



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:44 PM GMT

PDB ID : 4W4N
Title : Crystal structure of human Fc at 1.80 Å
Authors : Caaveiro, J.M.M.; Kiyoshi, M.; Tsumoto, K.
Deposited on : 2014-08-15
Resolution : 1.80 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

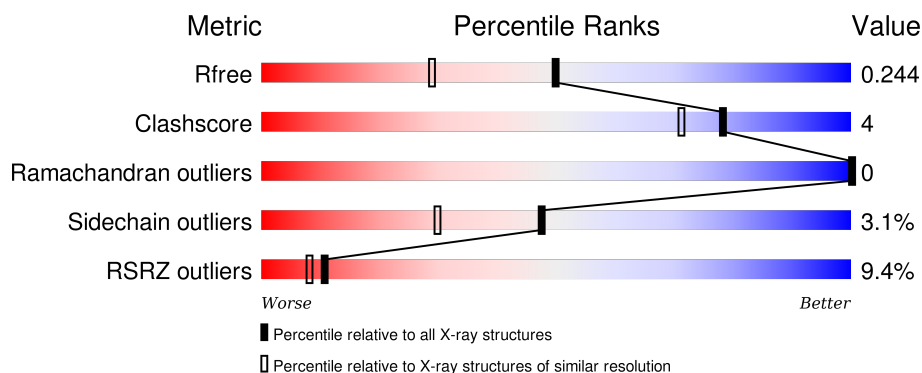
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	223	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 8%</div> </div> </div>
1	B	223	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 7%</div> </div> </div>

2 Entry composition [i](#)

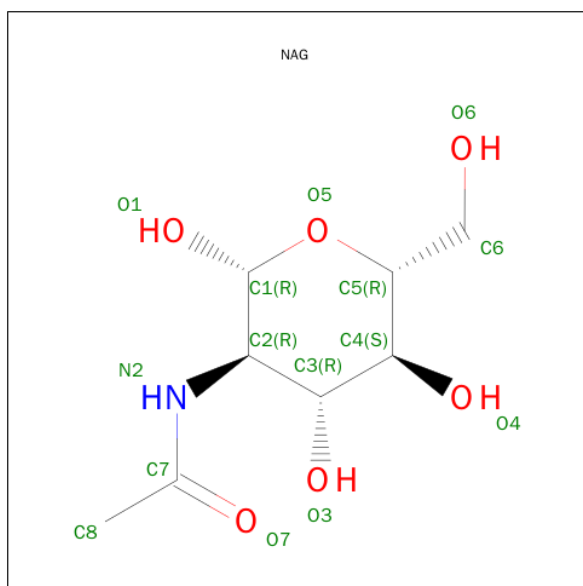
There are 7 unique types of molecules in this entry. The entry contains 3931 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	206	Total	C	N	O	S	0	3	0
			1666	1062	279	319	6			
1	B	207	Total	C	N	O	S	0	5	0
			1688	1077	283	322	6			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



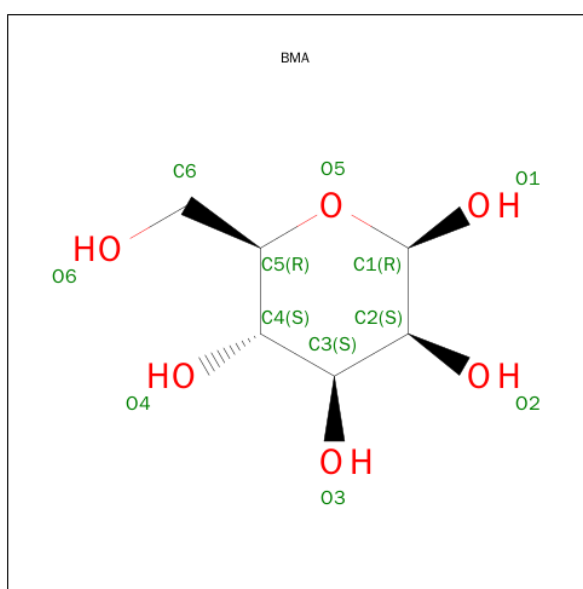
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



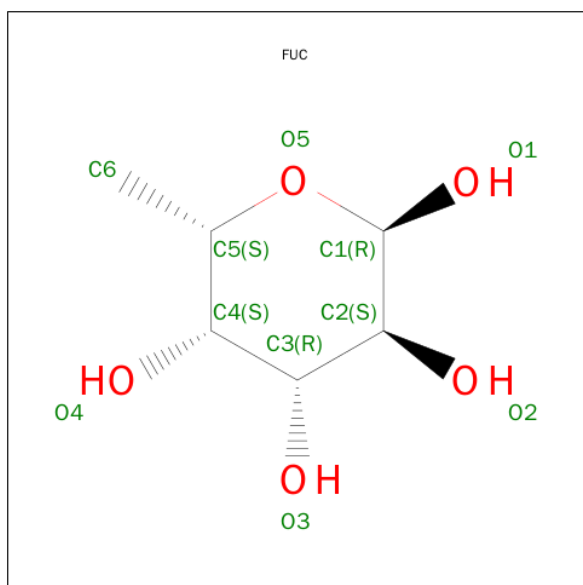
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	1
			12	6	6		

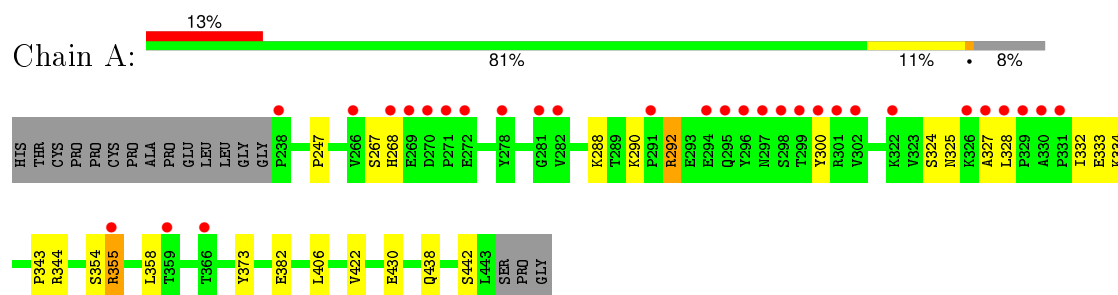
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	137	Total	O	0	0
			137	137		
7	B	237	Total	O	0	3
			240	240		

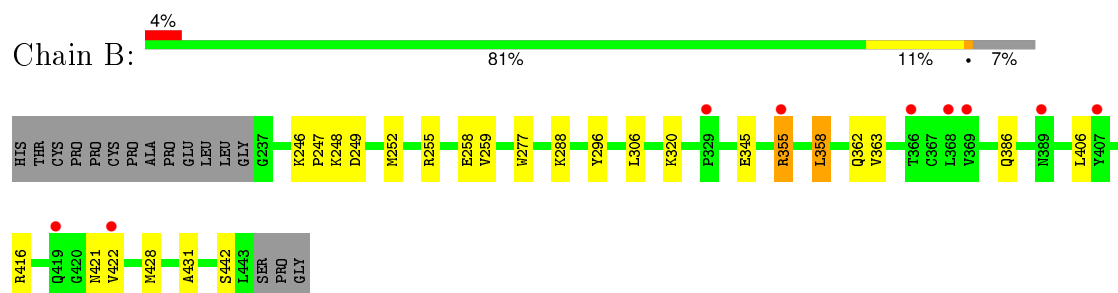
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Ig gamma-1 chain C region



- Molecule 1: 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	49.71 Å 79.29 Å 138.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.19 – 1.80 22.19 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (22.19-1.80) 99.0 (22.19-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.80 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.200 , 0.244 0.200 , 0.244	Depositor DCC
R_{free} test set	2087 reflections (4.26%)	DCC
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51118 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3931	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: MAN, GOL, 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	1.01	3/1721 (0.2%)	1.00	3/2344 (0.1%)
1	B	1.03	2/1749 (0.1%)	1.00	4/2383 (0.2%)
All	All	1.02	5/3470 (0.1%)	1.00	7/4727 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	SER	CB-OG	8.97	1.53	1.42
1	B	258	GLU	CD-OE2	-6.42	1.18	1.25
1	B	277	TRP	CE3-CZ3	6.41	1.49	1.38
1	A	324	SER	CB-OG	5.55	1.49	1.42
1	A	430	GLU	CD-OE1	-5.45	1.19	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	344	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	B	416	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	428	MET	CG-SD-CE	-7.29	88.53	100.20
1	B	248	LYS	CD-CE-NZ	-5.29	99.53	111.70
1	A	382	GLU	CB-CA-C	-5.26	99.88	110.40
1	B	320	LYS	CD-CE-NZ	-5.01	100.17	111.70

There are no chirality outliers.

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	1666	0	1641	14	0
1	B	1688	0	1667	11	0
2	A	56	0	50	0	0
2	B	56	0	49	0	0
3	A	11	0	8	0	0
3	B	11	0	8	0	0
4	A	22	0	18	0	0
4	B	22	0	18	0	0
5	B	10	0	10	0	0
6	B	12	0	16	0	0
7	A	137	0	0	2	0
7	B	240	0	0	2	0
All	All	3931	0	3485	25	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 4.

All (25) 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:A:333:GLU:O	1:A:334:LYS:HD2	1.89	0.72
1:A:438:GLN:NE2	7:A:601:HOH:O	2.27	0.65
1:A:328:LEU:HD22	1:A:332:ILE:HD11	1.80	0.64
1:A:292:ARG:HH11	1:A:292:ARG:H	1.47	0.60
1:B:422:VAL:HA	1:B:442:SER:HB3	1.89	0.54
1:A:438:GLN:HG3	7:A:639:HOH:O	2.12	0.50
1:A:406:LEU:HD12	1:A:406:LEU:C	2.32	0.50
1:A:325:ASN:ND2	1:A:327:ALA:H	2.10	0.49
1:A:343:PRO:HA	1:A:373:TYR:O	2.13	0.49
1:B:406:LEU:HD12	1:B:406:LEU:C	2.33	0.49
1:A:268:HIS:CD2	1:A:300:TYR:CE1	3.01	0.48
1:B:421:ASN:ND2	7:B:601:HOH:O	2.42	0.48
1:B:246:LYS:HB2	1:B:249:ASP:OD2	2.14	0.47
1:B:259[B]:VAL:HG23	1:B:306:LEU:HB3	1.97	0.47
1:A:328:LEU:HD13	1:A:332:ILE:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ARG:HA	1:A:358:LEU:HD12	1.99	0.44
1:B:358:LEU:HD13	1:B:363:VAL:HG11	1.99	0.44
1:B:249:ASP:OD1	1:B:255[A]:ARG:NE	2.45	0.43
1:B:345[A]:GLU:HG3	1:B:431:ALA:O	2.18	0.43
1:B:358:LEU:HD13	1:B:358:LEU:HA	1.77	0.43
1:A:355:ARG:HB2	1:A:355:ARG:HE	1.40	0.43
1:A:290:LYS:HD2	1:A:290:LYS:HA	1.92	0.42
1:B:355:ARG:HA	1:B:358:LEU:HD23	2.02	0.42
1:A:422:VAL:HA	1:A:442:SER:HB3	2.02	0.42
1:B:252:MET:HE2	7:B:735:HOH:O	2.21	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	207/223 (93%)	202 (98%)	5 (2%)	0	100	100
1	B	210/223 (94%)	208 (99%)	2 (1%)	0	100	100
All	All	417/446 (94%)	410 (98%)	7 (2%)	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	196/206 (95%)	191 (97%)	5 (3%)	54	37
1	B	198/206 (96%)	191 (96%)	7 (4%)	43	25
All	All	394/412 (96%)	382 (97%)	12 (3%)	47	31

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	PRO
1	A	288	LYS
1	A	292	ARG
1	A	354	SER
1	A	355	ARG
1	B	247	PRO
1	B	288	LYS
1	B	296	TYR
1	B	355	ARG
1	B	358	LEU
1	B	362	GLN
1	B	386	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	325	ASN
1	A	390	ASN
1	A	419	GLN
1	A	434	ASN
1	B	315	ASN
1	B	361	ASN
1	B	386	GLN
1	B	390	ASN
1	B	434	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

17 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	$\# Z > 2$
2	NAG	A	501	1,2	14,14,15	0.79	0	15,19,21	2.94	6 (40%)
2	NAG	A	502	3,2	14,14,15	0.75	0	15,19,21	1.36	1 (6%)
3	BMA	A	503	2,4	11,11,12	1.09	1 (9%)	14,15,17	1.76	3 (21%)
4	MAN	A	504	3,2	11,11,12	0.68	0	14,15,17	1.31	1 (7%)
2	NAG	A	505	4	14,14,15	0.48	0	15,19,21	2.93	5 (33%)
4	MAN	A	506	3,2	11,11,12	1.02	0	14,15,17	2.04	3 (21%)
2	NAG	A	507	4	14,14,15	0.50	0	15,19,21	2.43	3 (20%)
2	NAG	B	501	1,2,5	14,14,15	1.07	1 (7%)	15,19,21	0.99	0
2	NAG	B	502	3,2	14,14,15	1.10	2 (14%)	15,19,21	1.65	4 (26%)
3	BMA	B	503	2,4	11,11,12	1.08	1 (9%)	14,15,17	1.52	2 (14%)
4	MAN	B	504	3,2	11,11,12	0.90	1 (9%)	14,15,17	1.99	4 (28%)
2	NAG	B	505	4	14,14,15	1.43	2 (14%)	15,19,21	1.54	1 (6%)
4	MAN	B	506	3,2	11,11,12	1.23	2 (18%)	14,15,17	2.14	5 (35%)
2	NAG	B	507	4	14,14,15	0.58	0	15,19,21	2.12	6 (40%)
5	FUC	B	508	2	10,10,11	1.23	2 (20%)	14,14,16	1.37	1 (7%)
6	GOL	B	509[A]	-	5,5,5	0.16	0	5,5,5	0.52	0
6	GOL	B	509[B]	-	5,5,5	0.21	0	5,5,5	0.66	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	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	4	-	0/6/23/26	0/1/1/1
4	MAN	A	506	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	507	4	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1,2,5	-	0/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	505	4	-	0/6/23/26	0/1/1/1
4	MAN	B	506	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	507	4	-	0/6/23/26	0/1/1/1
5	FUC	B	508	2	-	0/0/17/20	0/1/1/1
6	GOL	B	509[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	B	509[B]	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	BMA	O5-C1	-2.33	1.39	1.43
4	B	506	MAN	O5-C1	-2.04	1.40	1.43
2	B	505	NAG	C4-C5	2.05	1.57	1.53
2	B	502	NAG	O7-C7	2.07	1.28	1.23
4	B	506	MAN	C4-C5	2.16	1.57	1.53
4	B	504	MAN	C2-C3	2.17	1.55	1.52
5	B	508	FUC	C1-C2	2.26	1.57	1.52
3	B	503	BMA	C2-C3	2.28	1.55	1.52
2	B	501	NAG	C1-C2	2.28	1.55	1.52
5	B	508	FUC	C6-C5	2.67	1.58	1.51
2	B	502	NAG	C3-C2	2.84	1.59	1.52
2	B	505	NAG	C1-C2	3.93	1.57	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	NAG	C6-C5-C4	-4.84	101.09	113.02
4	B	506	MAN	O2-C2-C3	-4.43	101.20	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	505	NAG	C1-O5-C5	-4.11	107.03	112.25
2	A	501	NAG	O7-C7-C8	-3.81	115.07	122.06
3	B	503	BMA	O3-C3-C2	-3.75	103.22	110.00
5	B	508	FUC	O5-C1-C2	-3.68	104.88	110.86
2	A	507	NAG	C4-C3-C2	-3.68	105.50	111.23
3	A	503	BMA	O6-C6-C5	-3.39	100.12	111.33
4	A	506	MAN	O2-C2-C3	-3.28	103.52	110.12
3	A	503	BMA	O4-C4-C3	-3.25	103.02	110.34
2	B	502	NAG	C8-C7-N2	-3.19	110.01	116.11
2	A	505	NAG	O3-C3-C4	-3.15	103.25	110.34
4	B	506	MAN	O5-C1-C2	-2.65	106.56	110.86
4	B	506	MAN	O4-C4-C3	-2.52	104.67	110.34
4	B	504	MAN	O6-C6-C5	-2.48	103.15	111.33
4	B	504	MAN	C6-C5-C4	-2.45	106.97	113.02
2	B	502	NAG	C2-N2-C7	-2.41	119.94	123.04
2	A	505	NAG	O6-C6-C5	-2.39	103.44	111.33
2	B	507	NAG	C6-C5-C4	-2.34	107.24	113.02
4	A	506	MAN	O3-C3-C4	-2.31	105.14	110.34
2	B	507	NAG	O3-C3-C2	-2.12	104.91	109.11
2	B	507	NAG	O6-C6-C5	-2.10	104.38	111.33
2	B	502	NAG	O4-C4-C5	-2.09	103.70	109.24
2	A	501	NAG	C3-C4-C5	2.05	113.77	110.20
2	A	505	NAG	C3-C4-C5	2.20	114.04	110.20
2	B	507	NAG	O7-C7-N2	2.22	126.39	121.86
2	A	502	NAG	C1-O5-C5	2.27	115.13	112.25
3	B	503	BMA	O2-C2-C3	2.48	115.11	110.12
2	A	501	NAG	O7-C7-N2	2.54	127.04	121.86
2	A	501	NAG	O5-C5-C6	2.64	113.06	107.35
4	B	504	MAN	O5-C5-C6	2.76	113.32	107.35
2	A	507	NAG	C8-C7-N2	2.76	121.40	116.11
3	A	503	BMA	C1-C2-C3	2.97	113.05	109.54
4	B	506	MAN	C1-O5-C5	3.01	116.07	112.25
4	A	504	MAN	C1-O5-C5	3.33	116.47	112.25
2	B	502	NAG	O7-C7-N2	3.35	128.69	121.86
2	B	507	NAG	C1-O5-C5	3.65	116.88	112.25
4	B	506	MAN	C1-C2-C3	3.73	113.95	109.54
2	B	507	NAG	C2-N2-C7	4.90	129.33	123.04
4	B	504	MAN	C1-O5-C5	4.92	118.49	112.25
2	A	501	NAG	C1-O5-C5	5.03	118.63	112.25
4	A	506	MAN	C1-O5-C5	5.36	119.05	112.25
2	A	507	NAG	C1-O5-C5	7.09	121.24	112.25
2	A	501	NAG	C2-N2-C7	7.61	132.81	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	NAG	C1-O5-C5	8.90	123.54	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	206/223 (92%)	0.66	30 (14%) 3 2	18, 45, 104, 135	0
1	B	207/223 (92%)	0.04	9 (4%) 39 32	17, 30, 63, 85	0
All	All	413/446 (92%)	0.35	39 (9%) 11 8	17, 35, 94, 135	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TYR	10.9
1	A	291	PRO	8.1
1	A	300	TYR	6.5
1	A	281	GLY	5.7
1	A	326	LYS	4.9
1	A	282	VAL	4.8
1	A	331	PRO	4.2
1	A	297	ASN	4.2
1	A	328	LEU	4.0
1	A	295	GLN	3.9
1	A	298	SER	3.7
1	B	368	LEU	3.7
1	A	299	THR	3.6
1	A	330	ALA	3.3
1	A	278	TYR	3.3
1	A	327	ALA	3.2
1	B	355	ARG	3.1
1	A	271	PRO	2.9
1	A	270	ASP	2.9
1	A	294	GLU	2.8
1	A	329	PRO	2.8
1	B	366	THR	2.7
1	B	407	TYR	2.7
1	A	355	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	366	THR	2.6
1	A	268	HIS	2.6
1	A	272	GLU	2.6
1	A	266	VAL	2.5
1	A	301	ARG	2.4
1	B	419	GLN	2.3
1	A	269	GLU	2.3
1	B	389	ASN	2.3
1	A	359	THR	2.3
1	A	238	PRO	2.2
1	B	369	VAL	2.2
1	A	322	LYS	2.2
1	B	329	PRO	2.1
1	B	422	VAL	2.1
1	A	302	VAL	2.1

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 carbohydrates 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. 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	A	505	14/15	0.92	0.17	1.35	54,57,60,62	0
6	GOL	B	509[B]	6/6	0.89	0.15	0.35	31,47,48,51	6
6	GOL	B	509[A]	6/6	0.89	0.15	0.35	38,49,52,52	6
2	NAG	B	505	14/15	0.93	0.11	-0.01	24,26,30,33	0
2	NAG	B	501	14/15	0.98	0.06	-2.30	27,30,34,34	0
2	NAG	B	507	14/15	0.82	0.30	-	45,48,53,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	507	14/15	0.88	0.31	-	61,71,80,82	0
2	NAG	A	501	14/15	0.63	0.28	-	73,81,89,90	0
3	BMA	A	503	11/12	0.90	0.11	-	46,47,51,52	0
4	MAN	B	504	11/12	0.96	0.09	-	25,27,31,32	0
4	MAN	B	506	11/12	0.94	0.10	-	28,32,39,42	0
4	MAN	A	504	11/12	0.92	0.13	-	51,57,61,65	0
4	MAN	A	506	11/12	0.89	0.15	-	45,47,53,58	0
5	FUC	B	508	10/11	0.94	0.14	-	30,34,37,42	0
2	NAG	B	502	14/15	0.98	0.06	-	24,25,27,28	0
3	BMA	B	503	11/12	0.96	0.07	-	23,25,26,26	0
2	NAG	A	502	14/15	0.70	0.22	-	54,61,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.