3	NAG	D	1080	14/15	0.84	0.32	180,208,220,227	0
3	NAG	B	1200	14/15	0.87	0.34	138,202,225,233	0
4	SO4	B	1	5/5	0.87	0.15	177,180,198,200	0
3	NAG	B	1215	14/15	0.88	0.13	169,193,208,209	0
4	SO4	B	2	5/5	0.90	0.14	163,197,199,212	0
4	SO4	A	3	5/5	0.96	0.11	95,131,184,201	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.