



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:57 PM GMT

PDB ID : 4DZ8
Title : human IgG1 Fc fragment Heterodimer
Authors : Strop, P.
Deposited on : 2012-02-29
Resolution : 1.91 Å(reported)

This is a Full wwPDB X-ray Structure 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/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

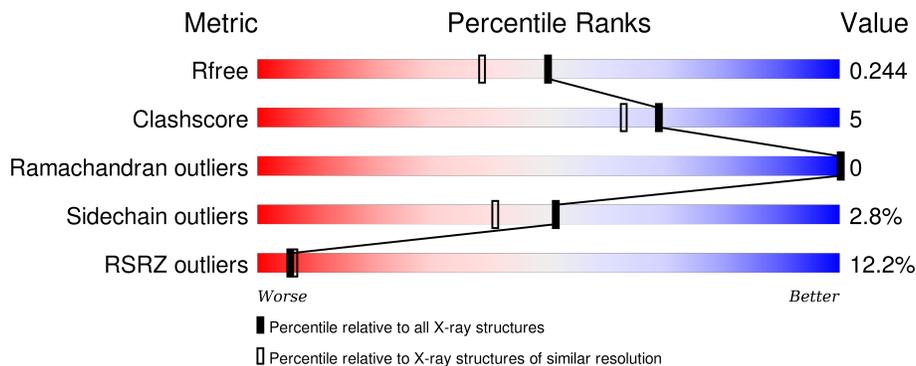
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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	225	
2	B	225	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3989 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	1688	1072	286	324	6	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ARG	PRO	ENGINEERED MUTATION	UNP P01857
A	368	GLU	LEU	MICROHETEROGENEITY	UNP P01857
A	409	ARG	LYS	MICROHETEROGENEITY	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	205	1667	1060	282	319	6	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	228	GLU	PRO	ENGINEERED MUTATION	UNP P01857
B	368	GLU	LEU	MICROHETEROGENEITY	UNP P01857
B	409	ARG	LYS	MICROHETEROGENEITY	UNP P01857

- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	8	99	56	4	39	0	0
3	B	8	99	56	4	39	0	0

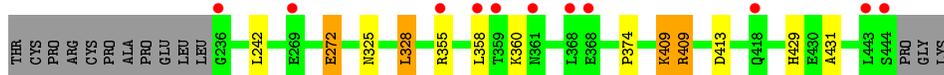
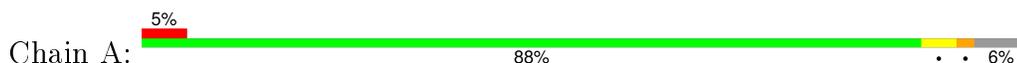
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	269	Total 269	O 269	0	0
4	B	167	Total 167	O 167	0	0

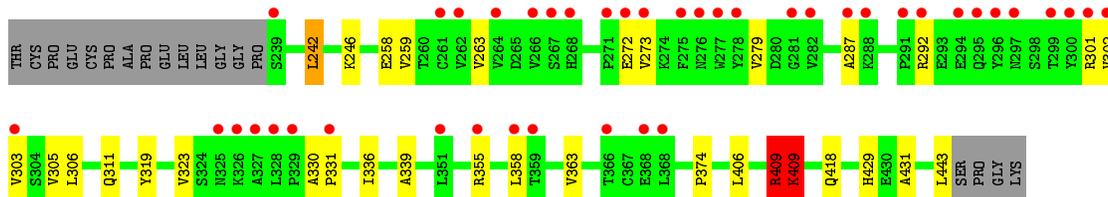
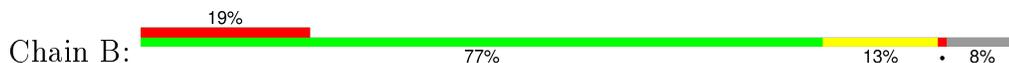
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: Ig gamma-1 chain C region



- Molecule 2: Ig gamma-1 chain C region



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.93Å 81.29Å 136.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.91 28.60 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.91) 99.5 (28.60-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.237 0.211 , 0.244	Depositor DCC
R_{free} test set	2201 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	29.6	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 43750 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3989	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: 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	0.43	0/1732	0.61	2/2355 (0.1%)
2	B	0.40	0/1710	0.57	2/2325 (0.1%)
All	All	0.42	0/3442	0.59	4/4680 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	409[B]	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	B	409[A]	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	A	409[B]	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	B	409[A]	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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	1688	0	1648	6	0
2	B	1667	0	1630	22	0
3	A	99	0	85	0	0
3	B	99	0	85	0	0
4	A	269	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	167	0	0	1	0
All	All	3989	0	3448	28	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 5.

All (28) 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:409[A]:ARG:HH11	2:B:409[A]:ARG:HG2	1.59	0.67
2:B:358:LEU:HD23	2:B:363:VAL:HG11	1.81	0.63
2:B:273:VAL:HG21	2:B:302:VAL:HG11	1.84	0.58
1:A:355:ARG:HA	1:A:358:LEU:HD12	1.87	0.57
1:A:429:HIS:CD2	1:A:431:ALA:H	2.22	0.56
2:B:259:VAL:HG13	2:B:336:ILE:HD11	1.88	0.55
2:B:409[A]:ARG:HH11	2:B:409[A]:ARG:CG	2.21	0.54
1:A:429:HIS:HD2	1:A:431:ALA:H	1.55	0.54
2:B:273:VAL:CG2	2:B:302:VAL:HG11	2.39	0.53
2:B:429:HIS:HD2	2:B:431:ALA:H	1.56	0.52
2:B:429:HIS:CD2	2:B:431:ALA:H	2.27	0.51
2:B:355:ARG:HA	2:B:358:LEU:HD12	1.95	0.49
2:B:406:LEU:HD12	2:B:406:LEU:C	2.33	0.49
1:A:374:PRO:O	1:A:429:HIS:HE1	1.96	0.48
2:B:263:VAL:HG22	2:B:323:VAL:HG21	1.96	0.48
2:B:287:ALA:HB2	2:B:306:LEU:HD13	1.96	0.47
2:B:242:LEU:HD13	2:B:336:ILE:HG12	1.96	0.47
2:B:311:GLN:NE2	4:B:764:HOH:O	2.46	0.47
2:B:258:GLU:HB3	2:B:305:VAL:HG13	1.95	0.47
2:B:330:ALA:HB1	2:B:331:PRO:HD2	1.97	0.46
1:A:272:GLU:HG2	4:A:754:HOH:O	2.16	0.44
2:B:242:LEU:HD13	2:B:336:ILE:HG23	2.00	0.44
2:B:301:ARG:NH1	2:B:303:VAL:HG21	2.33	0.43
2:B:339:ALA:HB3	2:B:374:PRO:HB3	2.01	0.43
1:A:325:ASN:HB3	1:A:328:LEU:HD22	2.00	0.43
2:B:418:GLN:HA	2:B:443:LEU:HD22	2.01	0.42
2:B:374:PRO:O	2:B:429:HIS:HE1	2.03	0.41
2:B:279:VAL:HG22	2:B:319:TYR:CD2	2.56	0.41

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	205/225 (91%)	205 (100%)	0	0	100	100
2	B	201/225 (89%)	201 (100%)	0	0	100	100
All	All	406/450 (90%)	406 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	196/208 (94%)	190 (97%)	6 (3%)	47	36
2	B	194/208 (93%)	189 (97%)	5 (3%)	54	44
All	All	390/416 (94%)	379 (97%)	11 (3%)	51	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	272	GLU
1	A	328	LEU
1	A	360	LYS
1	A	409[B]	ARG
1	A	413	ASP
2	B	242	LEU
2	B	246	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	272	GLU
2	B	292	ARG
2	B	409[A]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	325	ASN
1	A	362	GLN
1	A	418	GLN
1	A	429	HIS
1	A	434	ASN
2	B	311	GLN
2	B	315	ASN
2	B	325	ASN
2	B	429	HIS
2	B	434	ASN

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](#)

16 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	501	1,3	14,14,15	0.42	0	15,19,21	1.34	1 (6%)
3	NAG	A	502	3	14,14,15	0.63	0	15,19,21	1.00	1 (6%)
3	BMA	A	503	3	11,11,12	0.33	0	14,15,17	0.77	0
3	MAN	A	504	3	11,11,12	0.59	0	14,15,17	0.92	0
3	NAG	A	505	3	14,14,15	0.47	0	15,19,21	0.76	0
3	MAN	A	506	3	11,11,12	0.47	0	14,15,17	1.19	2 (14%)
3	NAG	A	507	3	14,14,15	0.53	0	15,19,21	0.76	1 (6%)
3	FUC	A	508	3	10,10,11	0.50	0	14,14,16	1.11	1 (7%)
3	NAG	B	501	3,2	14,14,15	0.55	0	15,19,21	0.79	0
3	NAG	B	502	3	14,14,15	0.56	0	15,19,21	0.80	0
3	BMA	B	503	3	11,11,12	0.52	0	14,15,17	1.43	1 (7%)
3	MAN	B	504	3	11,11,12	0.58	0	14,15,17	1.09	2 (14%)
3	NAG	B	505	3	14,14,15	0.52	0	15,19,21	0.92	1 (6%)
3	MAN	B	506	3	11,11,12	0.47	0	14,15,17	0.83	0
3	NAG	B	507	3	14,14,15	0.50	0	15,19,21	0.64	0
3	FUC	B	508	3	10,10,11	0.56	0	14,14,16	2.11	3 (21%)

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	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3	-	0/6/23/26	0/1/1/1
3	BMA	A	503	3	-	0/2/19/22	0/1/1/1
3	MAN	A	504	3	-	0/2/19/22	0/1/1/1
3	NAG	A	505	3	-	0/6/23/26	0/1/1/1
3	MAN	A	506	3	-	0/2/19/22	0/1/1/1
3	NAG	A	507	3	-	0/6/23/26	0/1/1/1
3	FUC	A	508	3	-	0/0/17/20	0/1/1/1
3	NAG	B	501	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3	-	0/6/23/26	0/1/1/1
3	BMA	B	503	3	-	0/2/19/22	0/1/1/1
3	MAN	B	504	3	-	0/2/19/22	0/1/1/1
3	NAG	B	505	3	-	0/6/23/26	0/1/1/1
3	MAN	B	506	3	-	0/2/19/22	0/1/1/1
3	NAG	B	507	3	-	0/6/23/26	0/1/1/1
3	FUC	B	508	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	MAN	O2-C2-C3	-2.30	105.49	110.12
3	A	507	NAG	C1-O5-C5	-2.13	109.55	112.25
3	A	502	NAG	O7-C7-C8	-2.01	118.38	122.06
3	B	504	MAN	O2-C2-C3	-2.00	106.09	110.12
3	B	505	NAG	C1-O5-C5	2.22	115.06	112.25
3	A	506	MAN	C1-O5-C5	2.29	115.15	112.25
3	B	504	MAN	C1-O5-C5	2.48	115.40	112.25
3	A	508	FUC	C1-O5-C5	2.67	116.50	112.38
3	B	508	FUC	O5-C1-C2	3.52	116.58	110.86
3	B	503	BMA	C1-C2-C3	3.99	114.26	109.54
3	B	508	FUC	O5-C5-C4	4.08	116.60	109.53
3	A	501	NAG	C1-O5-C5	4.32	117.73	112.25
3	B	508	FUC	C1-O5-C5	4.91	119.97	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	211/225 (93%)	0.24	11 (5%) 31 35	19, 30, 58, 67	4 (1%)
2	B	207/225 (92%)	0.96	40 (19%) 2 2	20, 44, 148, 201	4 (1%)
All	All	418/450 (92%)	0.59	51 (12%) 5 6	19, 33, 127, 201	8 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	296	TYR	9.9
2	B	291	PRO	8.0
1	A	444	SER	6.0
2	B	273	VAL	4.7
2	B	300	TYR	4.6
2	B	297	ASN	4.4
2	B	299	THR	4.4
2	B	282	VAL	4.3
2	B	329	PRO	3.7
2	B	359	THR	3.7
2	B	275	PHE	3.7
2	B	272	GLU	3.5
2	B	301	ARG	3.5
2	B	355	ARG	3.3
2	B	271	PRO	3.3
2	B	268	HIS	3.3
2	B	288	LYS	3.3
2	B	325	ASN	3.2
1	A	355	ARG	3.2
2	B	262	VAL	3.1
2	B	302	VAL	2.9
2	B	278	TYR	2.8
2	B	328	LEU	2.7
2	B	276	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	281	GLY	2.6
2	B	295	GLN	2.6
2	B	239	SER	2.6
2	B	326	LYS	2.6
2	B	266	VAL	2.6
1	A	358	LEU	2.5
2	B	366	THR	2.5
2	B	327	ALA	2.5
2	B	267	SER	2.4
1	A	418	GLN	2.4
1	A	236	GLY	2.3
1	A	443	LEU	2.3
2	B	294	GLU	2.2
2	B	261	CYS	2.2
2	B	292	ARG	2.2
1	A	368[A]	LEU	3.0
1	A	368[A]	LEU	3.0
2	B	303	VAL	2.2
2	B	331	PRO	2.2
2	B	358	LEU	2.1
2	B	287	ALA	2.1
2	B	351	LEU	2.1
1	A	359	THR	2.1
2	B	277	TRP	2.0
1	A	361	ASN	2.0
2	B	264	VAL	2.0
1	A	269	GLU	2.0

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(\AA^2)	Q<0.9
3	NAG	A	501	14/15	0.94	0.08	-0.48	27,30,36,37	0
3	NAG	B	507	14/15	0.93	0.12	-0.87	55,55,57,57	0
3	NAG	A	507	14/15	0.94	0.09	-1.29	28,30,31,32	0
3	MAN	A	504	11/12	0.90	0.10	-	38,42,45,48	0
3	FUC	A	508	10/11	0.91	0.11	-	34,35,37,38	0
3	NAG	A	505	14/15	0.82	0.25	-	53,56,57,57	0
3	MAN	B	504	11/12	0.88	0.13	-	44,47,49,53	0
3	NAG	B	505	14/15	0.84	0.18	-	57,59,60,60	0
3	FUC	B	508	10/11	0.71	0.44	-	74,76,77,77	0
3	MAN	A	506	11/12	0.94	0.08	-	27,28,30,32	0
3	BMA	A	503	11/12	0.96	0.08	-	26,27,29,32	0
3	NAG	A	502	14/15	0.95	0.09	-	23,25,27,28	0
3	MAN	B	506	11/12	0.90	0.13	-	53,55,55,56	0
3	NAG	B	502	14/15	0.77	0.23	-	54,58,60,61	0
3	NAG	B	501	14/15	0.65	0.32	-	63,65,68,72	0
3	BMA	B	503	11/12	0.87	0.14	-	47,50,51,52	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.