Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:16 PM GMT

PDB ID	:	4X98
Title	:	Immunoglobulin Fc heterodimer variant
Authors	:	Seok, S.H.; Choi, H.J.; Kim, Y.J.; Seo, M.D.; Kim, Y.S.
Deposited on	:	2014-12-11
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

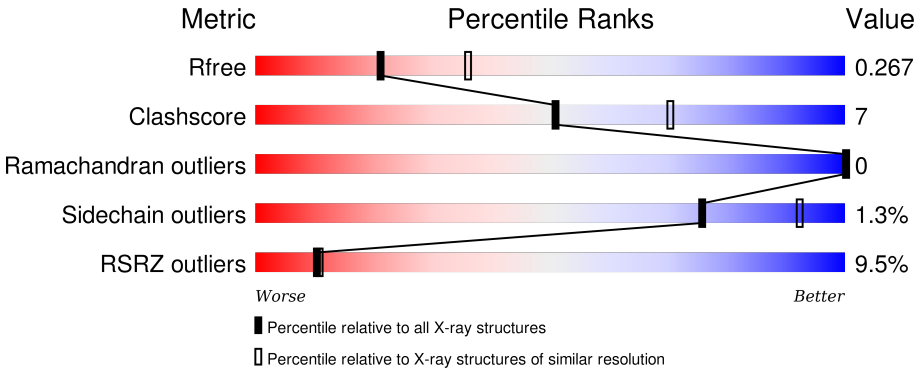
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	220	87% 8% 5%
2	B	207	19% 83% 14%

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
4	FUC	A	503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3542 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	208	Total	C	N	O	S	0	0	0
			1669	1063	279	321	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLU	LYS	engineered mutation	UNP P01857
A	409	TRP	LYS	engineered mutation	UNP P01857

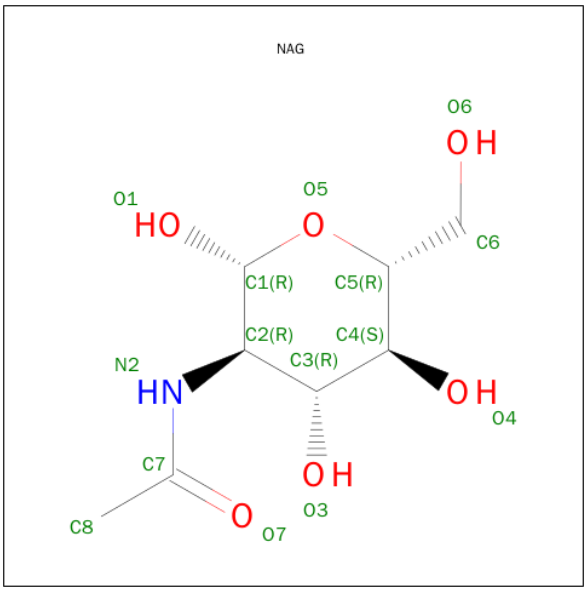
- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1604	1019	274	305	6			

There are 3 discrepancies between the modelled and reference sequences:

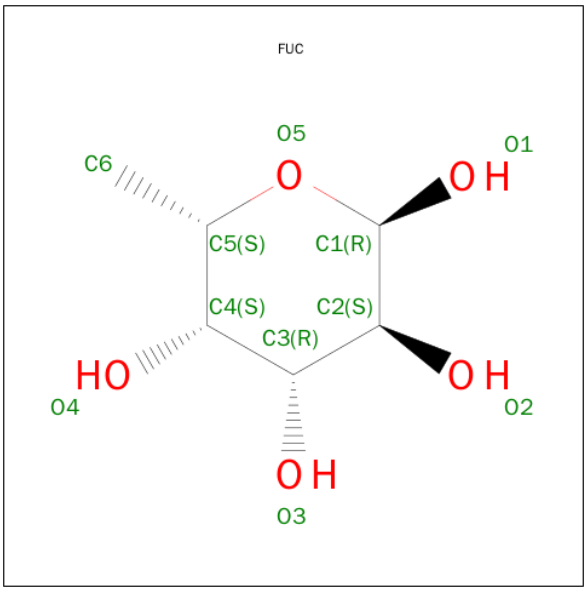
Chain	Residue	Modelled	Actual	Comment	Reference
B	347	ARG	GLN	engineered mutation	UNP P01857
B	399	VAL	ASP	engineered mutation	UNP P01857
B	405	THR	PHE	engineered mutation	UNP P01857

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



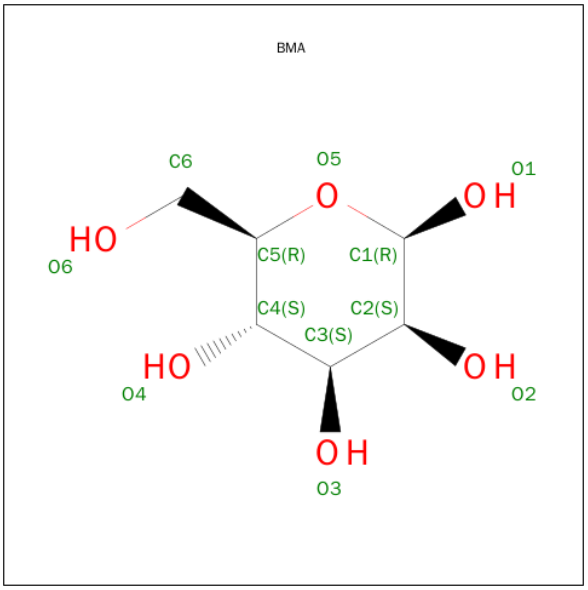
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



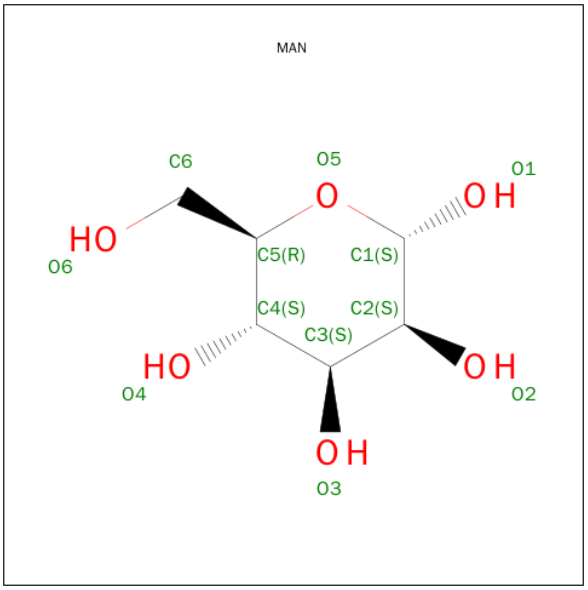
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is water.

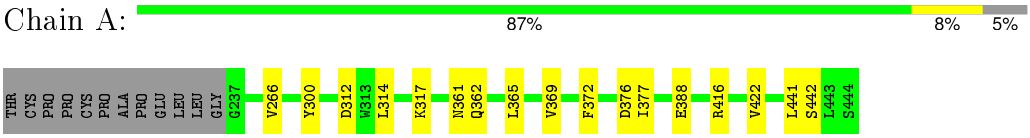
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	47	Total O 47 47	0	0
7	B	24	Total O 24 24	0	0

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.

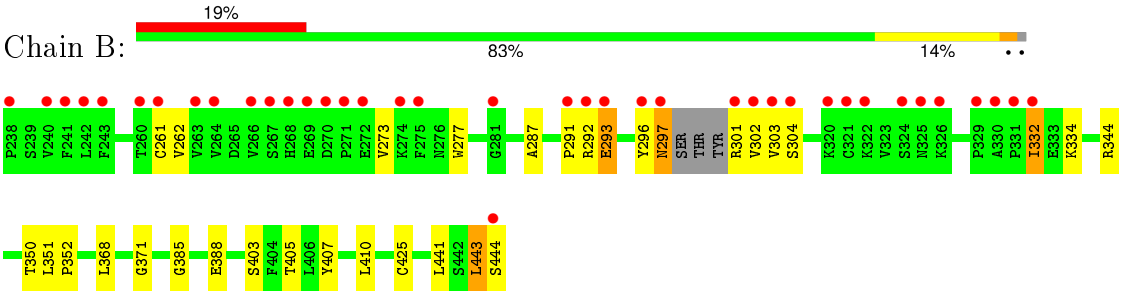
- Molecule 1: Ig gamma-1 chain C region

Chain A:



- Molecule 2: Ig gamma-1 chain C region

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	152.74Å 152.74Å 108.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.84 – 2.50 45.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.84-2.50) 95.5 (45.44-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.12 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.228 , 0.274 0.233 , 0.267	Depositor DCC
R_{free} test set	1900 reflections (7.52%)	DCC
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 26428 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3542	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 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.55	0/1717	0.68	0/2343
2	B	0.54	1/1645 (0.1%)	0.66	0/2241
All	All	0.54	1/3362 (0.0%)	0.67	0/4584

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	425	CYS	CB-SG	-5.19	1.73	1.81

There are no bond angle outliers.

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	1669	0	1619	10	0
2	B	1604	0	1578	22	0
3	A	56	0	48	11	0
3	B	56	0	49	4	0
4	A	10	0	10	6	0
4	B	10	0	10	4	0
5	A	11	0	7	0	0
5	B	11	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	22	0	17	4	0
6	B	22	0	18	0	0
7	A	47	0	0	0	0
7	B	24	0	0	1	0
All	All	3542	0	3364	47	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 7.

All (47) 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:296:TYR:O	2:B:297:ASN:HB3	1.53	1.09
3:A:502:NAG:H61	4:A:503:FUC:H5	1.36	1.07
6:A:507:MAN:C6	3:A:508:NAG:H83	1.98	0.93
6:A:507:MAN:O6	3:A:508:NAG:N2	2.00	0.93
6:A:507:MAN:H62	3:A:508:NAG:H83	1.53	0.89
3:B:502:NAG:H62	4:B:503:FUC:H5	1.54	0.87
3:A:502:NAG:H61	4:A:503:FUC:C5	2.07	0.84
2:B:292:ARG:C	2:B:293:GLU:HG2	2.02	0.79
2:B:291:PRO:O	2:B:293:GLU:HG2	1.87	0.74
2:B:371:GLY:H	2:B:405:THR:HG22	1.52	0.74
3:B:502:NAG:H62	4:B:503:FUC:C5	2.16	0.74
2:B:292:ARG:O	2:B:293:GLU:HG2	1.88	0.71
1:A:388:GLU:OE2	1:A:416:ARG:NH1	2.20	0.70
3:B:502:NAG:C6	4:B:503:FUC:H5	2.25	0.67
2:B:296:TYR:O	2:B:297:ASN:CB	2.38	0.65
3:A:502:NAG:C6	4:A:503:FUC:H5	2.22	0.63
2:B:350:THR:OG1	2:B:441:LEU:HB2	2.02	0.60
2:B:291:PRO:O	2:B:293:GLU:CG	2.49	0.59
3:B:502:NAG:C6	4:B:503:FUC:C5	2.85	0.54
1:A:369:VAL:HG12	1:A:372:PHE:CE1	2.43	0.54
2:B:262:VAL:HG22	2:B:303:VAL:HG22	1.91	0.52
2:B:344:ARG:NH1	2:B:403:SER:HB3	2.25	0.52
3:A:508:NAG:H3	3:A:508:NAG:O7	2.10	0.51
1:A:361:ASN:O	1:A:362:GLN:HG2	2.11	0.50
3:A:502:NAG:C6	4:A:503:FUC:C5	2.85	0.49
2:B:273:VAL:HG11	2:B:302:VAL:HG11	1.95	0.49
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.95	0.48
1:A:365:LEU:HB3	1:A:441:LEU:HD23	1.96	0.48
2:B:443:LEU:HD12	2:B:444:SER:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG12	1:A:372:PHE:CD1	2.51	0.46
2:B:261:CYS:HB2	2:B:277:TRP:CH2	2.51	0.44
2:B:334:LYS:HD3	2:B:334:LYS:HA	1.81	0.44
2:B:332:ILE:HA	2:B:332:ILE:HD12	1.82	0.44
1:A:422:VAL:HG22	1:A:442:SER:HB2	1.99	0.43
2:B:301:ARG:NH2	2:B:303:VAL:HG21	2.34	0.43
2:B:351:LEU:HA	2:B:352:PRO:HD3	1.84	0.43
2:B:388:GLU:HG2	2:B:410:LEU:HD11	2.00	0.43
6:A:507:MAN:C5	3:A:508:NAG:H83	2.48	0.43
2:B:368:LEU:HD13	2:B:407:TYR:CZ	2.54	0.42
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.78	0.42
3:A:502:NAG:H61	4:A:503:FUC:H3	2.03	0.41
3:A:502:NAG:O5	4:A:503:FUC:H5	2.21	0.41
2:B:287:ALA:HB1	2:B:304:SER:OG	2.21	0.41
2:B:261:CYS:HB2	2:B:277:TRP:CZ2	2.56	0.41
1:A:312:ASP:HB3	1:A:317:LYS:HD2	2.03	0.41
2:B:385:GLY:N	7:B:602:HOH:O	2.53	0.41
1:A:369:VAL:HG11	1:A:377:ILE:CD1	2.52	0.40

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	206/220 (94%)	202 (98%)	4 (2%)	0	100	100
2	B	200/207 (97%)	194 (97%)	6 (3%)	0	100	100
All	All	406/427 (95%)	396 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	194/204 (95%)	193 (100%)	1 (0%)	92 98
2	B	186/194 (96%)	182 (98%)	4 (2%)	60 84
All	All	380/398 (96%)	375 (99%)	5 (1%)	76 92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	ASP
2	B	293	GLU
2	B	297	ASN
2	B	332	ILE
2	B	443	LEU

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 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

16 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	501	3,5	14,14,15	1.46	2 (14%)	15,19,21	1.39	2 (13%)
3	NAG	A	502	1,3,4	14,14,15	1.72	3 (21%)	15,19,21	3.03	6 (40%)
4	FUC	A	503	3	10,10,11	1.96	5 (50%)	14,14,16	1.79	5 (35%)
5	BMA	A	504	3,6	11,11,12	1.87	4 (36%)	14,15,17	1.88	5 (35%)
6	MAN	A	505	3,5	11,11,12	1.87	5 (45%)	14,15,17	1.75	2 (14%)
3	NAG	A	506	6	14,14,15	1.38	3 (21%)	15,19,21	1.42	3 (20%)
6	MAN	A	507	3,5	11,11,12	1.13	0	14,15,17	3.81	6 (42%)
3	NAG	A	508	6	14,14,15	0.50	0	15,19,21	1.61	3 (20%)
3	NAG	B	501	3,5	14,14,15	0.54	0	15,19,21	0.86	0
3	NAG	B	502	3,2,4	14,14,15	0.91	0	15,19,21	1.01	2 (13%)
4	FUC	B	503	3	10,10,11	1.19	1 (10%)	14,14,16	1.62	6 (42%)
5	BMA	B	504	3,6	11,11,12	0.98	1 (9%)	14,15,17	1.53	3 (21%)
6	MAN	B	505	3,5	11,11,12	0.80	0	14,15,17	1.49	3 (21%)
3	NAG	B	506	6	14,14,15	0.83	0	15,19,21	1.25	2 (13%)
6	MAN	B	507	3,5	11,11,12	0.77	0	14,15,17	1.38	2 (14%)
3	NAG	B	508	6	14,14,15	0.70	0	15,19,21	0.96	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	501	3,5	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	503	3	-	0/0/17/20	0/1/1/1
5	BMA	A	504	3,6	-	0/2/19/22	0/1/1/1
6	MAN	A	505	3,5	-	0/2/19/22	0/1/1/1
3	NAG	A	506	6	-	0/6/23/26	0/1/1/1
6	MAN	A	507	3,5	-	0/2/19/22	0/1/1/1
3	NAG	A	508	6	-	0/6/23/26	0/1/1/1
3	NAG	B	501	3,5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	502	3,2,4	-	0/6/23/26	0/1/1/1
4	FUC	B	503	3	-	0/0/17/20	0/1/1/1
5	BMA	B	504	3,6	-	0/2/19/22	0/1/1/1
6	MAN	B	505	3,5	-	0/2/19/22	0/1/1/1
3	NAG	B	506	6	-	0/6/23/26	0/1/1/1
6	MAN	B	507	3,5	-	0/2/19/22	0/1/1/1
3	NAG	B	508	6	-	0/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	C1-C2	-3.43	1.47	1.52
4	A	503	FUC	C4-C5	-3.27	1.46	1.52
3	A	501	NAG	C1-C2	-3.15	1.48	1.52
3	A	501	NAG	O5-C1	-2.87	1.38	1.43
5	A	504	BMA	O4-C4	-2.87	1.36	1.43
6	A	505	MAN	C4-C5	-2.85	1.47	1.53
4	A	503	FUC	O5-C1	-2.80	1.39	1.43
3	A	506	NAG	O4-C4	-2.76	1.36	1.43
5	A	504	BMA	O2-C2	-2.69	1.37	1.43
6	A	505	MAN	O3-C3	-2.66	1.36	1.43
6	A	505	MAN	O2-C2	-2.66	1.37	1.43
4	B	503	FUC	C4-C5	-2.65	1.47	1.52
4	A	503	FUC	O2-C2	-2.63	1.37	1.43
5	A	504	BMA	C2-C3	-2.60	1.48	1.52
3	A	502	NAG	C3-C2	-2.60	1.46	1.52
3	A	506	NAG	O3-C3	-2.55	1.36	1.43
5	A	504	BMA	C4-C5	-2.40	1.48	1.53
4	A	503	FUC	O4-C4	-2.33	1.37	1.43
5	B	504	BMA	C2-C3	-2.33	1.49	1.52
4	A	503	FUC	O3-C3	-2.30	1.37	1.43
3	A	502	NAG	O4-C4	-2.30	1.37	1.43
6	A	505	MAN	O5-C1	-2.19	1.40	1.43
6	A	505	MAN	C2-C3	-2.06	1.49	1.52
3	A	506	NAG	C4-C5	-2.03	1.48	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	NAG	O5-C5-C6	-5.22	96.05	107.35
3	A	502	NAG	C6-C5-C4	-4.14	102.81	113.02
5	A	504	BMA	O3-C3-C2	-4.01	102.75	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	507	MAN	O5-C1-C2	-3.87	104.57	110.86
6	B	505	MAN	C3-C4-C5	-3.69	103.77	110.20
3	A	508	NAG	C1-O5-C5	-3.40	107.94	112.25
5	B	504	BMA	C1-C2-C3	-3.24	105.71	109.54
3	A	506	NAG	C2-N2-C7	-3.18	118.95	123.04
3	B	506	NAG	C2-N2-C7	-2.96	119.23	123.04
5	A	504	BMA	O2-C2-C3	-2.87	104.35	110.12
5	B	504	BMA	O5-C1-C2	-2.75	106.40	110.86
3	A	502	NAG	C3-C2-N2	-2.71	104.06	110.56
6	A	507	MAN	C6-C5-C4	-2.64	106.50	113.02
4	B	503	FUC	C3-C4-C5	-2.61	105.32	109.72
6	B	507	MAN	O5-C5-C6	-2.54	101.84	107.35
3	A	501	NAG	C6-C5-C4	-2.54	106.75	113.02
6	A	505	MAN	O3-C3-C4	-2.31	105.14	110.34
4	A	503	FUC	O5-C5-C4	-2.29	105.55	109.53
3	A	508	NAG	C6-C5-C4	-2.26	107.43	113.02
5	A	504	BMA	O5-C1-C2	-2.24	107.23	110.86
5	A	504	BMA	C3-C4-C5	-2.21	106.35	110.20
4	B	503	FUC	C6-C5-C4	-2.20	108.75	113.08
4	A	503	FUC	O3-C3-C2	-2.20	106.02	110.00
4	A	503	FUC	C6-C5-C4	-2.20	108.75	113.08
3	A	506	NAG	C3-C4-C5	-2.20	106.36	110.20
3	A	502	NAG	O3-C3-C2	-2.18	104.80	109.11
3	A	502	NAG	C2-N2-C7	-2.11	120.33	123.04
4	B	503	FUC	C1-C2-C3	-2.10	107.05	109.54
4	B	503	FUC	O2-C2-C1	-2.09	105.02	109.21
4	B	503	FUC	O5-C5-C4	-2.08	105.93	109.53
6	B	507	MAN	O2-C2-C3	-2.07	105.96	110.12
4	B	503	FUC	O4-C4-C5	-2.06	105.00	109.84
3	B	502	NAG	C3-C4-C5	-2.04	106.63	110.20
6	B	505	MAN	C1-O5-C5	-2.01	109.69	112.25
3	B	502	NAG	C2-N2-C7	-2.01	120.46	123.04
4	A	503	FUC	C1-C2-C3	2.21	112.16	109.54
5	B	504	BMA	C1-O5-C5	2.32	115.20	112.25
3	B	506	NAG	C1-O5-C5	2.43	115.33	112.25
3	A	508	NAG	O5-C5-C6	2.65	113.08	107.35
3	A	506	NAG	C1-O5-C5	2.66	115.63	112.25
5	A	504	BMA	C1-O5-C5	2.71	115.68	112.25
6	A	507	MAN	C2-C3-C4	2.79	115.78	111.04
6	B	505	MAN	O5-C5-C6	2.87	113.57	107.35
6	A	507	MAN	C3-C4-C5	2.95	115.35	110.20
3	A	501	NAG	C1-O5-C5	3.29	116.43	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	505	MAN	C1-O5-C5	3.48	116.67	112.25
4	A	503	FUC	C1-O5-C5	3.84	118.30	112.38
6	A	507	MAN	O5-C5-C6	7.17	122.86	107.35
3	A	502	NAG	C1-O5-C5	8.49	123.03	112.25
6	A	507	MAN	C1-O5-C5	10.03	124.97	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	6	0
4	A	503	FUC	6	0
6	A	507	MAN	4	0
3	A	508	NAG	5	0
3	B	502	NAG	4	0
4	B	503	FUC	4	0

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, 95^{th} 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	208/220 (94%)	0.20	0 100 100	39, 52, 80, 95	0
2	B	204/207 (98%)	1.16	39 (19%) 2 1	25, 69, 118, 135	0
All	All	412/427 (96%)	0.67	39 (9%) 10 11	25, 58, 110, 135	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	VAL	15.9
2	B	269	GLU	10.1
2	B	297	ASN	7.8
2	B	329	PRO	6.6
2	B	263	VAL	6.4
2	B	270	ASP	6.3
2	B	264	VAL	6.1
2	B	266	VAL	6.0
2	B	330	ALA	5.9
2	B	324	SER	5.8
2	B	267	SER	5.5
2	B	271	PRO	5.5
2	B	331	PRO	5.5
2	B	241	PHE	5.1
2	B	291	PRO	4.5
2	B	304	SER	4.3
2	B	272	GLU	4.2
2	B	243	PHE	4.1
2	B	296	TYR	4.0
2	B	332	ILE	4.0
2	B	281	GLY	3.9
2	B	240	VAL	3.9
2	B	326	LYS	3.7
2	B	292	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	268	HIS	3.4
2	B	322	LYS	3.3
2	B	274	LYS	3.1
2	B	325	ASN	2.9
2	B	238	PRO	2.9
2	B	303	VAL	2.8
2	B	301	ARG	2.7
2	B	444	SER	2.5
2	B	293	GLU	2.4
2	B	275	PHE	2.4
2	B	242	LEU	2.4
2	B	260	THR	2.3
2	B	321	CYS	2.3
2	B	320	LYS	2.3
2	B	261	CYS	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, 95^{th} 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
3	NAG	B	506	14/15	0.74	0.29	0.33	84,93,96,98	0
3	NAG	B	501	14/15	0.70	0.36	-0.13	93,102,106,107	0
3	NAG	A	506	14/15	0.90	0.14	-2.48	56,61,69,69	0
3	NAG	A	502	14/15	0.94	0.15	-	50,55,57,58	0
5	BMA	A	504	11/12	0.95	0.14	-	52,58,64,69	0
4	FUC	A	503	10/11	0.93	0.15	-	53,57,60,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MAN	A	507	11/12	0.85	0.19	-	71,77,82,85	0
6	MAN	B	505	11/12	0.76	0.17	-	90,98,100,103	0
6	MAN	B	507	11/12	0.79	0.23	-	87,95,99,102	0
3	NAG	B	502	14/15	0.73	0.41	-	100,106,107,108	0
3	NAG	B	508	14/15	0.39	0.41	-	90,99,103,107	0
4	FUC	B	503	10/11	0.84	0.16	-	96,100,102,103	0
3	NAG	A	508	14/15	0.79	0.23	-	77,79,88,89	0
5	BMA	B	504	11/12	0.72	0.17	-	89,98,102,104	0
3	NAG	A	501	14/15	0.94	0.14	-	50,54,60,62	0
6	MAN	A	505	11/12	0.95	0.15	-	60,64,68,80	0

6.5 Other polymers (i)

There are no such residues in this entry.