



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

PDB ID : 1GH7
Title : CRYSTAL STRUCTURE OF THE COMPLETE EXTRACELLULAR DOMAIN OF THE BETA-COMMON RECEPTOR OF IL-3, IL-5, AND GM-CSF
Authors : Carr, P.D.; Gustin, S.E.; Church, A.P.; Murphy, J.M.; Ford, S.C.; Mann, D.A.; Woltring, D.M.; Walker, I.; Ollis, D.L.; Young, I.G.
Deposited on : 2000-11-27
Resolution : 3.00 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

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

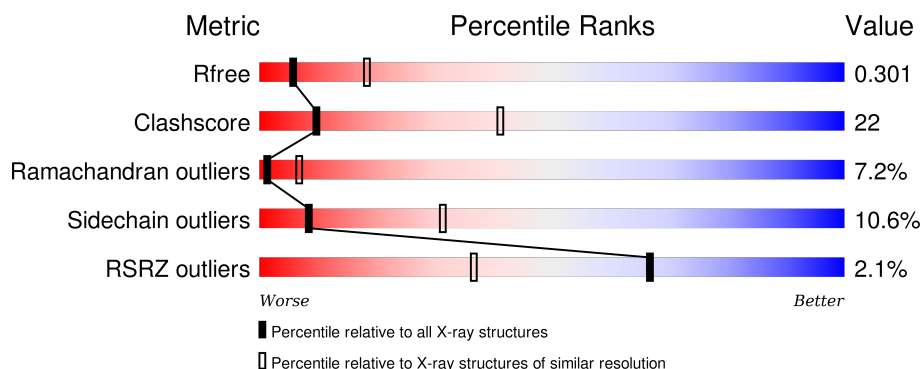
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	419	<div> <div>2%</div> <div>48%</div> <div>42%</div> <div>6%</div> <div>• •</div> </div>
1	B	419	<div> <div>2%</div> <div>51%</div> <div>40%</div> <div>6%</div> <div>•</div> </div>

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
2	NAG	A	1001	X	-	-	-
2	NAG	B	1001	X	-	-	-
3	NAG	A	1004	X	-	-	-
3	NAG	B	1004	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6470 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 CYTOKINE RECEPTOR COMMON BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3158	1973	567	600	18			
1	B	408	Total	C	N	O	S	0	0	0
			3158	1973	567	600	18			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	SER	-	INSERTION	UNP P32927
A	263	ALA	-	INSERTION	UNP P32927
A	264	VAL	-	INSERTION	UNP P32927
A	265	LEU	-	INSERTION	UNP P32927
A	266	LEU	-	INSERTION	UNP P32927
A	267	ARG	-	INSERTION	UNP P32927
A	328	GLN	ASN	ENGINEERED	UNP P32927
B	262	SER	-	INSERTION	UNP P32927
B	263	ALA	-	INSERTION	UNP P32927
B	264	VAL	-	INSERTION	UNP P32927
B	265	LEU	-	INSERTION	UNP P32927
B	266	LEU	-	INSERTION	UNP P32927
B	267	ARG	-	INSERTION	UNP P32927
B	328	GLN	ASN	ENGINEERED	UNP P32927

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

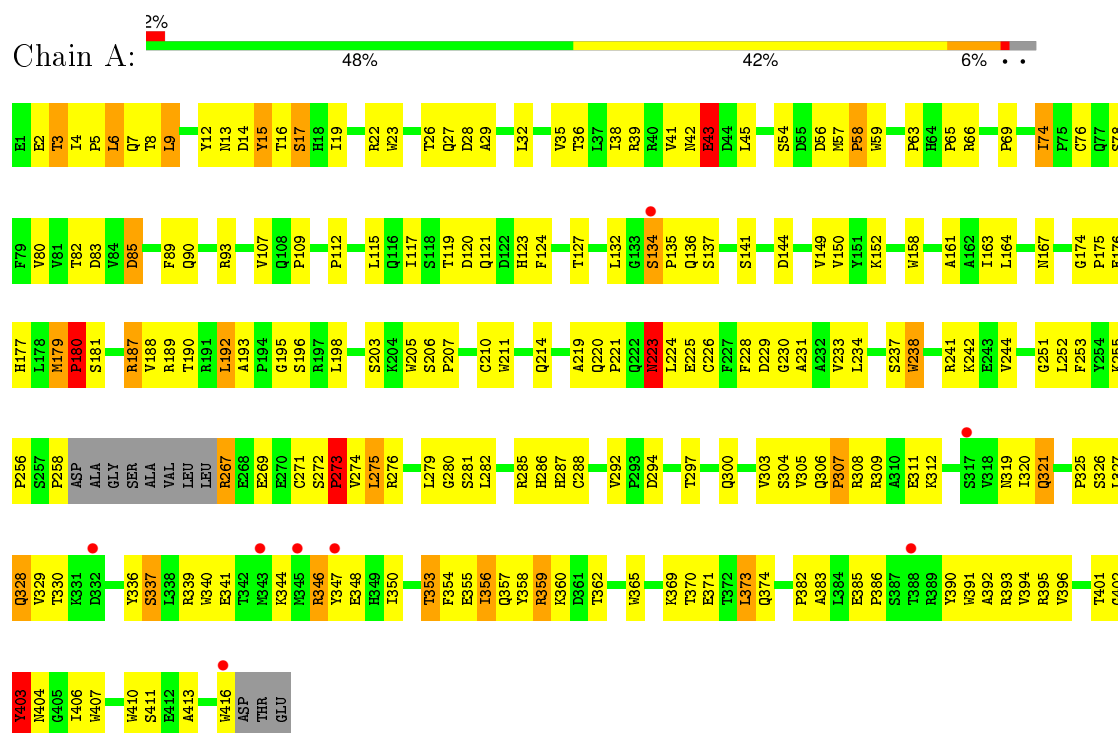
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		
3	B	3	Total	C	N	O	0	0
			38	22	2	14		

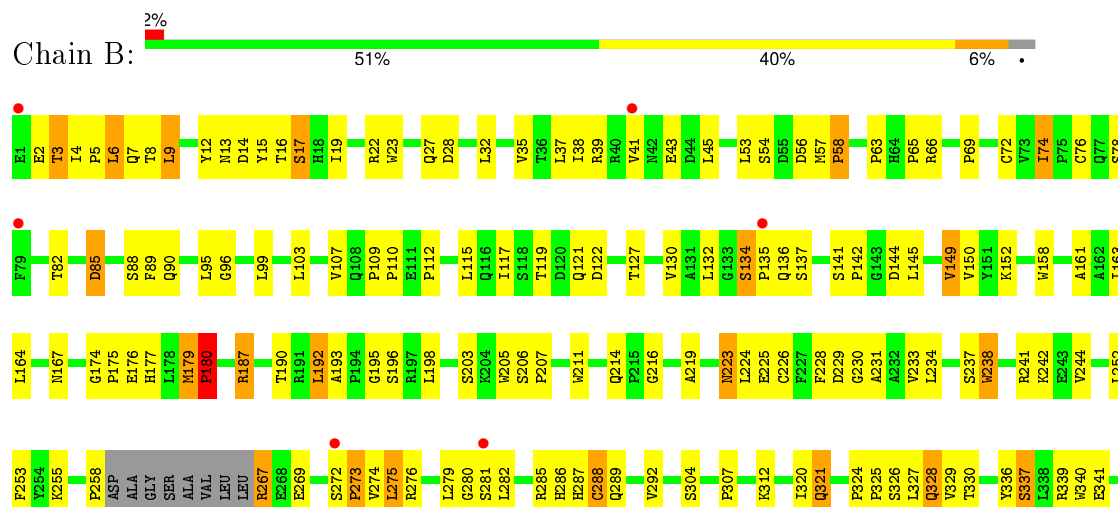
3 Residue-property plots

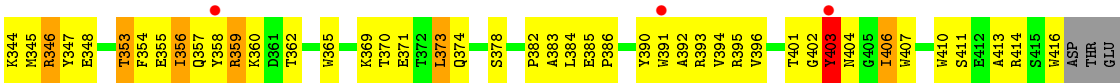
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: CYTOKINE RECEPTOR COMMON BETA CHAIN



• Molecule 1: CYTOKINE RECEPTOR COMMON BETA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	185.70Å 185.70Å 103.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 3.00 35.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	70.4 (35.00-3.00) 70.4 (35.09-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.29 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.307 0.268 , 0.301	Depositor DCC
R_{free} test set	816 reflections (4.36%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , -3.9	EDS
Estimated twinning fraction	0.078 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 18727 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	6470	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, FUC

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	0.44	0/3246	0.74	7/4446 (0.2%)
1	B	0.45	0/3246	0.75	7/4446 (0.2%)
All	All	0.45	0/6492	0.75	14/8892 (0.2%)

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
2	A	1	0
2	B	1	0
3	A	1	0
3	B	1	0
All	All	4	0

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	GLY	N-CA-C	-7.81	93.58	113.10
1	A	402	GLY	N-CA-C	-7.65	93.98	113.10
1	A	195	GLY	N-CA-C	-6.19	97.62	113.10
1	B	195	GLY	N-CA-C	-6.03	98.03	113.10
1	B	179	MET	C-N-CD	-6.00	107.39	120.60

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	NAG	C1

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Mol	Chain	Res	Type	Atom
3	A	1004	NAG	C1
2	B	1001	NAG	C1
3	B	1004	NAG	C1

There are no planarity outliers.

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	3158	0	2879	149	0
1	B	3158	0	2879	143	0
2	A	39	0	34	1	0
2	B	39	0	34	2	0
3	A	38	0	34	0	0
3	B	38	0	34	0	0
All	All	6470	0	5894	276	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 22.

The worst 5 of 276 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)
1:B:35:VAL:HG11	1:B:89:PHE:HB3	1.34	1.08
1:A:35:VAL:HG11	1:A:89:PHE:HB3	1.35	1.07
1:B:392:ALA:HB3	1:B:413:ALA:HA	1.39	1.04
1:A:392:ALA:HB3	1:A:413:ALA:HA	1.40	0.98
1:B:359:ARG:HG2	1:B:360:LYS:H	1.42	0.84

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	404/419 (96%)	324 (80%)	50 (12%)	30 (7%)	1	6
1	B	404/419 (96%)	323 (80%)	53 (13%)	28 (7%)	1	7
All	All	808/838 (96%)	647 (80%)	103 (13%)	58 (7%)	1	7

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	134	SER
1	A	136	GLN
1	A	180	PRO
1	A	328	GLN

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	331/379 (87%)	295 (89%)	36 (11%)	8	30
1	B	331/379 (87%)	297 (90%)	34 (10%)	9	33
All	All	662/758 (87%)	592 (89%)	70 (11%)	8	31

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	THR

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Mol	Chain	Res	Type
1	B	28	ASP
1	B	362	THR
1	A	373	LEU
1	A	406	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	404	ASN
1	B	105	GLN
1	B	214	GLN
1	A	214	GLN
1	B	108	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 ⓘ

12 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$
2	NAG	A	1001	1,2	14,14,15	1.42	1 (7%)	15,19,21	0.87	0
2	NAG	A	1002	2	14,14,15	0.86	0	15,19,21	1.01	1 (6%)
2	BMA	A	1003	2	11,11,12	1.74	3 (27%)	14,15,17	0.68	0
3	NAG	A	1004	1,3	14,14,15	1.47	2 (14%)	15,19,21	0.83	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	A	1005	3	10,10,11	1.99	4 (40%)	14,14,16	2.04	4 (28%)
3	NAG	A	1006	3	14,14,15	1.82	5 (35%)	15,19,21	0.90	0
2	NAG	B	1001	1,2	14,14,15	1.56	1 (7%)	15,19,21	0.70	0
2	NAG	B	1002	2	14,14,15	0.87	1 (7%)	15,19,21	1.02	1 (6%)
2	BMA	B	1003	2	11,11,12	1.71	3 (27%)	14,15,17	0.70	0
3	NAG	B	1004	1,3	14,14,15	1.54	2 (14%)	15,19,21	0.87	1 (6%)
3	FUC	B	1005	3	10,10,11	1.93	4 (40%)	14,14,16	2.03	4 (28%)
3	NAG	B	1006	3	14,14,15	1.90	5 (35%)	15,19,21	0.83	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
2	NAG	A	1001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
3	NAG	A	1004	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	FUC	A	1005	3	-	0/0/17/20	0/1/1/1
3	NAG	A	1006	3	-	0/6/23/26	0/1/1/1
2	NAG	B	1001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1003	2	-	0/2/19/22	0/1/1/1
3	NAG	B	1004	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	FUC	B	1005	3	-	0/0/17/20	0/1/1/1
3	NAG	B	1006	3	-	0/6/23/26	0/1/1/1

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	NAG	C4-C5	2.01	1.57	1.53
3	B	1006	NAG	C3-C2	2.04	1.57	1.52
3	A	1006	NAG	C3-C2	2.10	1.57	1.52
3	A	1004	NAG	O5-C5	2.17	1.48	1.43
3	A	1005	FUC	C4-C5	2.28	1.57	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1002	NAG	O4-C4-C3	-2.93	103.75	110.34
2	B	1002	NAG	O4-C4-C3	-2.88	103.86	110.34
3	B	1004	NAG	C4-C3-C2	-2.20	107.81	111.23
3	A	1004	NAG	C4-C3-C2	-2.10	107.97	111.23
3	A	1005	FUC	O5-C1-C2	-2.05	107.54	110.86

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1004	NAG	C1
3	A	1004	NAG	C1
2	B	1001	NAG	C1
2	A	1001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	1	0
2	A	1002	NAG	1	0
2	B	1001	NAG	2	0
2	B	1002	NAG	2	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	408/419 (97%)	-0.08	8 (1%) 68 39	10, 35, 86, 107	0
1	B	408/419 (97%)	-0.13	9 (2%) 65 35	10, 33, 88, 107	0
All	All	816/838 (97%)	-0.10	17 (2%) 67 36	10, 33, 88, 107	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	SER	3.6
1	A	347	TYR	3.4
1	B	403	TYR	3.2
1	B	135	PRO	2.7
1	A	388	THR	2.5

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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	1001	14/15	0.74	0.19	-0.63	17,45,51,70	0
2	NAG	A	1001	14/15	0.90	0.16	-0.69	10,32,46,67	0
3	NAG	B	1004	14/15	0.58	0.32	-	96,106,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1004	14/15	0.62	0.23	-	96,105,108,108	0
3	FUC	A	1005	10/11	0.59	0.23	-	107,108,108,108	0
2	BMA	B	1003	11/12	0.60	0.34	-	106,108,108,108	0
2	NAG	B	1002	14/15	0.79	0.22	-	91,101,107,107	0
3	NAG	A	1006	14/15	0.65	0.45	-	106,108,108,108	0
3	NAG	B	1006	14/15	0.62	0.39	-	105,108,108,108	0
2	BMA	A	1003	11/12	0.40	0.60	-	107,108,108,108	0
2	NAG	A	1002	14/15	0.68	0.28	-	89,100,103,107	0
3	FUC	B	1005	10/11	0.50	0.43	-	105,108,108,108	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.