Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:57 PM GMT

PDB ID	:	1I1C
Title	:	NON-FCRN BINDING FC FRAGMENT OF RAT IGG2A
Authors	:	Martin, W.L.; West Jr., A.P.; Gan, L.; Bjorkman, P.J.
Deposited on	:	2001-01-31
Resolution	:	2.70 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:

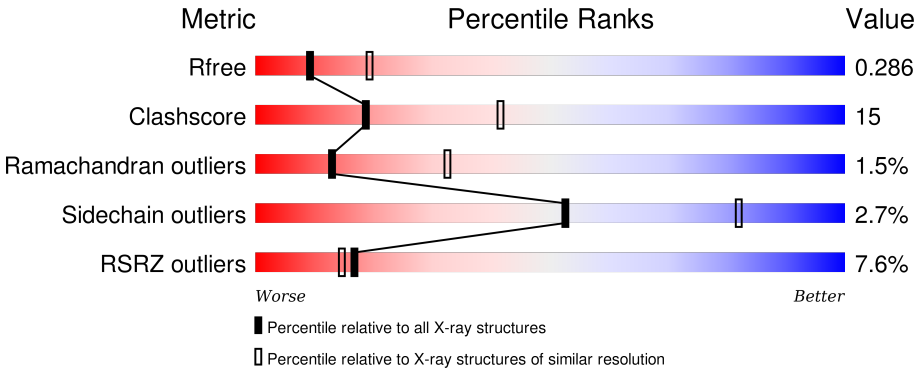
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	239	7%, 59%, 25%, ·, 14%
1	B	239	6%, 59%, 24%, ·, 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
3	FUC	B	202	X	-	-	-
3	NAG	B	206	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3440 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-2A CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1621	1027	268	317	9			
1	B	205	Total	C	N	O	S	0	0	0
			1621	1027	268	317	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	GLY	THR	ENGINEERED	UNP P20760
A	253	GLY	ILE	ENGINEERED	UNP P20760
A	254	GLY	THR	ENGINEERED	UNP P20760
A	310	GLU	HIS	ENGINEERED	UNP P20760
A	433	GLU	HIS	ENGINEERED	UNP P20760
A	435	GLU	HIS	ENGINEERED	UNP P20760
A	448	GLY	-	CLONING ARTIFACT	UNP P20760
A	449	ILE	-	CLONING ARTIFACT	UNP P20760
A	450	GLU	-	CLONING ARTIFACT	UNP P20760
A	451	GLY	-	CLONING ARTIFACT	UNP P20760
A	452	ARG	-	CLONING ARTIFACT	UNP P20760
A	453	GLY	-	CLONING ARTIFACT	UNP P20760
A	454	SER	-	CLONING ARTIFACT	UNP P20760
A	455	SER	-	CLONING ARTIFACT	UNP P20760
A	456	HIS	-	CLONING ARTIFACT	UNP P20760
A	457	HIS	-	CLONING ARTIFACT	UNP P20760
A	458	HIS	-	CLONING ARTIFACT	UNP P20760
A	459	HIS	-	CLONING ARTIFACT	UNP P20760
A	460	HIS	-	CLONING ARTIFACT	UNP P20760
A	461	HIS	-	CLONING ARTIFACT	UNP P20760
B	252	GLY	THR	ENGINEERED	UNP P20760
B	253	GLY	ILE	ENGINEERED	UNP P20760
B	254	GLY	THR	ENGINEERED	UNP P20760
B	310	GLU	HIS	ENGINEERED	UNP P20760
B	433	GLU	HIS	ENGINEERED	UNP P20760

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	435	GLU	HIS	ENGINEERED	UNP P20760
B	448	GLY	-	CLONING ARTIFACT	UNP P20760
B	449	ILE	-	CLONING ARTIFACT	UNP P20760
B	450	GLU	-	CLONING ARTIFACT	UNP P20760
B	451	GLY	-	CLONING ARTIFACT	UNP P20760
B	452	ARG	-	CLONING ARTIFACT	UNP P20760
B	453	GLY	-	CLONING ARTIFACT	UNP P20760
B	454	SER	-	CLONING ARTIFACT	UNP P20760
B	455	SER	-	CLONING ARTIFACT	UNP P20760
B	456	HIS	-	CLONING ARTIFACT	UNP P20760
B	457	HIS	-	CLONING ARTIFACT	UNP P20760
B	458	HIS	-	CLONING ARTIFACT	UNP P20760
B	459	HIS	-	CLONING ARTIFACT	UNP P20760
B	460	HIS	-	CLONING ARTIFACT	UNP P20760
B	461	HIS	-	CLONING ARTIFACT	UNP P20760

- Molecule 2 is a polymer of unknown type called SUGAR ((NAG)(FUC)(NAG)(MAN)(MAN)(NAG)(MAN)(NAG)).

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

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

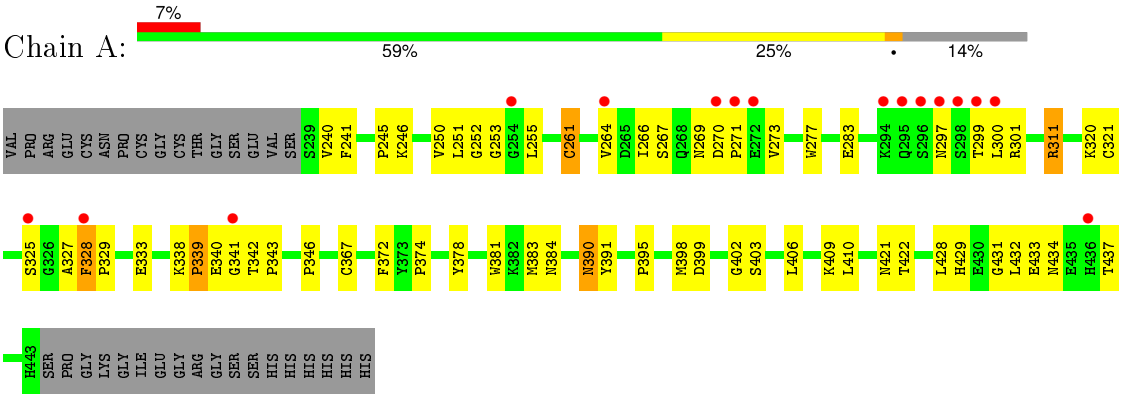
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	8	Total	C	N	O	0	0
			99	56	4	39		

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.

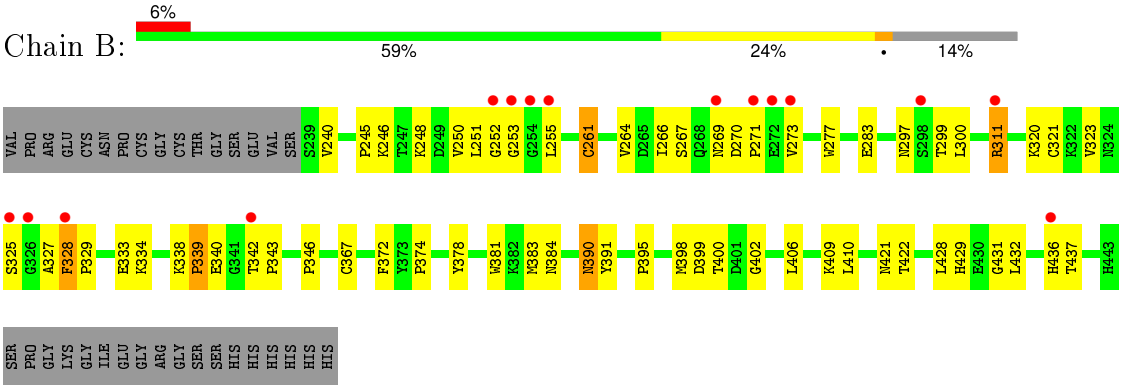
- Molecule 1: IG GAMMA-2A CHAIN C REGION

Chain A:



- Molecule 1: IG GAMMA-2A CHAIN C REGION

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.50Å 73.36Å 82.16Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	29.81 – 2.70 29.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.81-2.70) 98.6 (29.81-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.13 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.279 0.251 , 0.286	Depositor DCC
R_{free} test set	1375 reflections (10.21%)	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.0	EDS
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 13471 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3440	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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, FUL, 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	0.40	0/1666	0.69	2/2267 (0.1%)
1	B	0.42	1/1666 (0.1%)	0.64	0/2267
All	All	0.41	1/3332 (0.0%)	0.66	2/4534 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	C-N	5.14	1.42	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	GLU	N-CA-C	8.14	132.98	111.00
1	A	341	GLY	N-CA-C	6.02	128.14	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	202	FUC	C1

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	1621	0	1570	52	0
1	B	1621	0	1570	49	0
2	A	99	0	85	6	0
3	B	99	0	85	5	0
All	All	3440	0	3310	104	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 15.

All (104) 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:325:SER:HB2	1:A:328:PHE:HB2	1.36	1.06
1:B:325:SER:HB2	1:B:328:PHE:HB2	1.36	1.01
1:B:248:LYS:HD2	1:B:378:TYR:CE1	2.10	0.86
1:A:384:ASN:HD21	1:A:421:ASN:HD22	1.22	0.83
1:B:384:ASN:HD21	1:B:421:ASN:HD22	1.26	0.82
1:B:325:SER:CB	1:B:328:PHE:HB2	2.11	0.81
1:A:325:SER:CB	1:A:328:PHE:HB2	2.11	0.80
1:A:271:PRO:HB3	1:A:300:LEU:HD12	1.64	0.79
1:B:271:PRO:HB3	1:B:300:LEU:HD12	1.65	0.77
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.71	0.72
1:B:398:MET:HE3	1:B:399:ASP:N	2.05	0.71
1:B:429:HIS:CD2	1:B:431:GLY:H	2.09	0.71
1:A:429:HIS:CD2	1:A:431:GLY:H	2.10	0.70
1:A:246:LYS:HE2	2:A:106:NAG:O4	1.91	0.70
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.75	0.69
1:A:398:MET:HE3	1:A:399:ASP:N	2.10	0.66
1:A:271:PRO:HB3	1:A:300:LEU:CD1	2.28	0.63
1:B:271:PRO:HB3	1:B:300:LEU:CD1	2.28	0.63
1:B:398:MET:HE2	1:B:402:GLY:HA2	1.82	0.62
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.36	0.61
1:B:398:MET:HE2	1:B:402:GLY:CA	2.31	0.61
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.36	0.60
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ILE:HB	1:B:300:LEU:HB2	1.83	0.59
1:B:311:ARG:HE	1:B:311:ARG:HA	1.68	0.59
1:A:266:ILE:HB	1:A:300:LEU:HB2	1.84	0.59
1:A:311:ARG:HA	1:A:311:ARG:HE	1.68	0.57
1:A:398:MET:HE2	1:A:402:GLY:HA2	1.85	0.57
1:B:398:MET:HE3	1:B:399:ASP:H	1.70	0.56
1:A:398:MET:HE2	1:A:402:GLY:CA	2.35	0.56
1:B:390:ASN:O	1:B:410:LEU:HD12	2.07	0.55
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.40	0.55
1:A:429:HIS:HD2	1:A:431:GLY:H	1.54	0.55
1:A:266:ILE:HD13	1:A:273:VAL:HG21	1.88	0.54
1:B:248:LYS:HB2	1:B:378:TYR:CD1	2.43	0.54
1:A:390:ASN:O	1:A:410:LEU:HD12	2.07	0.54
1:B:429:HIS:HD2	1:B:431:GLY:H	1.54	0.53
1:B:432:LEU:HD13	1:B:437:THR:HG22	1.91	0.53
1:B:266:ILE:HD13	1:B:273:VAL:HG21	1.89	0.53
1:A:432:LEU:HD13	1:A:437:THR:HG22	1.91	0.53
1:A:264:VAL:HG11	2:A:103:NAG:H2	1.90	0.52
1:B:297:ASN:O	1:B:299:THR:HG23	2.10	0.51
1:B:264:VAL:HG11	3:B:203:NAG:H2	1.91	0.51
1:B:248:LYS:HD2	1:B:378:TYR:CZ	2.46	0.49
1:A:301:ARG:NE	2:A:103:NAG:O7	2.39	0.49
1:A:406:LEU:HD12	1:A:406:LEU:C	2.33	0.49
1:A:297:ASN:O	1:A:299:THR:HG23	2.13	0.49
1:A:338:LYS:O	1:A:339:PRO:O	2.31	0.48
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.48	0.48
1:B:406:LEU:HD12	1:B:406:LEU:C	2.35	0.47
1:B:328:PHE:CD2	1:B:329:PRO:HD2	2.50	0.47
1:A:398:MET:HE3	1:A:399:ASP:H	1.77	0.47
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.50	0.47
1:B:246:LYS:HE2	3:B:206:NAG:O4	2.16	0.46
1:B:320:LYS:HE2	1:B:333:GLU:OE2	2.16	0.45
1:A:320:LYS:HE2	1:A:333:GLU:OE2	2.16	0.45
1:A:328:PHE:CD2	1:A:329:PRO:HD2	2.52	0.45
2:A:103:NAG:H83	2:A:105:MAN:C3	2.47	0.45
1:B:398:MET:CE	1:B:402:GLY:C	2.85	0.45
1:A:395:PRO:HD2	1:B:395:PRO:HD2	1.99	0.45
3:B:203:NAG:H83	3:B:205:MAN:C3	2.47	0.44
1:A:267:SER:C	1:A:269:ASN:N	2.70	0.44
1:B:391:TYR:HA	1:B:409:LYS:O	2.17	0.44
1:B:383:MET:HA	1:B:422:THR:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:O	1:B:253:GLY:N	2.50	0.44
1:B:338:LYS:O	1:B:339:PRO:O	2.36	0.44
1:A:391:TYR:HA	1:A:409:LYS:O	2.18	0.44
1:A:342:THR:HA	1:A:343:PRO:HD3	1.74	0.44
1:B:270:ASP:OD2	1:B:327:ALA:HB2	2.17	0.44
1:A:398:MET:CE	1:A:402:GLY:C	2.87	0.43
3:B:203:NAG:H83	3:B:205:MAN:H3	1.99	0.43
1:B:384:ASN:ND2	1:B:421:ASN:HD22	2.06	0.43
1:A:267:SER:C	1:A:269:ASN:H	2.22	0.43
2:A:109:NAG:H61	3:B:202:FUC:H4	1.98	0.43
1:A:378:TYR:HB3	1:A:428:LEU:HB2	2.00	0.43
1:B:267:SER:C	1:B:269:ASN:N	2.71	0.43
1:A:270:ASP:OD2	1:A:327:ALA:HB2	2.19	0.42
1:A:374:PRO:O	1:A:429:HIS:HE1	2.02	0.42
1:A:383:MET:HA	1:A:422:THR:O	2.19	0.42
1:A:245:PRO:HB2	1:A:250:VAL:CG2	2.49	0.42
2:A:103:NAG:H83	2:A:105:MAN:H3	1.99	0.42
1:B:398:MET:HE2	1:B:402:GLY:C	2.39	0.42
1:B:270:ASP:CG	1:B:327:ALA:HB2	2.39	0.42
1:A:251:LEU:O	1:A:253:GLY:N	2.53	0.42
1:B:240:VAL:HG21	1:B:323:VAL:CG1	2.49	0.42
1:B:374:PRO:O	1:B:429:HIS:HE1	2.02	0.42
1:B:342:THR:HA	1:B:343:PRO:HD3	1.70	0.42
1:A:384:ASN:ND2	1:A:421:ASN:HD22	2.02	0.42
1:A:277:TRP:O	1:A:283:GLU:HA	2.19	0.42
1:B:428:LEU:HD23	1:B:436:HIS:HB3	2.01	0.42
1:B:245:PRO:HB2	1:B:250:VAL:CG2	2.49	0.42
1:B:267:SER:C	1:B:269:ASN:H	2.23	0.41
1:A:270:ASP:CG	1:A:327:ALA:HB2	2.40	0.41
1:B:277:TRP:O	1:B:283:GLU:HA	2.20	0.41
1:A:398:MET:HE2	1:A:402:GLY:C	2.41	0.41
1:A:433:GLU:O	1:A:434:ASN:HB2	2.20	0.41
1:A:266:ILE:CD1	1:A:273:VAL:HG21	2.51	0.41
1:B:334:LYS:HA	1:B:334:LYS:HD3	1.87	0.41
1:A:390:ASN:ND2	1:B:400:THR:HG21	2.36	0.40
1:A:338:LYS:C	1:A:339:PRO:O	2.60	0.40
1:A:240:VAL:HG12	1:A:241:PHE:N	2.37	0.40
1:A:406:LEU:HD12	1:A:406:LEU:O	2.21	0.40
1:A:320:LYS:HE2	1:A:333:GLU:CD	2.42	0.40
1:A:398:MET:HE1	1:A:403:SER:O	2.21	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	203/239 (85%)	190 (94%)	10 (5%)	3 (2%)	13 32
1	B	203/239 (85%)	190 (94%)	10 (5%)	3 (2%)	13 32
All	All	406/478 (85%)	380 (94%)	20 (5%)	6 (2%)	13 32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	LEU
1	B	255	LEU
1	A	252	GLY
1	A	339	PRO
1	B	252	GLY
1	B	339	PRO

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	188/216 (87%)	183 (97%)	5 (3%)	52 82
1	B	188/216 (87%)	183 (97%)	5 (3%)	52 82
All	All	376/432 (87%)	366 (97%)	10 (3%)	52 82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	CYS
1	A	311	ARG
1	A	321	CYS
1	A	328	PHE
1	A	390	ASN
1	B	261	CYS
1	B	311	ARG
1	B	321	CYS
1	B	328	PHE
1	B	390	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	390	ASN
1	A	421	ASN
1	A	429	HIS
1	B	268	GLN
1	B	390	ASN
1	B	421	ASN
1	B	429	HIS

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	$\#\|Z\| > 2$
2	NAG	A	101	1,2	14,14,15	0.51	0	15,19,21	0.74	1 (6%)
2	FUL	A	102	2	10,10,11	0.46	0	14,14,16	0.50	0
2	NAG	A	103	2	14,14,15	0.45	0	15,19,21	0.77	1 (6%)
2	BMA	A	104	2	11,11,12	0.41	0	14,15,17	0.80	1 (7%)
2	MAN	A	105	2	11,11,12	0.50	0	14,15,17	0.62	0
2	NAG	A	106	2	14,14,15	0.48	0	15,19,21	0.75	1 (6%)
2	MAN	A	108	2	11,11,12	0.49	0	14,15,17	0.49	0
2	NAG	A	109	2	14,14,15	0.48	0	15,19,21	0.68	1 (6%)
3	NAG	B	201	1,3	14,14,15	0.56	0	15,19,21	0.78	1 (6%)
3	FUC	B	202	3	10,10,11	0.41	0	14,14,16	0.49	0
3	NAG	B	203	3	14,14,15	0.42	0	15,19,21	0.77	1 (6%)
3	BMA	B	204	3	11,11,12	0.41	0	14,15,17	0.79	1 (7%)
3	MAN	B	205	3	11,11,12	0.52	0	14,15,17	0.56	0
3	NAG	B	206	3	14,14,15	0.50	0	15,19,21	0.77	1 (6%)
3	MAN	B	208	3	11,11,12	0.49	0	14,15,17	0.48	0
3	NAG	B	209	3	14,14,15	0.51	0	15,19,21	0.68	1 (6%)

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	101	1,2	-	0/6/23/26	0/1/1/1
2	FUL	A	102	2	-	0/0/17/20	0/1/1/1
2	NAG	A	103	2	-	0/6/23/26	0/1/1/1
2	BMA	A	104	2	-	0/2/19/22	0/1/1/1
2	MAN	A	105	2	-	0/2/19/22	0/1/1/1
2	NAG	A	106	2	-	0/6/23/26	0/1/1/1
2	MAN	A	108	2	-	0/2/19/22	0/1/1/1
2	NAG	A	109	2	-	0/6/23/26	0/1/1/1
3	NAG	B	201	1,3	-	0/6/23/26	0/1/1/1
3	FUC	B	202	3	1/1/4/5	0/0/17/20	0/1/1/1
3	NAG	B	203	3	-	0/6/23/26	0/1/1/1
3	BMA	B	204	3	-	0/2/19/22	0/1/1/1
3	MAN	B	205	3	-	0/2/19/22	0/1/1/1
3	NAG	B	206	3	-	0/6/23/26	0/1/1/1
3	MAN	B	208	3	-	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	B	209	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	NAG	C2-N2-C7	-2.50	119.83	123.04
2	A	103	NAG	C2-N2-C7	-2.49	119.84	123.04
3	B	203	NAG	C2-N2-C7	-2.42	119.94	123.04
3	B	206	NAG	C2-N2-C7	-2.41	119.95	123.04
2	A	101	NAG	C2-N2-C7	-2.32	120.05	123.04
2	A	106	NAG	C2-N2-C7	-2.30	120.09	123.04
3	B	209	NAG	C2-N2-C7	-2.11	120.33	123.04
2	A	109	NAG	C2-N2-C7	-2.05	120.41	123.04
3	B	204	BMA	C1-C2-C3	2.44	112.43	109.54
2	A	104	BMA	C1-C2-C3	2.49	112.49	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	202	FUC	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	103	NAG	4	0
2	A	105	MAN	2	0
2	A	106	NAG	1	0
2	A	109	NAG	1	0
3	B	202	FUC	1	0
3	B	203	NAG	3	0
3	B	205	MAN	2	0
3	B	206	NAG	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	205/239 (85%)	0.35	16 (7%)	16	14	11, 32, 86, 119	0
1	B	205/239 (85%)	0.32	15 (7%)	18	16	7, 34, 81, 116	0
All	All	410/478 (85%)	0.33	31 (7%)	17	15	7, 33, 86, 119	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	PRO	10.9
1	A	298	SER	5.7
1	A	325	SER	4.7
1	A	299	THR	4.6
1	B	328	PHE	4.5
1	B	254	GLY	4.4
1	B	325	SER	4.4
1	B	253	GLY	4.1
1	B	269	ASN	3.9
1	A	297	ASN	3.6
1	B	271	PRO	3.5
1	B	272	GLU	3.4
1	A	296	SER	3.3
1	A	341	GLY	3.2
1	B	298	SER	3.1
1	A	300	LEU	3.0
1	B	252	GLY	2.9
1	A	294	LYS	2.9
1	A	295	GLN	2.7
1	A	272	GLU	2.7
1	A	328	PHE	2.7
1	B	326	GLY	2.6
1	B	311	ARG	2.6
1	B	436	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	342	THR	2.4
1	A	264	VAL	2.2
1	A	270	ASP	2.2
1	B	273	VAL	2.1
1	B	255	LEU	2.1
1	A	436	HIS	2.1
1	A	254	GLY	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)

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	206	14/15	0.80	0.27	3.04	78,80,88,89	0
2	NAG	A	101	14/15	0.72	0.37	-0.18	100,112,117,123	0
3	NAG	B	201	14/15	0.82	0.21	-1.65	87,96,104,112	0
3	BMA	B	204	11/12	0.77	0.24	-	83,98,102,108	0
2	MAN	A	105	11/12	0.89	0.20	-	60,62,64,64	0
2	NAG	A	109	14/15	0.77	0.26	-	93,103,106,106	0
2	MAN	A	108	11/12	0.79	0.26	-	88,92,94,98	0
2	NAG	A	106	14/15	0.84	0.23	-	46,65,74,77	0
3	NAG	B	203	14/15	0.83	0.23	-	80,94,101,104	0
2	NAG	A	103	14/15	0.74	0.33	-	78,86,90,91	0
3	FUC	B	202	10/11	0.79	0.23	-	117,121,123,124	0
3	MAN	B	205	11/12	0.91	0.19	-	72,75,79,80	0
3	MAN	B	208	11/12	0.59	0.34	-	105,110,114,118	0
3	NAG	B	209	14/15	0.42	0.46	-	113,119,121,121	0
2	BMA	A	104	11/12	0.86	0.20	-	65,76,77,82	0
2	FUL	A	102	10/11	0.46	0.70	-	128,130,131,132	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.