



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 03:29 PM GMT

PDB ID : 1IVO  
Title : Crystal Structure of the Complex of Human Epidermal Growth Factor and Receptor Extracellular Domains.  
Authors : Ogiso, H.; Ishitani, R.; Nureki, O.; Fukai, S.; Yamanaka, M.; Kim, J.H.; Saito, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2002-03-28  
Resolution : 3.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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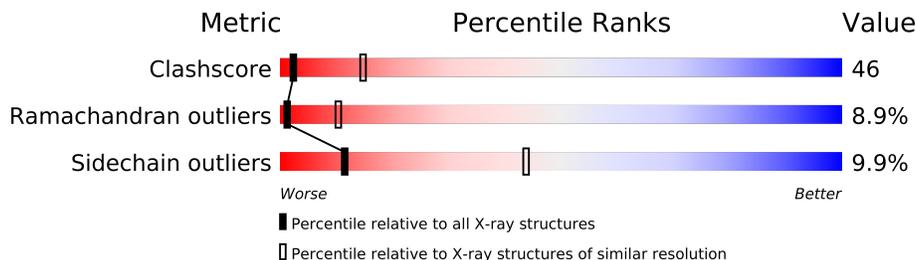
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 3.30 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))
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	
2	C	53	
2	D	53	

## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8892 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.

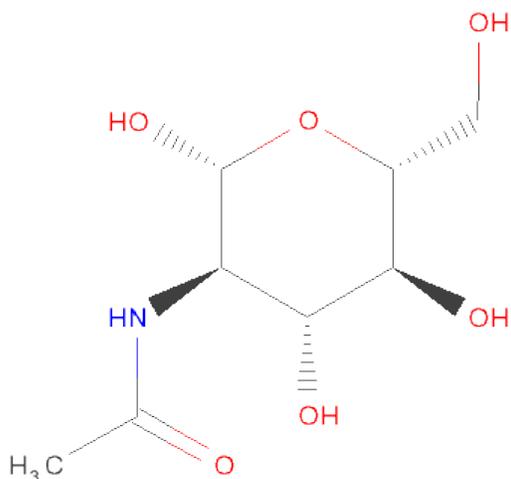
- Molecule 1 is a protein called Epidermal Growth Factor Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	Total 3956	C 2446	N 706	O 760	S 44	111	0	0
1	B	510	Total 3947	C 2441	N 705	O 757	S 44	62	0	0

- Molecule 2 is a protein called Epidermal growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	47	Total 385	C 244	N 63	O 71	S 7	0	0	0
2	D	47	Total 385	C 244	N 63	O 71	S 7	0	0	0

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		
5	C	6	Total	O	0	0
			6	6		
5	D	6	Total	O	0	0
			6	6		

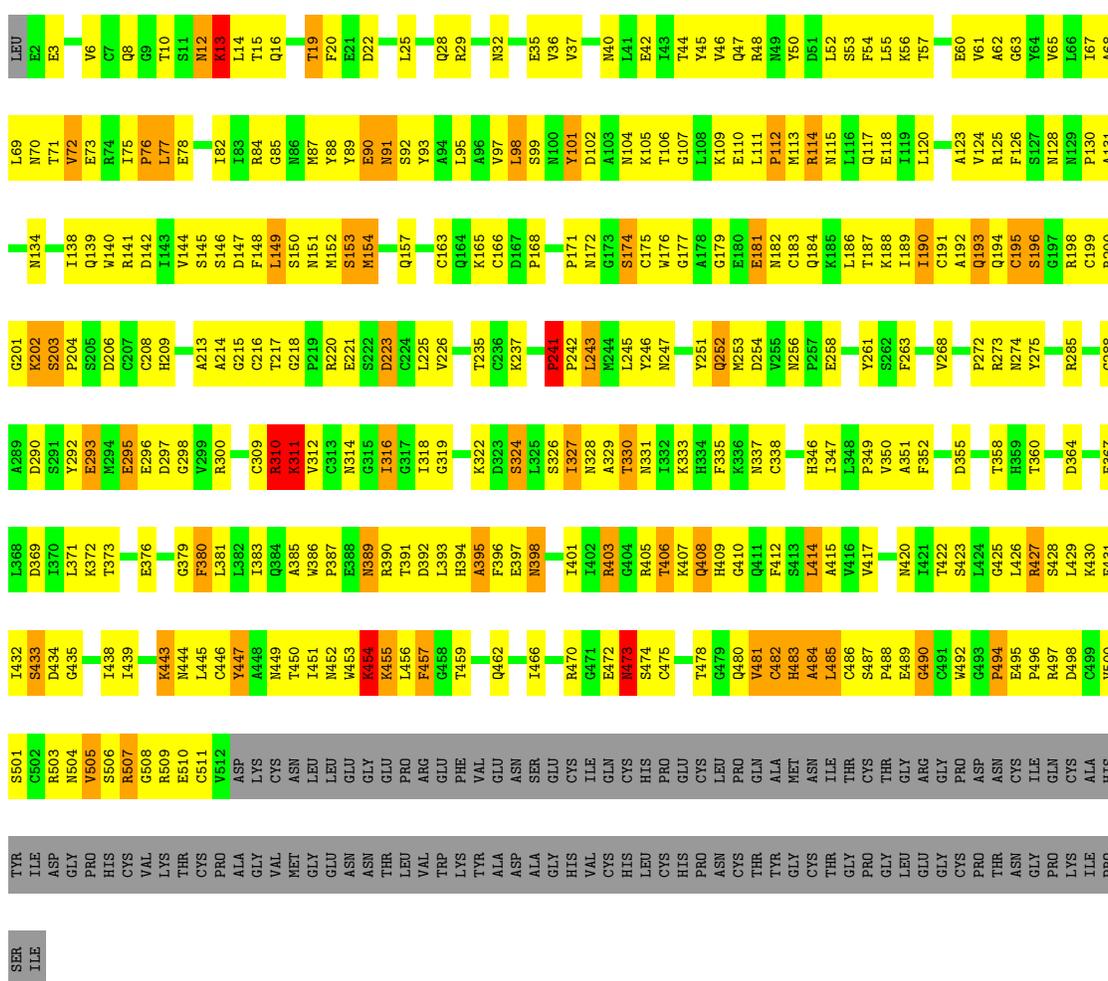
### 3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: Epidermal Growth Factor Receptor

Chain A:



- Molecule 1: Epidermal Growth Factor Receptor

Chain B:



I75	I76	I77	I78	I79	I80	I81	I82	I83	I84	M87	M88	M89	E90	N91	S92	Y93	A94	L95	A96	V97	L98	S99	M100	Y101	I102	A103	N104	K105	T106	K109	E110	L111	P112	M113	R114	N115	L116	Q117	E118	I119	L120	A123	V124	R125	F126	S127	M128	N129	P130	A131	M134	V135	E136	S137	I138
Q139	W140	R141	D142	I143	L144	S145	S146	D147	I148	L149	S150	M151	M152	S153	M154	F155	F156	Q157	C163	Q164	K165	P171	C175	W176	A180	E181	M182	Q184	L185	L186	T187	K188	I189	L190	C191	A192	Q193	S196	G197	R198	C199	R200	F201	K202	S203	P204	S205	D206	C207	C208	H209	N210	S211	Q211	
G212	A213	A214	G215	C216	T217	G218	P219	R220	E221	S222	D223	M224	L225	V226	D231	R232	K237	C240	P241	P242	L243	M244	L245	Y246	N247	P248	T249	T250	Y251	M252	M253	N256	P257	E258	G259	F263	K270	C271	P272	R273	N274	Y275	V276	V277	R285	G288	A289	D290	S291	Y292	E293				
K294	E295	E296	D297	G298	V299	R300	K301	K302	K303	K304	C305	E306	G307	P308	C309	K311	N314	G315	I318	G319	E320	F321	S324	L325	S326	I327	N328	A329	T330	N331	I332	K333	H334	F335	K336	T339	S340	I341	S342	H346	I347	L348	P349	V350	A351	R352	G354	D355	T358	L363					
K364	P365	Q366	E367	L368	D369	I370	L371	K372	V373	V374	C375	E376	L377	G378	G379	F380	L381	L382	L383	Q384	A385	K386	P387	E388	K389	R390	T391	L392	L393	H394	A395	L399	E400	L401	L402	R403	G404	R405	Q408	H409	G410	Q411	F412	S413	V416	V417	S418	L419	M420	L421	T422	G423	L424	K430	E431
I432	S433	D436	V437	I438	I439	S440	G441	N442	K443	N444	M445	L446	Y447	A448	N449	I451	M452	M453	K454	K455	L456	F457	G458	T459	Q462	K463	T464	K465	I466	I467	N469	M470	G471	E472	M473	A474	S475	K476	A477	Q480	V481	C482	H483	A484	L485	C486	S487	P488	C491	W492	G493	P494	E495		
P496	R497	D498	C499	V500	S501	C502	R503	N504	V505	S506	R507	E508	E510	C511	V512	LYS	CYS	ASN	LEU	GLU	GLY	GLN	GLU	PRO	ARG	GLU	PHE	VAL	VAL	GLU	ASN	ILE	GLN	CYS	HIS	PRO	CYS	LEU	PRO	ASN	PRO	GLN	ALA	ALA	MET	GLY	ASN	THR	ILE	THR	CYS	PRO	ASP	ASN	CYS
ILE	GLN	CYS	ALA	HIS	TRP	ILE	ASP	GLY	PRO	HIS	VAL	LYS	THR	CYS	PRO	ALA	GLY	VAL	MET	GLY	GLU	ASN	THR	LEU	VAL	TRP	TRP	VAL	TRP	ALA	HIS	VAL	CYS	HIS	PRO	CYS	LEU	PRO	ASN	CYS	THR	TRP	THR	GLY	CYS	THR	GLY	GLY	CYS	THR	ASN	CYS			
GLY	PRO	LYS	ILE	PRO	SER	SER	ILE	ASP	GLY	PRO	VAL	THR	ILE	PRO	ALA	GLY	VAL	MET	GLY	GLU	ASN	THR	LEU	VAL	TRP	TRP	VAL	TRP	ALA	HIS	VAL	CYS	HIS	PRO	CYS	LEU	PRO	ASN	CYS	THR	TRP	THR	GLY	CYS	THR	GLY	GLY	CYS	THR	ASN	CYS				

• Molecule 2: Epidermal growth factor

Chain C:



ASN	SER	ASP	SER	E5	C6	P7	L8	S9	H10	D11	G12	Y13	G14	H15	H16	V19	E24	A25	L26	D27	K28	Y29	N32	Y37	I38	G39	Q43	Y44	R45	D46	L47	K48	W50	E51	LEU	ARG
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• Molecule 2: Epidermal growth factor

Chain D:



ASN	SER	ASP	SER	E5	C6	P7	L8	S9	H10	D11	L15	H16	G18	V19	Y22	I23	E24	A25	L26	D27	K28	Y29	A30	C31	N32	G33	V34	V35	I38	G39	E40	R41	G42	Q43	Y44	R45	D46	L47	K48	W49	E51	LEU	ARG
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.16Å 220.16Å 113.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	98.0 (10.00-3.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.255 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

## 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

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	0.33	0/4027	0.67	1/5438 (0.0%)
1	B	0.34	0/4018	0.67	1/5426 (0.0%)
2	C	0.36	0/396	0.64	0/536
2	D	0.35	0/396	0.63	0/536
All	All	0.34	0/8837	0.67	2/11936 (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	A	195	CYS	CA-CB-SG	-5.07	104.87	114.00
1	B	240	CYS	CA-CB-SG	-5.06	104.90	114.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	3956	0	3843	342	0
1	B	3947	0	3843	397	0
2	C	385	0	344	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	385	0	344	42	0
3	A	70	0	65	9	0
3	B	42	0	39	21	0
4	A	28	0	25	4	0
5	A	35	0	0	2	0
5	B	32	0	0	5	0
5	C	6	0	0	1	0
5	D	6	0	0	2	0
All	All	8892	0	8503	788	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 46.

The worst 5 of 788 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:243:LEU:HA	1:B:256:ASN:HB3	1.34	1.09
1:A:174:SER:HB3	1:A:184:GLN:HB3	1.39	1.02
1:A:481:VAL:HG12	1:A:482:CYS:H	1.24	0.99
1:B:328:ASN:H	3:B:1328:NAG:H82	1.27	0.97
1:A:331:ASN:HB2	3:A:1328:NAG:HN2	1.29	0.96

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	509/622 (82%)	368 (72%)	93 (18%)	48 (9%)	<b>1</b> <b>9</b>
1	B	508/622 (82%)	369 (73%)	98 (19%)	41 (8%)	<b>1</b> <b>13</b>
2	C	45/53 (85%)	35 (78%)	9 (20%)	1 (2%)	<b>10</b> <b>55</b>
2	D	45/53 (85%)	31 (69%)	6 (13%)	8 (18%)	<b>0</b> <b>1</b>
All	All	1107/1350 (82%)	803 (72%)	206 (19%)	98 (9%)	<b>1</b> <b>10</b>

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	LEU
1	A	146	SER
1	A	171	PRO
1	A	203	SER

### 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	449/543 (83%)	408 (91%)	41 (9%)	14 49
1	B	448/543 (82%)	402 (90%)	46 (10%)	10 41
2	C	41/47 (87%)	37 (90%)	4 (10%)	12 45
2	D	41/47 (87%)	35 (85%)	6 (15%)	5 23
All	All	979/1180 (83%)	882 (90%)	97 (10%)	11 44

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	LYS
1	B	219	PRO
2	C	24	GLU
1	B	30	MET
1	B	139	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	GLN
1	B	128	ASN
1	B	469	ASN
1	B	47	GLN
1	A	252	GLN

### 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 ⓘ

2 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
4	NAG	A	1420	1,4	12,14,15	0.66	0	15,19,21	1.04	1 (6%)
4	NAG	A	2420	4	12,14,15	0.50	0	15,19,21	0.68	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
4	NAG	A	1420	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2420	4	-	0/6/23/26	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(°)
4	A	1420	NAG	C3-C2-N2	-2.14	108.50	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry (i)

8 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	A	1032	1	12,14,15	0.38	0	15,19,21	0.73	0
3	NAG	A	1151	1	12,14,15	0.48	0	15,19,21	0.77	0
3	NAG	A	1172	1	12,14,15	0.49	0	15,19,21	0.67	0
3	NAG	A	1328	1	12,14,15	0.40	0	15,19,21	1.12	1 (6%)
3	NAG	A	1337	1	12,14,15	0.51	0	15,19,21	0.55	0
3	NAG	B	1032	1	12,14,15	0.44	0	15,19,21	0.73	1 (6%)
3	NAG	B	1151	1	12,14,15	0.43	0	15,19,21	0.62	0
3	NAG	B	1328	1	12,14,15	0.64	0	15,19,21	1.00	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	A	1032	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1172	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1328	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1337	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1032	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1328	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1328	NAG	C3-C4-C5	-2.63	105.51	110.20
3	B	1032	NAG	C2-N2-C7	-2.02	119.70	123.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1328	NAG	C1-C2-N2-C7
3	A	1172	NAG	O7-C7-N2-C2
3	A	1328	NAG	O7-C7-N2-C2
3	A	1172	NAG	C8-C7-N2-C2

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.