



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:10 PM GMT

PDB ID : 3QWQ
Title : Crystal structure of the extracellular domain of the epidermal growth factor receptor in complex with an adnectin
Authors : Sheriff, S.
Deposited on : 2011-02-28
Resolution : 2.75 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

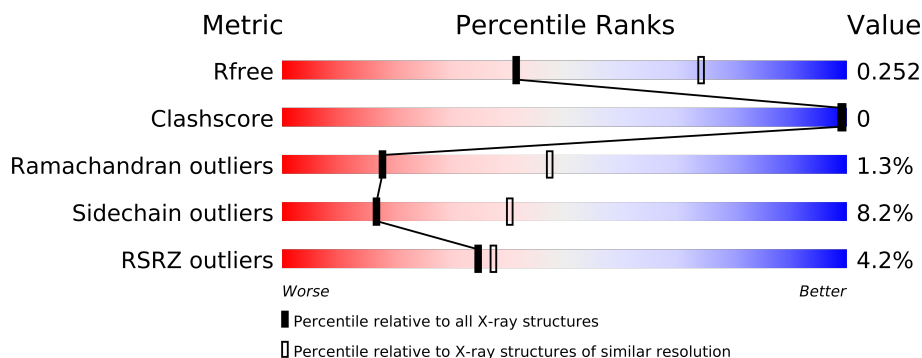
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.75 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	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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 ≥ 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	648	
2	B	114	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5610 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
1	A	613	Total	C	N	O	S	0	0	0
			4612	2844	815	893	60			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	HIS	-	EXPRESSION TAG	UNP P00533
A	620	HIS	-	EXPRESSION TAG	UNP P00533
A	621	HIS	-	EXPRESSION TAG	UNP P00533
A	622	HIS	-	EXPRESSION TAG	UNP P00533
A	623	HIS	-	EXPRESSION TAG	UNP P00533
A	624	HIS	-	EXPRESSION TAG	UNP P00533

- Molecule 2 is a protein called ADNECTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	0	0	0
			747	475	124	148			

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			71	40	2	29		
3	A	6	Total	C	N	O	0	0
			71	40	2	29		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	HIS	-	EXPRESSION TAG	UNP P00533
A	620	HIS	-	EXPRESSION TAG	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
A	621	HIS	-	EXPRESSION TAG	UNP P00533
A	622	HIS	-	EXPRESSION TAG	UNP P00533
A	623	HIS	-	EXPRESSION TAG	UNP P00533
A	624	HIS	-	EXPRESSION TAG	UNP P00533
A	619	HIS	-	EXPRESSION TAG	UNP P00533
A	620	HIS	-	EXPRESSION TAG	UNP P00533
A	621	HIS	-	EXPRESSION TAG	UNP P00533
A	622	HIS	-	EXPRESSION TAG	UNP P00533
A	623	HIS	-	EXPRESSION TAG	UNP P00533
A	624	HIS	-	EXPRESSION TAG	UNP P00533

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	HIS	-	EXPRESSION TAG	UNP P00533
A	620	HIS	-	EXPRESSION TAG	UNP P00533
A	621	HIS	-	EXPRESSION TAG	UNP P00533
A	622	HIS	-	EXPRESSION TAG	UNP P00533
A	623	HIS	-	EXPRESSION TAG	UNP P00533
A	624	HIS	-	EXPRESSION TAG	UNP P00533

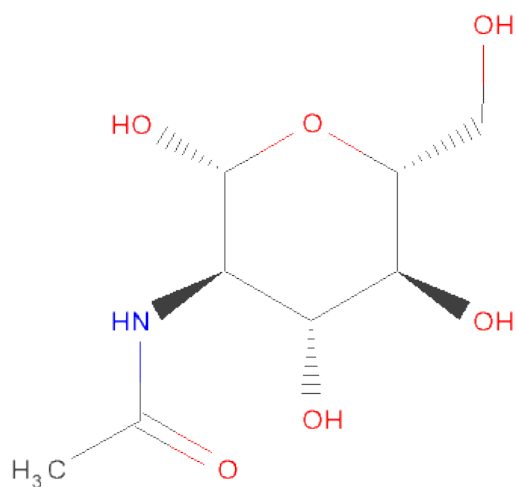
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	HIS	-	EXPRESSION TAG	UNP P00533
A	620	HIS	-	EXPRESSION TAG	UNP P00533
A	621	HIS	-	EXPRESSION TAG	UNP P00533
A	622	HIS	-	EXPRESSION TAG	UNP P00533
A	623	HIS	-	EXPRESSION TAG	UNP P00533
A	624	HIS	-	EXPRESSION TAG	UNP P00533

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

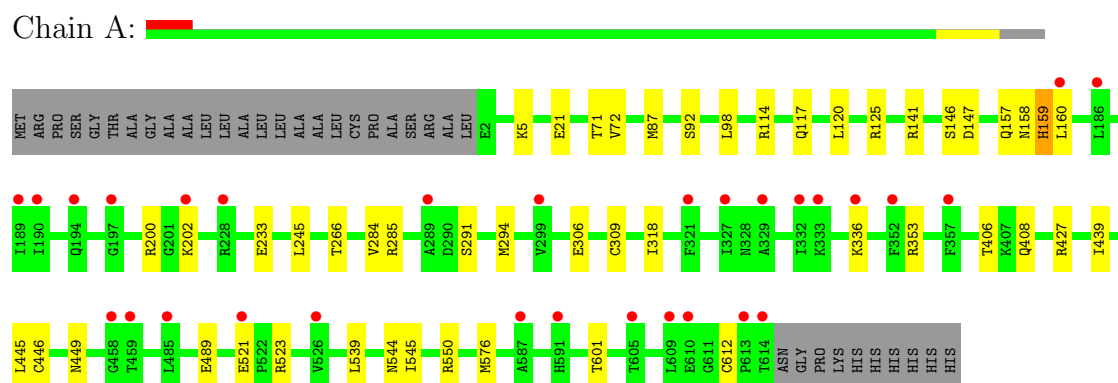
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	2	Total	O	0	0
			2	2		

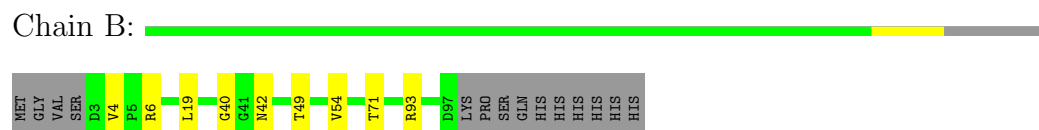
3 Residue-property plots

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: Epidermal growth factor receptor



- Molecule 2: ADNECTIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.00Å 72.10Å 262.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 2.75 49.47 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.47-2.75) 99.6 (49.47-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.13.0	Depositor
R, R_{free}	0.202 , 0.246 0.210 , 0.252	Depositor DCC
R_{free} test set	1058 reflections (3.19%)	DCC
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 34224 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5610	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: FUC, BMA, 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	0.53	0/4702	0.80	1/6383 (0.0%)
2	B	0.54	0/770	0.84	0/1062
All	All	0.53	0/5472	0.80	1/7445 (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	159	HIS	C-N-CA	6.14	137.05	121.70

There are no chirality outliers.

There are no planarity outliers.

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	4612	0	0	1	0
2	B	747	0	0	0	0
3	A	142	0	0	0	0
4	A	39	0	0	0	0
5	A	28	0	0	0	0
6	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	0	0	0
7	B	2	0	0	0	0
All	All	5610	0	0	1	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 0.

All (1) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:87:MET:SD	1:A:87:MET:CE	2.04	1.46

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	611/648 (94%)	559 (92%)	46 (8%)	6 (1%)	22	56
2	B	98/114 (86%)	91 (93%)	4 (4%)	3 (3%)	7	18
All	All	709/762 (93%)	650 (92%)	50 (7%)	9 (1%)	18	47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	GLU
1	A	336	LYS
2	B	4	VAL
1	A	159	HIS
2	B	40	GLY
1	A	160	LEU
1	A	601	THR
2	B	42	ASN
1	A	521	GLU

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	508/559 (91%)	466 (92%)	42 (8%)	16	39
2	B	77/99 (78%)	71 (92%)	6 (8%)	18	42
All	All	585/658 (89%)	537 (92%)	48 (8%)	17	40

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	21	GLU
1	A	71	THR
1	A	72	VAL
1	A	92	SER
1	A	98	LEU
1	A	114	ARG
1	A	117	GLN
1	A	120	LEU
1	A	125	ARG
1	A	141	ARG
1	A	146	SER
1	A	147	ASP
1	A	157	GLN
1	A	158	ASN
1	A	200	ARG
1	A	202	LYS
1	A	233	GLU
1	A	245	LEU
1	A	266	THR
1	A	284	VAL
1	A	285	ARG
1	A	291	SER
1	A	294	MET
1	A	309	CYS
1	A	318	ILE
1	A	353	ARG
1	A	406	THR
1	A	408	GLN

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Mol	Chain	Res	Type
1	A	427	ARG
1	A	439	ILE
1	A	445	LEU
1	A	446	CYS
1	A	449	ASN
1	A	489	GLU
1	A	523	ARG
1	A	539	LEU
1	A	544	ASN
1	A	545	ILE
1	A	550	ARG
1	A	576	MET
1	A	612	CYS
2	B	6	ARG
2	B	19	LEU
2	B	49	THR
2	B	54	VAL
2	B	71	THR
2	B	93	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

17 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
3	NAG	A	1032	1,3	12,14,15	0.27	0	15,19,21	0.64	0
3	NAG	A	1033	3	12,14,15	0.36	0	15,19,21	0.82	0
3	BMA	A	1034	3	10,11,12	0.33	0	11,15,17	0.94	0
3	MAN	A	1035	3	10,11,12	0.41	0	11,15,17	1.02	1 (9%)
3	MAN	A	1036	3	10,11,12	0.37	0	11,15,17	0.96	1 (9%)
3	FUC	A	1037	3	9,10,11	0.38	0	10,14,16	0.46	0
4	NAG	A	1328	1,4	12,14,15	0.25	0	15,19,21	0.41	0
4	NAG	A	1329	4	12,14,15	0.21	0	15,19,21	0.61	0
4	BMA	A	1330	4	10,11,12	0.36	0	11,15,17	0.56	0
5	NAG	A	1337	1,5	12,14,15	0.25	0	15,19,21	1.07	1 (6%)
5	NAG	A	1338	5	12,14,15	0.23	0	15,19,21	0.97	2 (13%)
3	NAG	A	1504	1,3	12,14,15	0.25	0	15,19,21	0.40	0
3	NAG	A	1505	3	12,14,15	0.25	0	15,19,21	0.42	0
3	BMA	A	1506	3	10,11,12	0.35	0	11,15,17	1.42	1 (9%)
3	MAN	A	1507	3	10,11,12	0.36	0	11,15,17	0.87	0
3	MAN	A	1508	3	10,11,12	0.35	0	11,15,17	1.00	0
3	FUC	A	1509	3	9,10,11	0.38	0	10,14,16	0.37	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1033	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1034	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1035	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1036	3	-	0/2/19/22	0/1/1/1
3	FUC	A	1037	3	-	0/0/17/20	0/1/1/1
4	NAG	A	1328	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1329	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1330	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1337	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1338	5	-	0/6/23/26	0/1/1/1
3	NAG	A	1504	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1505	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1506	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1507	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1508	3	-	0/2/19/22	0/1/1/1
3	FUC	A	1509	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1506	BMA	O3-C3-C2	3.80	116.89	109.94
3	A	1035	MAN	C3-C4-C5	2.25	114.22	110.20
5	A	1338	NAG	C3-C4-C5	2.06	113.88	110.20
3	A	1036	MAN	O5-C5-C6	2.04	109.12	106.98
5	A	1337	NAG	O5-C5-C4	2.04	113.24	110.65
5	A	1338	NAG	O5-C5-C6	2.01	109.08	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
6	NAG	A	1389	1	12,14,15	0.23	0	15,19,21	1.05	1 (6%)
6	NAG	A	1420	1	12,14,15	0.22	0	15,19,21	1.04	2 (13%)

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
6	NAG	A	1389	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1420	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1420	NAG	O5-C5-C4	2.42	113.72	110.65
6	A	1389	NAG	C3-C4-C5	2.11	113.98	110.20
6	A	1420	NAG	C3-C4-C5	2.02	113.81	110.20

There are no chirality outliers.

There are no torsion outliers.

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, 95th 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 ²)	Q<0.9
1	A	613/648 (94%)	0.48	30 (4%) 28 30	32, 65, 95, 141	0
2	B	100/114 (87%)	0.26	0 100 100	32, 45, 74, 107	0
All	All	713/762 (93%)	0.45	30 (4%) 35 37	32, 63, 94, 141	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	614	THR	6.8
1	A	160	LEU	5.2
1	A	336	LYS	4.7
1	A	202	LYS	4.5
1	A	610	GLU	4.4
1	A	194	GLN	4.2
1	A	521	GLU	3.3
1	A	332	ILE	3.1
1	A	289	ALA	3.0
1	A	329	ALA	3.0
1	A	321	PHE	2.9
1	A	333	LYS	2.7
1	A	591	HIS	2.7
1	A	190	ILE	2.6
1	A	605	THR	2.6
1	A	458	GLY	2.5
1	A	459	THR	2.5
1	A	186	LEU	2.4
1	A	189	ILE	2.4
1	A	357	PHE	2.4
1	A	526	VAL	2.4
1	A	327	ILE	2.3
1	A	587	ALA	2.3
1	A	299	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	613	PRO	2.2
1	A	197	GLY	2.2
1	A	228	ARG	2.1
1	A	352	PHE	2.1
1	A	485	LEU	2.1
1	A	609	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 ⓘ

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, 95th 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 ²)	Q<0.9
3	NAG	A	1505	14/15	0.20	-	76,80,83,87	0
3	MAN	A	1508	11/12	0.39	-	112,116,119,119	0
3	NAG	A	1032	14/15	0.18	-	31,53,70,70	0
3	FUC	A	1037	10/11	0.14	-	66,71,75,76	0
3	BMA	A	1034	11/12	0.19	-	97,99,102,106	0
3	BMA	A	1506	11/12	0.14	-	93,96,102,107	0
4	BMA	A	1330	11/12	0.19	-	102,106,108,108	0
3	NAG	A	1504	14/15	0.19	-	74,84,93,97	0
5	NAG	A	1338	14/15	0.45	-	121,126,128,129	0
4	NAG	A	1329	14/15	0.23	-	82,89,96,96	0
3	MAN	A	1036	11/12	0.24	-	104,106,108,108	0
3	MAN	A	1507	11/12	0.20	-	105,106,109,109	0
3	NAG	A	1033	14/15	0.22	-	81,89,94,97	0
5	NAG	A	1337	14/15	0.40	-	124,129,130,130	0
3	FUC	A	1509	10/11	0.29	-	100,102,102,103	0
3	MAN	A	1035	11/12	0.21	-	102,106,108,109	0
4	NAG	A	1328	14/15	0.20	-	65,72,76,78	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, 95th 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 ²)	Q<0.9
6	NAG	A	1420	14/15	0.55	-	115,123,127,128	0
6	NAG	A	1389	14/15	0.26	-	138,140,142,144	0

6.5 Other polymers

There are no such residues in this entry.