Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:16 PM GMT

PDB ID	:	4X99
Title	:	Immunoglobulin Fc heterodimers 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:

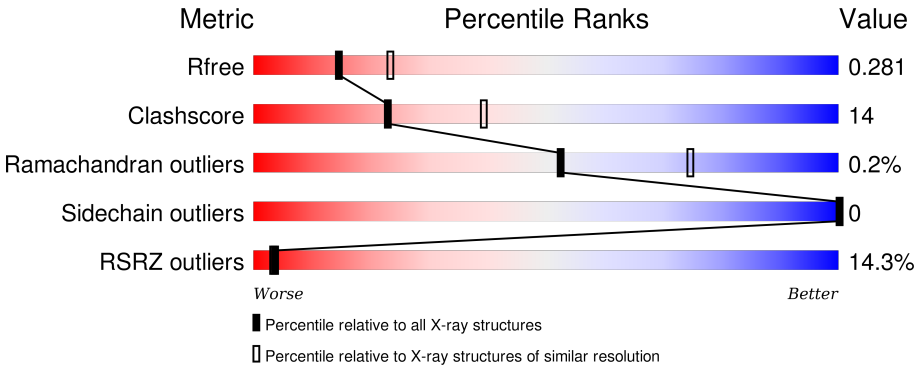
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	223	% 72% 21% 7%
2	B	223	25% 68% 23% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3502 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
			1663	1057	279	320	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	CYS	TYR	engineered mutation	UNP P01857
A	360	GLU	LYS	engineered mutation	UNP P01857
A	409	TRP	LYS	engineered mutation	UNP P01857

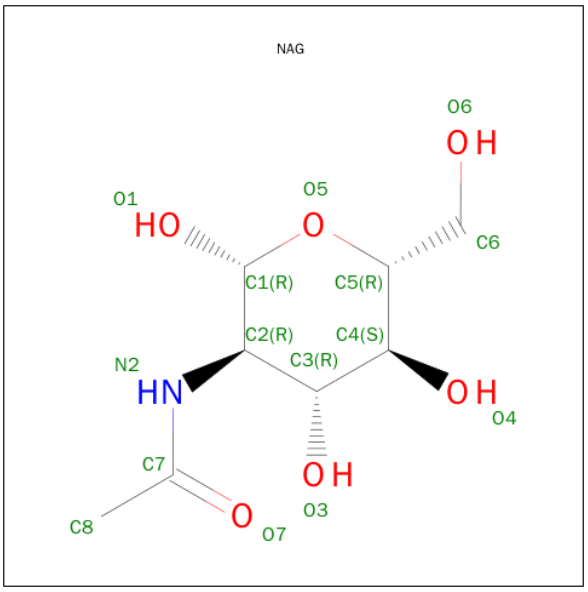
- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	205	Total	C	N	O	S	0	0	0
			1600	1018	273	302	7			

There are 4 discrepancies between the modelled and reference sequences:

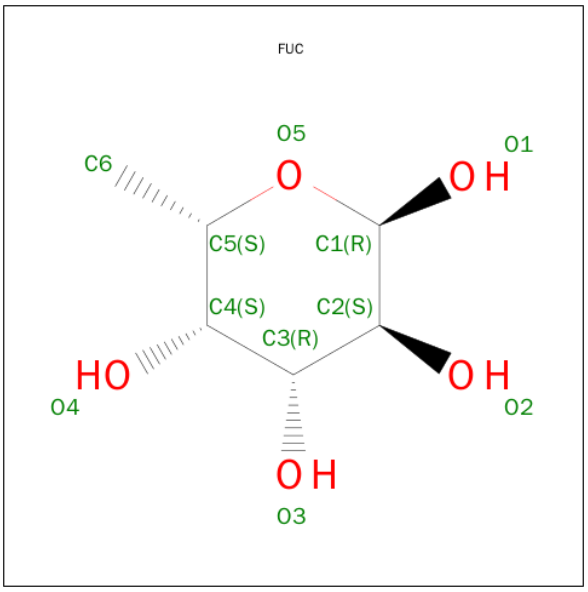
Chain	Residue	Modelled	Actual	Comment	Reference
B	347	ARG	GLN	engineered mutation	UNP P01857
B	354	CYS	SER	engineered mutation	UNP P01857
B	399	VAL	ASP	engineered mutation	UNP P01857
B	405	THR	PHE	engineered mutation	UNP P01857

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



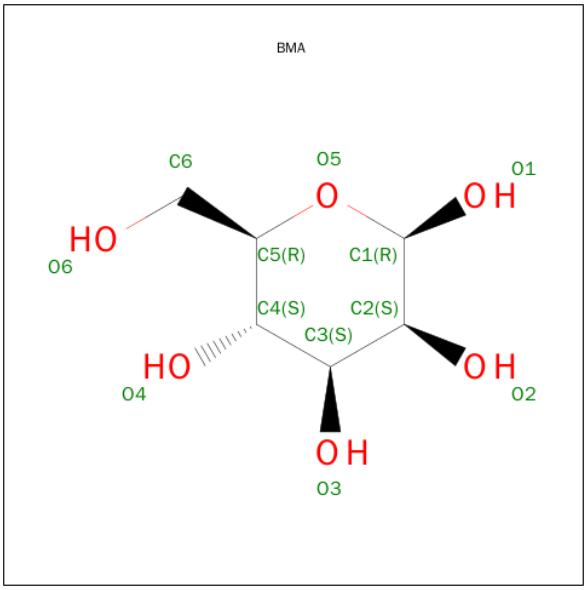
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

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



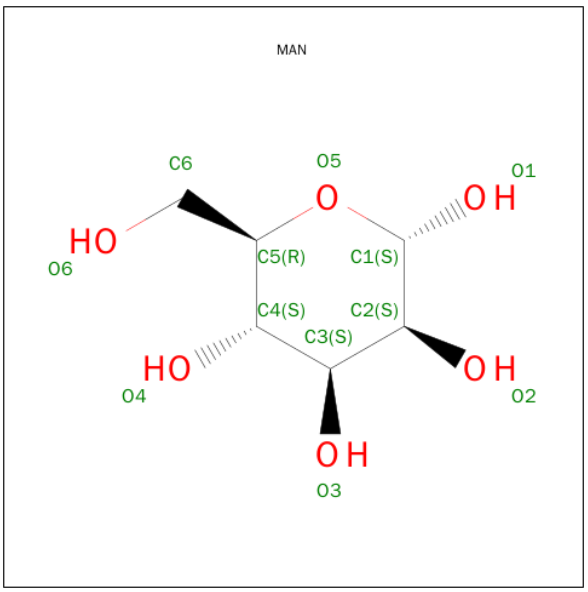
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0

- 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.

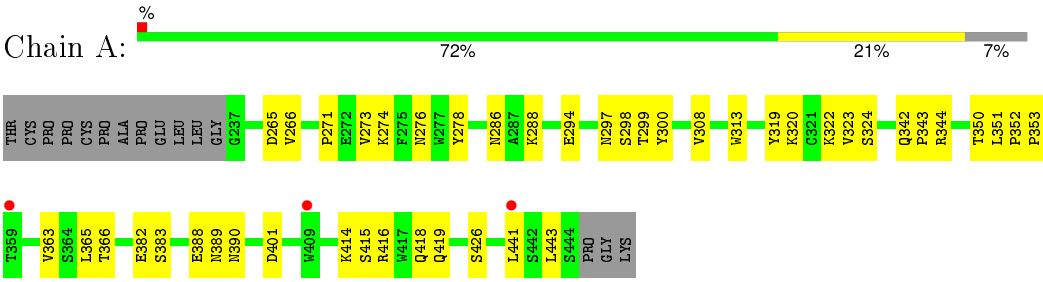
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	30	Total O 30 30	0	0
7	B	11	Total O 11 11	0	0

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.

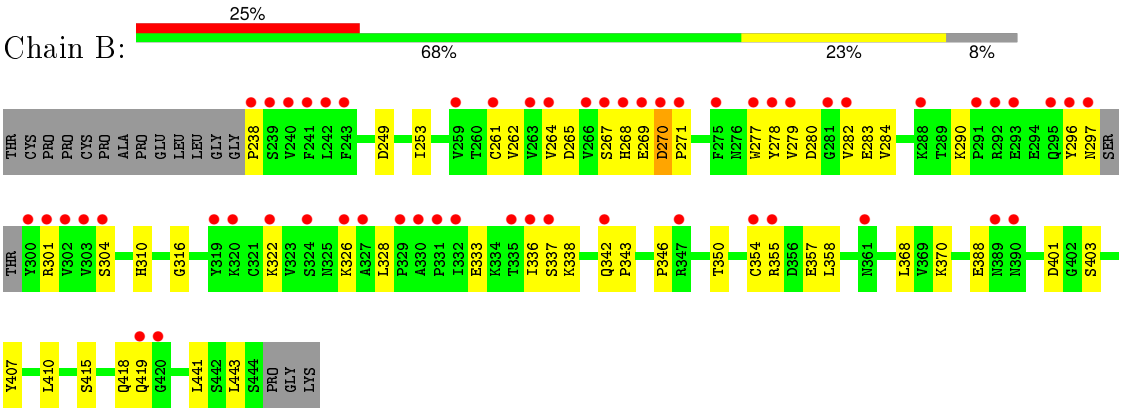
- Molecule 1: Ig gamma-1 chain C region

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	152.77Å 152.77Å 109.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.63 – 2.50 45.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.63-2.50) 93.4 (45.52-2.50)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.09 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.248 , 0.283 0.255 , 0.281	Depositor DCC
R_{free} test set	1869 reflections (7.50%)	DCC
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 26577 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3502	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.63	0/1710	0.70	0/2333
2	B	0.63	0/1642	0.78	3/2241 (0.1%)
All	All	0.63	0/3352	0.74	3/4574 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	268	HIS	CB-CA-C	-10.77	88.87	110.40
2	B	290	LYS	C-N-CD	5.86	140.70	128.40
2	B	270	ASP	C-N-CD	5.59	140.15	128.40

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	1663	0	1614	30	0
2	B	1600	0	1555	47	0
3	A	56	0	48	7	0
3	B	56	0	49	10	0
4	A	10	0	10	0	0
4	B	10	0	10	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	11	0	8	0	0
5	B	11	0	8	0	0
6	A	22	0	17	5	0
6	B	22	0	18	3	0
7	A	30	0	0	1	0
7	B	11	0	0	1	0
All	All	3502	0	3337	92	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 14.

All (92) 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:278:TYR:CE1	2:B:283:GLU:HB2	1.30	1.56
2:B:278:TYR:CE1	2:B:283:GLU:CB	2.23	1.20
2:B:267:SER:HB2	2:B:271:PRO:HG2	1.33	1.05
1:A:265:ASP:OD1	3:A:502:NAG:O7	1.83	0.96
2:B:278:TYR:HE1	2:B:283:GLU:HB2	1.28	0.94
6:A:507:MAN:H4	3:A:508:NAG:H83	1.50	0.94
2:B:278:TYR:CD1	2:B:283:GLU:CA	2.55	0.90
2:B:278:TYR:CZ	2:B:283:GLU:HB2	2.06	0.88
2:B:267:SER:O	2:B:271:PRO:HD2	1.75	0.87
2:B:278:TYR:CD1	2:B:283:GLU:HB2	2.09	0.86
3:B:502:NAG:H62	4:B:503:FUC:H5	1.59	0.83
1:A:350:THR:HB	1:A:441:LEU:HD13	1.61	0.81
1:A:294:GLU:OE2	1:A:298:SER:HA	1.84	0.77
2:B:269:GLU:C	2:B:271:PRO:HD3	2.06	0.76
2:B:278:TYR:CD1	2:B:283:GLU:N	2.55	0.75
2:B:253:ILE:H	2:B:253:ILE:HD12	1.52	0.74
2:B:278:TYR:HD1	2:B:282:VAL:C	1.90	0.74
6:A:507:MAN:O2	3:A:508:NAG:H83	1.87	0.73
2:B:278:TYR:CD1	2:B:283:GLU:HA	2.21	0.73
2:B:278:TYR:HD1	2:B:283:GLU:N	1.87	0.72
3:B:502:NAG:H62	4:B:503:FUC:C5	2.21	0.70
1:A:418:GLN:HA	1:A:443:LEU:HD22	1.75	0.69
2:B:278:TYR:CD1	2:B:283:GLU:CB	2.69	0.69
3:B:502:NAG:C6	4:B:503:FUC:H5	2.23	0.68
6:A:507:MAN:H4	3:A:508:NAG:C8	2.22	0.68
6:B:507:MAN:H4	3:B:508:NAG:H4	1.78	0.66
1:A:415:SER:O	1:A:419:GLN:HG3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:507:MAN:O3	3:B:508:NAG:H61	1.96	0.65
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.79	0.65
1:A:353:PRO:HB3	1:A:363:VAL:HG13	1.79	0.64
1:A:355:ARG:HA	1:A:358:LEU:HD12	1.79	0.64
2:B:265:ASP:OD1	3:B:502:NAG:H83	1.98	0.63
2:B:279:VAL:O	2:B:280:ASP:HB2	2.01	0.61
1:A:308:VAL:HG11	1:A:313:TRP:HB2	1.83	0.60
2:B:354:CYS:SG	2:B:357:GLU:HB2	2.42	0.60
6:A:507:MAN:C4	3:A:508:NAG:H83	2.30	0.59
2:B:279:VAL:O	2:B:279:VAL:HG23	2.02	0.58
2:B:262:VAL:CG1	2:B:301:ARG:HH21	2.17	0.57
1:A:308:VAL:HG22	1:A:319:TYR:CE1	2.40	0.57
2:B:267:SER:HB2	2:B:271:PRO:CG	2.21	0.57
2:B:261:CYS:HB2	2:B:277:TRP:CH2	2.41	0.55
1:A:350:THR:CB	1:A:441:LEU:HD13	2.35	0.54
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.88	0.54
2:B:418:GLN:HA	2:B:443:LEU:HD22	1.90	0.54
2:B:322:LYS:HG3	2:B:333:GLU:HG2	1.90	0.54
1:A:388:GLU:OE2	1:A:416:ARG:NH1	2.40	0.54
6:A:507:MAN:O2	3:A:508:NAG:O6	2.27	0.53
3:B:506:NAG:O7	3:B:506:NAG:O3	2.26	0.53
3:B:508:NAG:O7	3:B:508:NAG:H5	2.08	0.53
2:B:316:GLY:O	2:B:337:SER:HB2	2.10	0.51
3:B:502:NAG:C6	4:B:503:FUC:C5	2.85	0.51
2:B:238:PRO:HB2	2:B:328:LEU:HD11	1.93	0.50
2:B:278:TYR:CE1	2:B:283:GLU:CA	2.84	0.50
1:A:297:ASN:OD1	1:A:299:THR:OG1	2.27	0.50
2:B:338:LYS:HE3	7:B:606:HOH:O	2.13	0.48
2:B:238:PRO:HA	2:B:264:VAL:O	2.14	0.48
1:A:351:LEU:HB2	1:A:366:THR:HB	1.95	0.48
2:B:262:VAL:HG11	2:B:301:ARG:HH21	1.77	0.48
2:B:355:ARG:HA	2:B:358:LEU:HD12	1.96	0.48
6:B:505:MAN:O3	3:B:506:NAG:N2	2.48	0.47
1:A:308:VAL:CG1	1:A:313:TRP:HB2	2.44	0.47
2:B:388:GLU:HG2	2:B:410:LEU:HD11	1.95	0.47
1:A:271:PRO:HD2	7:A:628:HOH:O	2.15	0.47
2:B:253:ILE:CD1	2:B:253:ILE:H	2.24	0.47
2:B:401:ASP:HB3	2:B:403:SER:H	1.80	0.47
1:A:358:LEU:O	1:A:414:LYS:NZ	2.23	0.47
2:B:346:PRO:HA	2:B:370:LYS:O	2.17	0.45
2:B:350:THR:OG1	2:B:441:LEU:HD22	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:OE1	1:A:426:SER:OG	2.35	0.44
2:B:262:VAL:HG13	2:B:301:ARG:HH21	1.82	0.44
1:A:286:ASN:O	1:A:288:LYS:NZ	2.37	0.44
2:B:368:LEU:HD13	2:B:407:TYR:CZ	2.53	0.44
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.91	0.44
1:A:344:ARG:HH12	1:A:401:ASP:CG	2.21	0.43
2:B:296:TYR:O	2:B:297:ASN:C	2.56	0.43
1:A:276:ASN:HB2	1:A:322:LYS:HB3	2.01	0.43
2:B:283:GLU:HG2	2:B:284:VAL:N	2.34	0.43
1:A:353:PRO:HD3	1:A:365:LEU:HD23	2.01	0.43
1:A:383:SER:HB2	1:A:388:GLU:OE1	2.19	0.43
2:B:415:SER:O	2:B:419:GLN:HG3	2.19	0.42
1:A:308:VAL:HG22	1:A:319:TYR:CZ	2.54	0.42
2:B:337:SER:O	2:B:338:LYS:C	2.57	0.42
1:A:278:TYR:CD1	1:A:320:LYS:HD2	2.55	0.42
2:B:336:ILE:O	2:B:337:SER:HB3	2.20	0.41
2:B:249:ASP:O	2:B:310:HIS:HE1	2.03	0.41
1:A:389:ASN:O	1:A:390:ASN:HB2	2.20	0.41
1:A:351:LEU:HA	1:A:352:PRO:HD2	1.83	0.41
1:A:273:VAL:HG13	1:A:323:VAL:HG13	2.03	0.41
2:B:342:GLN:OE1	2:B:343:PRO:HD2	2.20	0.41
2:B:277:TRP:HZ2	2:B:304:SER:HB3	1.86	0.40
2:B:326:LYS:C	2:B:328:LEU:H	2.24	0.40
3:A:502:NAG:C3	3:A:502:NAG:O7	2.70	0.40

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	206/223 (92%)	200 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	201/223 (90%)	188 (94%)	12 (6%)	1 (0%)	34 55
All	All	407/446 (91%)	388 (95%)	18 (4%)	1 (0%)	52 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	ASP

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	194/206 (94%)	194 (100%)	0	100 100
2	B	183/206 (89%)	183 (100%)	0	100 100
All	All	377/412 (92%)	377 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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

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)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1.30	2 (14%)	15,19,21	1.16	2 (13%)
3	NAG	A	502	1,3,4	14,14,15	1.33	1 (7%)	15,19,21	1.86	4 (26%)
4	FUC	A	503	3	10,10,11	1.81	5 (50%)	14,14,16	1.27	1 (7%)
5	BMA	A	504	3,6	11,11,12	1.56	2 (18%)	14,15,17	1.64	3 (21%)
6	MAN	A	505	3,5	11,11,12	1.98	4 (36%)	14,15,17	2.26	4 (28%)
3	NAG	A	506	6	14,14,15	1.42	3 (21%)	15,19,21	1.21	1 (6%)
6	MAN	A	507	3,5	11,11,12	1.39	0	14,15,17	2.05	6 (42%)
3	NAG	A	508	6	14,14,15	0.94	1 (7%)	15,19,21	1.66	3 (20%)
3	NAG	B	501	3,5	14,14,15	0.95	1 (7%)	15,19,21	1.14	1 (6%)
3	NAG	B	502	3,2,4	14,14,15	0.78	0	15,19,21	0.95	1 (6%)
4	FUC	B	503	3	10,10,11	1.18	1 (10%)	14,14,16	1.53	5 (35%)
5	BMA	B	504	3,6	11,11,12	1.23	1 (9%)	14,15,17	2.37	5 (35%)
6	MAN	B	505	3,5	11,11,12	1.00	1 (9%)	14,15,17	1.81	3 (21%)
3	NAG	B	506	6	14,14,15	1.01	1 (7%)	15,19,21	1.43	2 (13%)
6	MAN	B	507	3,5	11,11,12	0.76	0	14,15,17	1.78	3 (21%)
3	NAG	B	508	6	14,14,15	1.36	3 (21%)	15,19,21	1.92	3 (20%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	505	MAN	O3-C3	-3.43	1.34	1.43
3	A	502	NAG	C1-C2	-3.36	1.47	1.52
4	A	503	FUC	O5-C1	-3.14	1.38	1.43
6	A	505	MAN	O5-C1	-3.06	1.38	1.43
3	A	506	NAG	O4-C4	-3.01	1.35	1.43
4	B	503	FUC	C4-C5	-2.92	1.46	1.52
6	A	505	MAN	C2-C3	-2.81	1.48	1.52
3	B	501	NAG	C1-C2	-2.70	1.48	1.52
3	A	501	NAG	O5-C1	-2.70	1.39	1.43
4	A	503	FUC	C4-C5	-2.55	1.47	1.52
5	B	504	BMA	C4-C3	-2.50	1.45	1.52
5	A	504	BMA	O2-C2	-2.49	1.37	1.43
5	A	504	BMA	O3-C3	-2.42	1.37	1.43
3	A	506	NAG	C4-C5	-2.35	1.48	1.53
3	B	506	NAG	C1-C2	-2.25	1.49	1.52
6	A	505	MAN	C4-C5	-2.24	1.48	1.53
4	A	503	FUC	O4-C4	-2.23	1.37	1.43
3	A	501	NAG	C1-C2	-2.17	1.49	1.52
3	A	506	NAG	C1-C2	-2.12	1.49	1.52
4	A	503	FUC	O3-C3	-2.10	1.37	1.43
3	A	508	NAG	C3-C2	-2.03	1.47	1.52
4	A	503	FUC	O2-C2	-2.02	1.38	1.43
6	B	505	MAN	O5-C1	2.12	1.47	1.43
3	B	508	NAG	C1-C2	2.17	1.55	1.52
3	B	508	NAG	C4-C5	2.35	1.58	1.53
3	B	508	NAG	C3-C2	2.76	1.58	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	504	BMA	C1-C2-C3	-5.09	103.52	109.54
6	B	507	MAN	O5-C5-C6	-3.99	98.70	107.35
6	A	507	MAN	O5-C5-C6	-3.06	100.73	107.35
3	A	502	NAG	C4-C3-C2	-3.03	106.52	111.23
6	B	507	MAN	O2-C2-C1	-3.00	103.19	109.21
3	B	501	NAG	C2-N2-C7	-2.88	119.34	123.04
3	B	506	NAG	C2-N2-C7	-2.85	119.38	123.04
6	A	507	MAN	C3-C4-C5	-2.84	105.25	110.20
6	A	505	MAN	O5-C5-C6	-2.83	101.23	107.35
6	A	507	MAN	O2-C2-C3	-2.81	104.46	110.12
3	A	506	NAG	C2-N2-C7	-2.77	119.48	123.04
5	A	504	BMA	O5-C1-C2	-2.66	106.55	110.86
4	B	503	FUC	C1-C2-C3	-2.57	106.50	109.54
3	B	508	NAG	C3-C4-C5	-2.54	105.77	110.20
6	B	505	MAN	C1-O5-C5	-2.39	109.22	112.25
5	A	504	BMA	O2-C2-C1	-2.35	104.49	109.21
4	B	503	FUC	C6-C5-C4	-2.34	108.47	113.08
5	B	504	BMA	C6-C5-C4	-2.31	107.32	113.02
5	B	504	BMA	O4-C4-C3	-2.27	105.23	110.34
6	A	505	MAN	C6-C5-C4	-2.23	107.51	113.02
3	A	508	NAG	C4-C3-C2	-2.22	107.78	111.23
4	B	503	FUC	O5-C1-C2	-2.20	107.29	110.86
6	A	505	MAN	C1-C2-C3	-2.18	106.96	109.54
4	B	503	FUC	C3-C4-C5	-2.17	106.05	109.72
6	A	507	MAN	O4-C4-C3	-2.15	105.49	110.34
3	A	502	NAG	C3-C4-C5	-2.09	106.56	110.20
4	B	503	FUC	O4-C4-C5	-2.07	104.98	109.84
4	A	503	FUC	O5-C5-C4	-2.02	106.02	109.53
3	B	502	NAG	C3-C2-N2	-2.01	105.74	110.56
3	A	501	NAG	C6-C5-C4	-2.01	108.06	113.02
6	A	507	MAN	O5-C1-C2	-2.01	107.60	110.86
5	B	504	BMA	O3-C3-C4	-2.00	105.83	110.34
3	B	508	NAG	C2-N2-C7	2.14	125.79	123.04
3	A	501	NAG	C1-O5-C5	2.26	115.11	112.25
3	A	508	NAG	C3-C4-C5	2.27	114.16	110.20
6	B	507	MAN	C1-O5-C5	2.29	115.16	112.25
3	A	502	NAG	C3-C2-N2	2.62	116.83	110.56
6	B	505	MAN	O5-C5-C6	3.03	113.90	107.35
5	A	504	BMA	C1-O5-C5	3.33	116.48	112.25
6	A	507	MAN	C1-O5-C5	3.45	116.62	112.25
6	B	505	MAN	O2-C2-C1	3.75	116.72	109.21
3	B	506	NAG	C1-O5-C5	4.28	117.67	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	508	NAG	C1-O5-C5	4.97	118.56	112.25
3	A	502	NAG	C1-O5-C5	5.08	118.70	112.25
3	B	508	NAG	C1-O5-C5	5.45	119.17	112.25
5	B	504	BMA	C1-O5-C5	5.63	119.39	112.25
6	A	505	MAN	C1-O5-C5	6.35	120.30	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	2	0
6	A	507	MAN	5	0
3	A	508	NAG	5	0
3	B	502	NAG	5	0
4	B	503	FUC	4	0
6	B	505	MAN	1	0
3	B	506	NAG	2	0
6	B	507	MAN	2	0
3	B	508	NAG	3	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	208/223 (93%)	0.50	3 (1%) 78 80	39, 52, 82, 95	0
2	B	205/223 (91%)	1.46	56 (27%) 1 1	37, 71, 109, 132	0
All	All	413/446 (92%)	0.97	59 (14%) 4 3	37, 59, 104, 132	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	VAL	21.9
2	B	270	ASP	10.5
2	B	241	PHE	7.5
2	B	263	VAL	7.2
2	B	266	VAL	5.6
2	B	296	TYR	5.6
2	B	242	LEU	5.4
2	B	268	HIS	5.1
2	B	264	VAL	5.0
2	B	240	VAL	5.0
2	B	291	PRO	4.9
2	B	301	ARG	4.7
2	B	297	ASN	4.7
2	B	331	PRO	4.6
2	B	326	LYS	4.6
2	B	303	VAL	4.5
2	B	332	ILE	4.5
2	B	281	GLY	4.3
2	B	330	ALA	4.2
2	B	267	SER	4.0
2	B	335	THR	3.9
2	B	336	ILE	3.9
2	B	319	TYR	3.7
2	B	278	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	271	PRO	3.7
2	B	324	SER	3.6
2	B	304	SER	3.6
2	B	347	ARG	3.5
2	B	239	SER	3.5
2	B	275	PHE	3.4
2	B	277	TRP	3.3
2	B	269	GLU	3.1
2	B	420	GLY	3.1
2	B	238	PRO	3.0
2	B	419	GLN	3.0
2	B	292	ARG	2.8
2	B	390	ASN	2.8
2	B	293	GLU	2.8
1	A	359	THR	2.7
2	B	329	PRO	2.7
2	B	243	PHE	2.7
2	B	327	ALA	2.5
2	B	322	LYS	2.4
2	B	295	GLN	2.3
2	B	361	ASN	2.3
2	B	279	VAL	2.2
2	B	389	ASN	2.2
2	B	320	LYS	2.2
2	B	288	LYS	2.1
2	B	337	SER	2.1
2	B	261	CYS	2.1
2	B	300	TYR	2.1
2	B	259	VAL	2.1
2	B	282	VAL	2.1
2	B	355	ARG	2.1
2	B	342	GLN	2.0
1	A	409	TRP	2.0
2	B	354	CYS	2.0
1	A	441	LEU	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)

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	A	502	14/15	0.89	0.16	-0.35	44,49,54,54	0
3	NAG	A	506	14/15	0.94	0.17	-2.81	53,59,66,70	0
3	NAG	A	501	14/15	0.91	0.11	-	43,51,57,59	0
6	MAN	B	505	11/12	0.62	0.29	-	94,101,106,108	0
3	NAG	B	508	14/15	0.44	0.38	-	97,105,112,113	0
3	NAG	A	508	14/15	0.82	0.15	-	74,83,91,91	0
6	MAN	B	507	11/12	0.70	0.23	-	92,100,105,106	0
6	MAN	A	507	11/12	0.89	0.17	-	73,79,87,87	0
3	NAG	B	502	14/15	0.72	0.40	-	95,109,112,113	0
4	FUC	A	503	10/11	0.94	0.13	-	48,52,56,59	0
3	NAG	B	506	14/15	0.65	0.32	-	96,101,106,107	0
3	NAG	B	501	14/15	0.54	0.46	-	103,106,111,112	0
5	BMA	B	504	11/12	0.76	0.20	-	97,104,109,110	0
4	FUC	B	503	10/11	0.72	0.24	-	97,104,108,109	0
5	BMA	A	504	11/12	0.93	0.14	-	50,56,62,71	0
6	MAN	A	505	11/12	0.96	0.15	-	56,58,64,75	0

6.5 Other polymers (i)

There are no such residues in this entry.