



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2017 – 07:46 PM EDT

PDB ID : 4WI3  
Title : Structural mapping of the human IgG1 binding site for FcRn: hu3S193 Fc mutation I253A  
Authors : Farrugia, W.; Burvenich, I.J.G.; Scott, A.M.; Ramsland, P.A.  
Deposited on : unknown  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

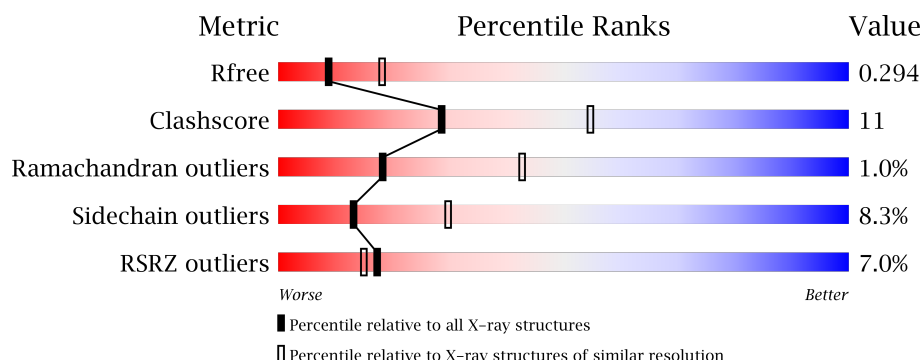
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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  $\geq 3$ , 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	208	<div> <div>7%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
1	B	208	<div> <div>7%</div> <div>72%</div> <div>23%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3552 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.

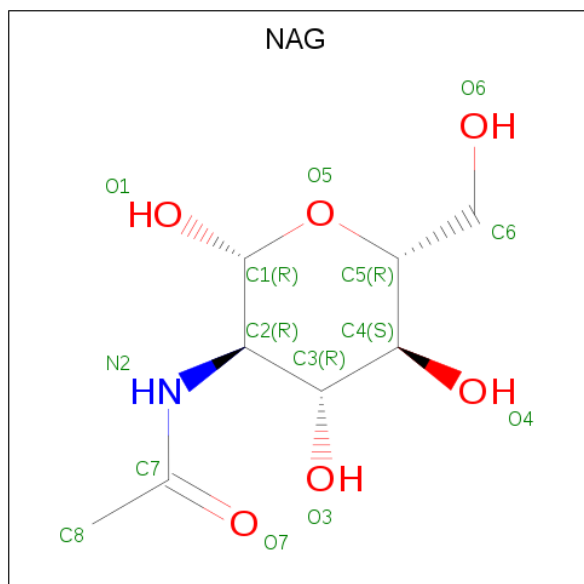
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1661	1056	280	319	6			
1	B	208	Total	C	N	O	S	0	0	0
			1661	1056	280	319	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	ALA	ILE	engineered mutation	UNP P01857
B	253	ALA	ILE	engineered mutation	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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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	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:  $C_6H_{12}O_6$ ).



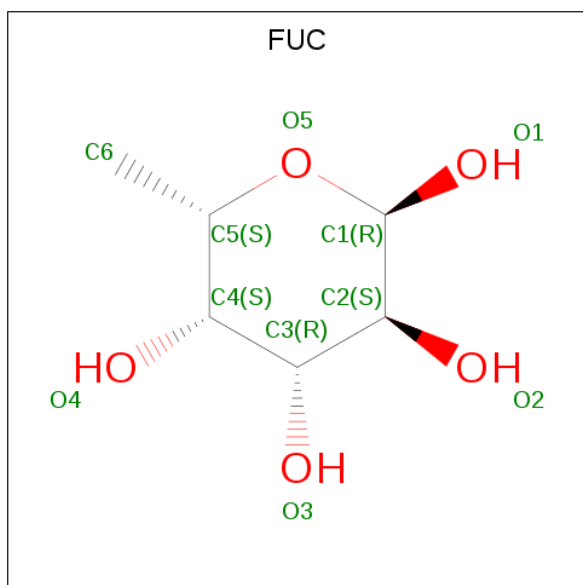
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



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	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

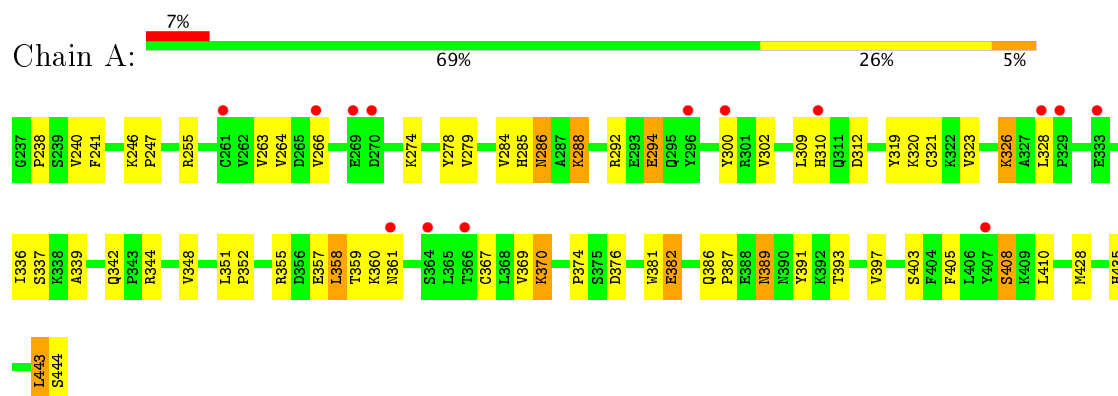
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	18	Total	O	0	0
			18	18		

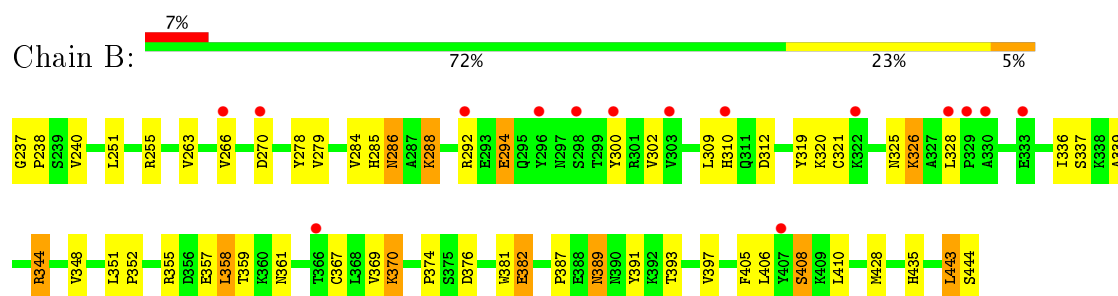
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



GLOBAL-STATISTICS INFOmissingINFO

## 4 Model quality

### 4.1 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	0.39	0/1707	0.57	0/2326
1	B	0.39	0/1707	0.56	0/2326
All	All	0.39	0/3414	0.56	0/4652

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	1661	0	1624	40	0
1	B	1661	0	1624	37	0
2	A	56	0	49	2	0
2	B	56	0	49	1	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	A	10	0	10	0	0
5	B	10	0	10	0	0
6	A	14	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	0	3	0
All	All	3552	0	3418	76	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 11.

All (76) 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:B:344:ARG:NH1	6:B:613:HOH:O	2.12	0.82
1:B:443:LEU:HD12	1:B:444:SER:H	1.52	0.74
1:A:443:LEU:HD12	1:A:444:SER:H	1.54	0.71
1:A:393:THR:OG1	1:A:408:SER:OG	2.09	0.70
1:B:393:THR:OG1	1:B:408:SER:OG	2.10	0.69
1:A:240:VAL:HG22	1:A:263:VAL:HG22	1.77	0.66
1:B:240:VAL:HG22	1:B:263:VAL:HG22	1.78	0.65
1:A:339:ALA:HB3	1:A:374:PRO:HB3	1.80	0.63
1:A:274:LYS:O	6:A:605:HOH:O	2.15	0.63
1:B:339:ALA:HB3	1:B:374:PRO:HB3	1.82	0.61
1:B:381:TRP:HE1	1:B:408:SER:HB3	1.67	0.60
1:A:294:GLU:HG2	1:A:300:TYR:HE1	1.67	0.59
1:B:294:GLU:HG2	1:B:300:TYR:HE1	1.68	0.59
1:B:355:ARG:HA	1:B:358:LEU:HD13	1.84	0.59
1:A:355:ARG:HA	1:A:358:LEU:HD13	1.85	0.59
1:A:444:SER:O	6:A:607:HOH:O	2.17	0.57
1:A:381:TRP:HE1	1:A:408:SER:HB3	1.68	0.57
1:A:323:VAL:HG13	6:A:605:HOH:O	2.06	0.56
1:B:255:ARG:O	1:B:310:HIS:NE2	2.37	0.56
1:A:370:LYS:HE2	1:B:357:GLU:OE2	2.06	0.56
1:A:255:ARG:O	1:A:310:HIS:NE2	2.40	0.52
1:A:397:VAL:HB	1:A:405:PHE:CE2	2.44	0.52
1:A:357:GLU:OE2	1:B:370:LYS:HE2	2.09	0.52
1:A:360:LYS:NZ	6:A:611:HOH:O	2.42	0.52
1:A:278:TYR:HD1	1:A:320:LYS:HD3	1.75	0.51
1:A:292:ARG:HB3	1:A:302:VAL:HG22	1.93	0.51
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.46	0.51
1:B:278:TYR:HD1	1:B:320:LYS:HD3	1.76	0.50
1:B:393:THR:O	6:B:612:HOH:O	2.19	0.50
1:B:292:ARG:HB3	1:B:302:VAL:HG22	1.92	0.50
1:A:403:SER:OG	6:A:606:HOH:O	2.20	0.49
1:B:309:LEU:HB2	1:B:312:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG11	2:A:501:NAG:O4	2.14	0.48
1:A:286:ASN:OD1	1:A:286:ASN:N	2.45	0.48
1:A:326:LYS:H	1:A:326:LYS:HD2	1.79	0.48
1:B:286:ASN:OD1	1:B:286:ASN:N	2.46	0.48
1:A:309:LEU:HB2	1:A:312:ASP:HB2	1.95	0.47
1:A:241:PHE:CE2	2:A:502:NAG:H4	2.49	0.47
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.49	0.47
1:B:326:LYS:H	1:B:326:LYS:HD2	1.80	0.47
1:B:389:ASN:OD1	1:B:389:ASN:N	2.43	0.47
1:A:278:TYR:HB2	1:A:320:LYS:HG2	1.97	0.47
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.50	0.47
1:A:382:GLU:HB3	1:A:387:PRO:HA	1.97	0.47
1:B:382:GLU:HB3	1:B:387:PRO:HA	1.97	0.46
1:A:428:MET:HA	1:A:435:HIS:O	2.16	0.46
1:A:357:GLU:O	1:A:359:THR:N	2.46	0.46
1:B:348:VAL:HG22	1:B:369:VAL:HG13	1.97	0.46
1:A:391:TYR:HB3	1:A:410:LEU:CD1	2.46	0.46
1:B:278:TYR:HB2	1:B:320:LYS:HG2	1.98	0.46
1:B:288:LYS:HE2	1:B:288:LYS:HB2	1.55	0.45
1:A:279:VAL:HG22	1:A:319:TYR:CD1	2.53	0.44
1:A:389:ASN:N	1:A:389:ASN:OD1	2.46	0.44
1:A:238:PRO:HD2	1:A:328:LEU:HG	2.00	0.43
1:B:428:MET:HA	1:B:435:HIS:O	2.18	0.43
1:B:391:TYR:HB3	1:B:410:LEU:CD1	2.49	0.43
1:B:443:LEU:HA	1:B:443:LEU:HD13	1.91	0.43
1:A:336:ILE:HG12	1:A:337:SER:N	2.34	0.43
1:A:351:LEU:HA	1:A:352:PRO:HD2	1.74	0.43
1:B:443:LEU:HD12	1:B:444:SER:N	2.27	0.42
1:A:386:GLN:HA	1:A:387:PRO:HD3	1.88	0.42
1:B:238:PRO:HD2	1:B:328:LEU:HG	2.02	0.42
1:B:279:VAL:HG22	1:B:319:TYR:CD1	2.54	0.42
1:B:255:ARG:HD2	6:B:602:HOH:O	2.20	0.42
1:B:339:ALA:HB3	1:B:374:PRO:CB	2.49	0.42
1:A:342:GLN:HG2	1:A:342:GLN:H	1.70	0.42
1:B:270:ASP:O	1:B:325:ASN:ND2	2.35	0.42
1:B:237:GLY:HA3	1:B:238:PRO:HD3	1.89	0.41
1:B:357:GLU:O	1:B:359:THR:N	2.46	0.41
2:B:507:NAG:H83	2:B:507:NAG:H2	1.90	0.41
1:A:288:LYS:HB2	1:A:288:LYS:HE2	1.57	0.41
1:A:348:VAL:HG22	1:A:369:VAL:HG13	2.03	0.41
1:A:246:LYS:HA	1:A:247:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ALA:HB3	1:A:374:PRO:CB	2.48	0.41
1:B:336:ILE:HG12	1:B:337:SER:N	2.34	0.41
1:B:351:LEU:HA	1:B:352:PRO:HD2	1.76	0.40

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 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	206/208 (99%)	193 (94%)	11 (5%)	2 (1%)	18	43
1	B	206/208 (99%)	194 (94%)	10 (5%)	2 (1%)	18	43
All	All	412/416 (99%)	387 (94%)	21 (5%)	4 (1%)	18	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLU
1	A	358	LEU
1	B	294	GLU
1	B	358	LEU

### 4.3.2 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	193/193 (100%)	178 (92%)	15 (8%)	15	33
1	B	193/193 (100%)	176 (91%)	17 (9%)	12	27
All	All	386/386 (100%)	354 (92%)	32 (8%)	13	30

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	VAL
1	A	284	VAL
1	A	285	HIS
1	A	286	ASN
1	A	288	LYS
1	A	321	CYS
1	A	326	LYS
1	A	344	ARG
1	A	361	ASN
1	A	370	LYS
1	A	376	ASP
1	A	382	GLU
1	A	389	ASN
1	A	408	SER
1	A	443	LEU
1	B	251	LEU
1	B	266	VAL
1	B	284	VAL
1	B	285	HIS
1	B	286	ASN
1	B	288	LYS
1	B	321	CYS
1	B	326	LYS
1	B	344	ARG
1	B	361	ASN
1	B	370	LYS
1	B	376	ASP
1	B	382	GLU
1	B	389	ASN
1	B	406	LEU
1	B	408	SER
1	B	443	LEU

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

### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 4.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 4.6 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	$\# Z  > 2$
2	NAG	A	501	1,2,5	14,14,15	0.53	0	15,19,21	1.41	3 (20%)
2	NAG	A	502	3,2	14,14,15	0.55	0	15,19,21	1.25	2 (13%)
3	BMA	A	503	2,4	11,11,12	0.67	0	13,15,17	0.91	1 (7%)
4	MAN	A	504	3,2	11,11,12	0.61	0	13,15,17	0.89	1 (7%)
2	NAG	A	505	4	14,14,15	0.59	0	15,19,21	0.43	0
4	MAN	A	506	3,2	11,11,12	0.63	0	13,15,17	1.14	1 (7%)
2	NAG	A	507	4	14,14,15	0.43	0	15,19,21	0.89	1 (6%)
5	FUC	A	508	2	9,10,11	0.62	0	13,14,16	0.81	0
2	NAG	B	501	1,2,5	14,14,15	0.49	0	15,19,21	0.95	1 (6%)
2	NAG	B	502	3,2	14,14,15	0.50	0	15,19,21	1.10	1 (6%)
3	BMA	B	503	2,4	11,11,12	0.67	0	13,15,17	1.18	1 (7%)
4	MAN	B	504	3,2	11,11,12	0.55	0	13,15,17	0.90	0
2	NAG	B	505	4	14,14,15	0.50	0	15,19,21	0.63	0
4	MAN	B	506	3,2	11,11,12	0.63	0	13,15,17	1.05	0
2	NAG	B	507	4	14,14,15	0.42	0	15,19,21	1.50	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FUC	B	508	2	9,10,11	0.61	0	13,14,16	0.99	1 (7%)

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	1,2,5	-	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
5	FUC	A	508	2	-	0/0/17/20	0/1/1/1
2	NAG	B	501	1,2,5	-	2/6/23/26	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	-	2/6/23/26	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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	507	NAG	C2-N2-C7	-2.61	119.13	122.94
2	B	501	NAG	O5-C1-C2	-2.57	107.89	111.47
4	A	504	MAN	O5-C1-C2	-2.54	106.81	110.79
2	B	507	NAG	C4-C3-C2	-2.48	107.38	111.02
4	A	506	MAN	O2-C2-C3	-2.06	106.14	110.17
2	B	502	NAG	C3-C4-C5	2.05	113.82	110.22
2	A	501	NAG	C3-C4-C5	2.16	114.03	110.22
5	B	508	FUC	C1-O5-C5	2.21	117.28	112.39
3	A	503	BMA	C1-C2-C3	2.32	112.59	109.65
2	A	501	NAG	C4-C3-C2	2.37	114.48	111.02
2	A	502	NAG	C4-C3-C2	2.62	114.85	111.02
2	A	502	NAG	C3-C4-C5	2.72	115.00	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	BMA	C1-C2-C3	2.77	113.16	109.65
2	A	507	NAG	C1-O5-C5	2.84	116.08	112.17
2	A	501	NAG	C1-O5-C5	2.95	116.23	112.17
2	B	507	NAG	C1-O5-C5	3.87	117.51	112.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	505	NAG	C8-C7-N2-C2
2	B	501	NAG	O7-C7-N2-C2
2	B	501	NAG	C8-C7-N2-C2
2	B	505	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	A	502	NAG	1	0
2	B	507	NAG	1	0

## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/208 (100%)	0.32	14 (6%)	19 16	51, 104, 183, 213	0
1	B	208/208 (100%)	0.32	15 (7%)	16 14	53, 106, 183, 213	0
All	All	416/416 (100%)	0.32	29 (6%)	17 15	51, 105, 183, 213	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	TYR	5.7
1	B	300	TYR	5.3
1	A	310	HIS	3.2
1	B	266	VAL	3.1
1	B	333	GLU	2.9
1	B	296	TYR	2.9
1	B	329	PRO	2.8
1	A	407	TYR	2.8
1	A	329	PRO	2.7
1	B	366	THR	2.7
1	B	310	HIS	2.7
1	A	270	ASP	2.6
1	A	266	VAL	2.6
1	B	322	LYS	2.6
1	A	366	THR	2.5
1	A	261	CYS	2.4
1	B	407	TYR	2.3
1	B	328	LEU	2.3
1	A	333	GLU	2.2
1	A	364	SER	2.2
1	A	296	TYR	2.2
1	B	270	ASP	2.2
1	B	330	ALA	2.2
1	B	303	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	2.1
1	B	292	ARG	2.0
1	A	361	ASN	2.0
1	A	269	GLU	2.0
1	B	298	SER	2.0

## 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.4 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	A	507	14/15	0.88	0.17	-1.01	107,126,138,139	0
2	NAG	B	502	14/15	0.87	0.23	-	129,178,203,208	0
4	MAN	B	506	11/12	0.95	0.15	-	119,131,146,156	0
2	NAG	B	501	14/15	0.79	0.25	-	104,158,186,212	0
2	NAG	A	501	14/15	0.87	0.23	-	131,161,190,211	0
2	NAG	B	505	14/15	0.85	0.16	-	121,159,173,178	0
2	NAG	A	505	14/15	0.87	0.17	-	131,160,185,185	0
4	MAN	B	504	11/12	0.93	0.20	-	158,170,190,204	0
2	NAG	A	502	14/15	0.83	0.26	-	124,171,201,208	0
3	BMA	A	503	11/12	0.92	0.15	-	107,141,164,167	0
5	FUC	B	508	10/11	0.58	0.44	-	146,175,208,221	0
5	FUC	A	508	10/11	0.71	0.38	-	171,192,202,203	0
4	MAN	A	504	11/12	0.96	0.20	-	139,161,181,194	0
2	NAG	B	507	14/15	0.85	0.18	-	109,132,139,152	0
4	MAN	A	506	11/12	0.93	0.17	-	113,128,152,154	0
3	BMA	B	503	11/12	0.92	0.15	-	111,143,164,176	0

## 5.5 Other polymers [i](#)

There are no such residues in this entry.