



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:41 PM GMT

PDB ID : 4WI9  
Title : Structural mapping of the human IgG1 binding site for FcRn: hu3S193 Fc mutation I253A/H310A  
Authors : Farrugia, W.; Burvenich, I.J.G.; Scott, A.M.; Ramsland, P.A.  
Deposited on : 2014-09-25  
Resolution : 2.65 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

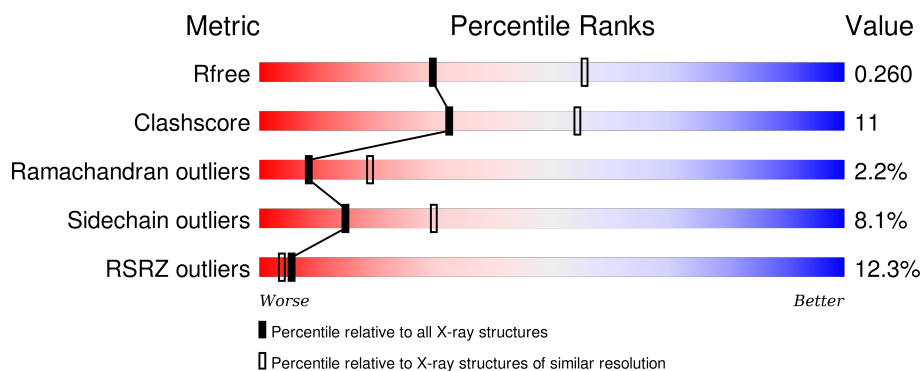
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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>12%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	B	208	<div> <div>13%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>

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
2	NAG	B	501	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3540 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.

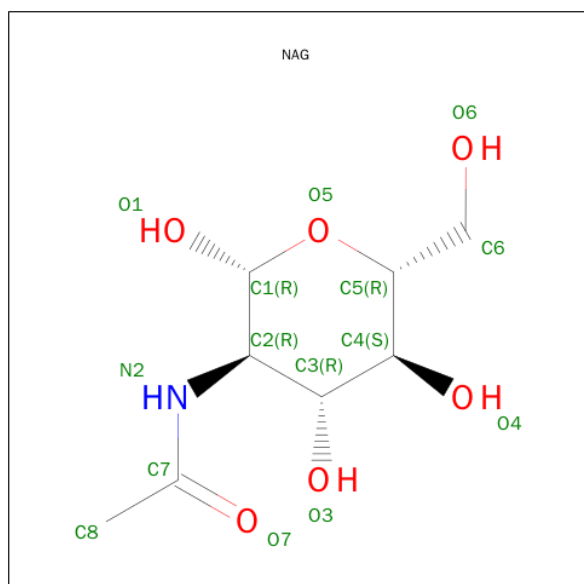
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1656	1053	278	319	6			
1	B	208	Total	C	N	O	S	0	0	0
			1656	1053	278	319	6			

There are 4 discrepancies between the modelled and reference sequences:

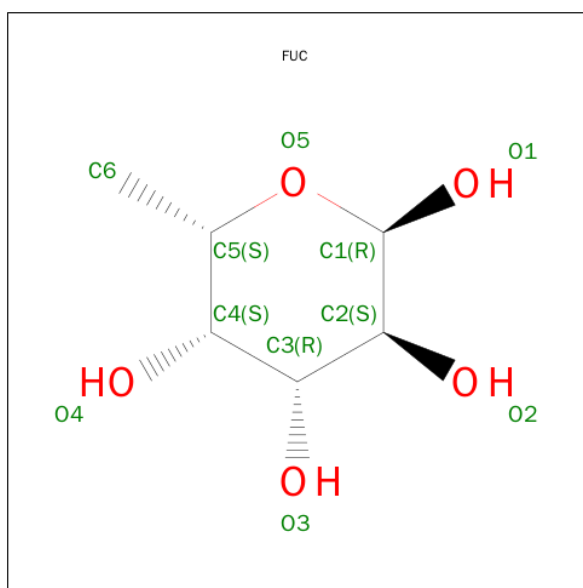
Chain	Residue	Modelled	Actual	Comment	Reference
A	253	ALA	ILE	engineered mutation	UNP P01857
A	310	ALA	HIS	engineered mutation	UNP P01857
B	253	ALA	ILE	engineered mutation	UNP P01857
B	310	ALA	HIS	engineered mutation	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



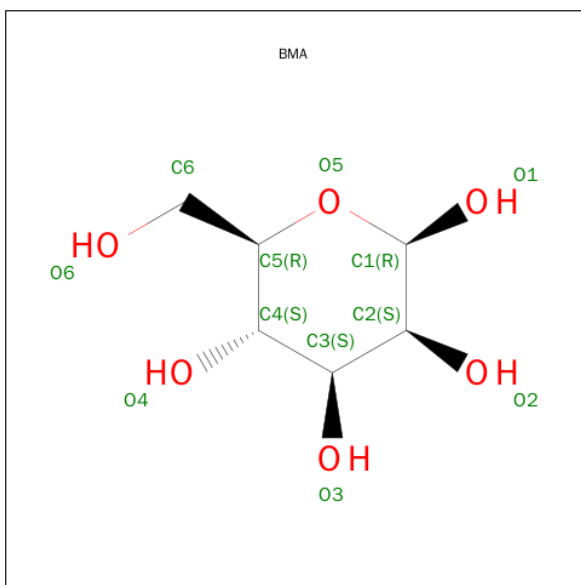
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



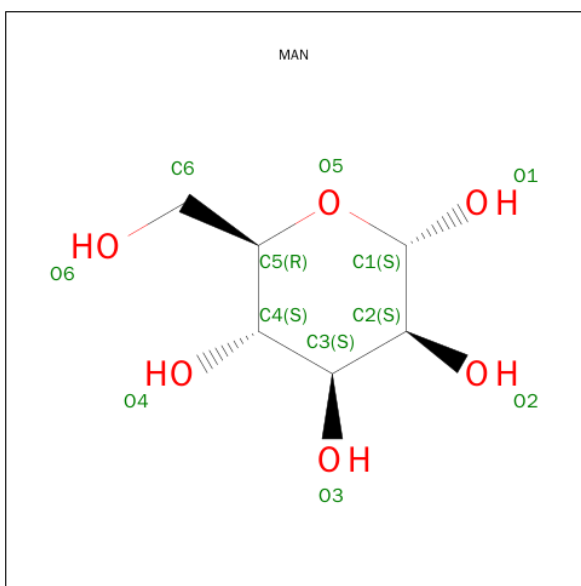
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

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



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

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

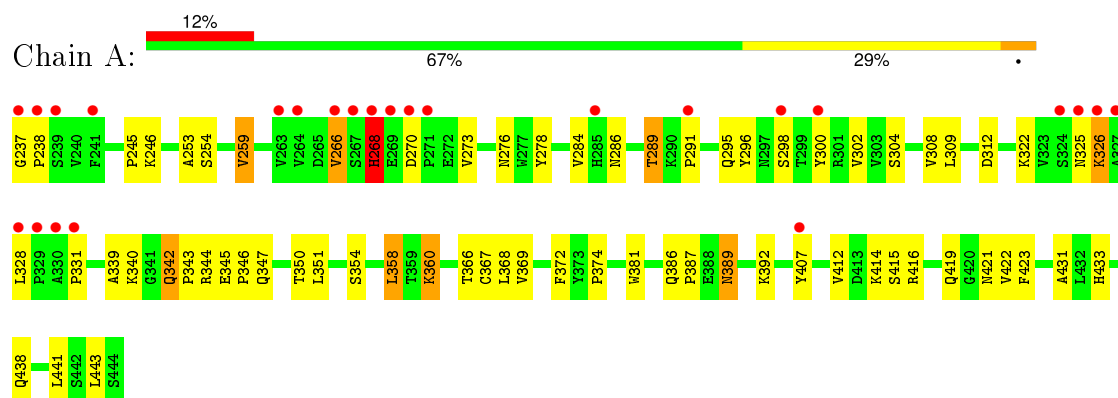
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	12	Total	O	0	0
			12	12		

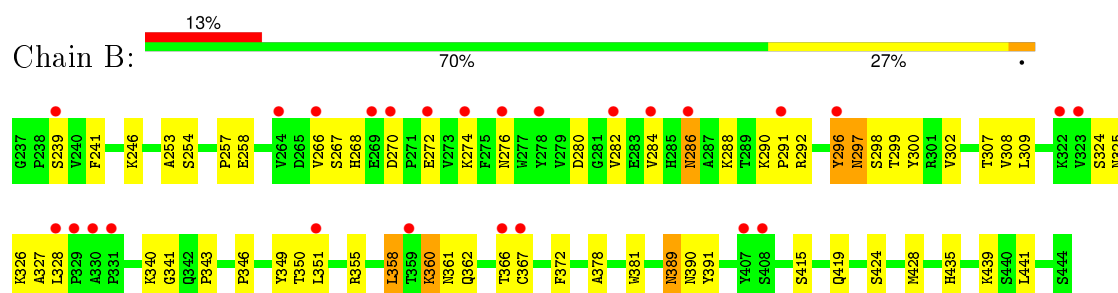
### 3 Residue-property plots

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



- Molecule 1: Ig gamma-1 chain C region



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.16 Å 77.65 Å 140.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.65 29.78 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.78-2.65) 99.8 (29.78-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.64 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.206 , 0.274 0.196 , 0.260	Depositor DCC
$R_{free}$ test set	1627 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 16289 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.42	0/1701	0.58	0/2318
1	B	0.44	0/1701	0.58	0/2318
All	All	0.43	0/3402	0.58	0/4636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	1656	0	1622	40	0
1	B	1656	0	1622	33	0
2	A	56	0	50	1	0
2	B	56	0	49	5	0
3	A	10	0	10	1	0
3	B	10	0	10	0	0
4	A	11	0	8	0	0
4	B	11	0	8	0	0
5	A	22	0	18	0	0
5	B	22	0	18	0	0
6	A	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	0	0	0
All	All	3540	0	3415	73	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 (73) 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:392:LYS:NZ	6:A:614:HOH:O	1.83	1.09
1:B:299:THR:HG21	2:B:501:NAG:HN2	1.46	0.80
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.74	0.70
1:A:358:LEU:O	1:A:414:LYS:NZ	2.25	0.68
1:B:350:THR:HB	1:B:441:LEU:HD22	1.78	0.64
1:B:325:ASN:HB3	1:B:328:LEU:HG	1.78	0.64
1:B:325:ASN:H	1:B:328:LEU:HD12	1.63	0.63
1:A:284:VAL:HG22	1:A:286:ASN:H	1.64	0.62
1:B:288:LYS:HG2	1:B:290:LYS:HG3	1.80	0.62
1:A:389:ASN:N	1:A:389:ASN:OD1	2.33	0.60
1:B:292:ARG:HD2	1:B:302:VAL:HG22	1.84	0.60
1:B:246:LYS:NZ	2:B:507:NAG:O3	2.31	0.59
1:B:415:SER:O	1:B:419:GLN:HG2	2.04	0.58
1:A:415:SER:O	1:A:419:GLN:HG2	2.04	0.58
1:A:273:VAL:HG21	1:A:302:VAL:HG21	1.86	0.57
1:A:273:VAL:HG12	1:A:325:ASN:HD22	1.68	0.57
1:B:296:TYR:O	1:B:298:SER:N	2.33	0.56
1:B:360:LYS:HE3	1:B:361:ASN:H	1.69	0.56
1:B:241:PHE:CZ	2:B:502:NAG:H61	2.42	0.55
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.42	0.55
1:B:284:VAL:HG22	1:B:286:ASN:H	1.72	0.54
1:A:350:THR:HB	1:A:441:LEU:HD22	1.90	0.53
1:B:389:ASN:OD1	1:B:389:ASN:N	2.42	0.53
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.90	0.53
1:A:296:TYR:HB2	3:A:502:FUC:H63	1.91	0.53
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.44	0.52
1:B:286:ASN:OD1	1:B:286:ASN:N	2.42	0.51
1:B:351:LEU:HB2	1:B:366:THR:HB	1.92	0.50
1:A:289:THR:HA	1:A:304:SER:HA	1.94	0.49
1:B:274:LYS:HB3	1:B:324:SER:HB2	1.96	0.48
1:B:257:PRO:HG2	1:B:308:VAL:O	2.14	0.48
1:B:325:ASN:OD1	1:B:327:ALA:N	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLU:HG3	1:A:431:ALA:O	2.14	0.47
1:A:268:HIS:NE2	1:A:298:SER:OG	2.47	0.47
1:A:351:LEU:HB2	1:A:366:THR:HB	1.96	0.47
1:A:328:LEU:HD13	1:A:331:PRO:HA	1.97	0.46
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.96	0.46
1:A:246:LYS:HA	1:A:246:LYS:HD2	1.64	0.46
1:A:339:ALA:HB3	1:A:374:PRO:HB3	1.98	0.45
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.98	0.45
1:A:245:PRO:HD3	1:A:259:VAL:HG12	1.98	0.45
1:B:378:ALA:HB3	1:B:428:MET:HB2	1.99	0.44
1:B:272:GLU:O	1:B:326:LYS:NZ	2.46	0.44
1:A:259:VAL:HG13	1:A:308:VAL:HG11	1.99	0.43
1:A:347:GLN:O	1:A:369:VAL:HA	2.18	0.43
1:B:267:SER:OG	1:B:268:HIS:N	2.51	0.43
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.89	0.43
1:B:428:MET:HA	1:B:435:HIS:O	2.18	0.43
1:A:266:VAL:HG21	1:A:300:TYR:HB2	2.00	0.43
1:B:241:PHE:CE2	2:B:502:NAG:H61	2.53	0.43
1:A:270:ASP:HB3	1:A:326:LYS:HZ3	1.83	0.43
1:A:295:GLN:HE21	2:A:501:NAG:C6	2.32	0.43
1:B:355:ARG:HA	1:B:358:LEU:HD22	2.01	0.42
1:A:289:THR:O	1:A:289:THR:OG1	2.30	0.42
1:B:341:GLY:O	1:B:343:PRO:HD3	2.19	0.42
1:A:386:GLN:HA	1:A:387:PRO:HD3	1.89	0.42
1:A:278:TYR:HE1	1:A:322:LYS:HB2	1.84	0.42
1:A:237:GLY:HA3	1:A:238:PRO:HD2	1.86	0.42
1:A:266:VAL:HG22	1:A:300:TYR:H	1.84	0.41
1:B:361:ASN:OD1	1:B:362:GLN:HG3	2.20	0.41
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.55	0.41
1:A:326:LYS:HZ3	1:A:326:LYS:H	1.68	0.41
1:A:416:ARG:O	1:A:421:ASN:HB2	2.21	0.41
1:A:412:VAL:HG11	1:A:423:PHE:CE2	2.56	0.41
1:B:389:ASN:O	1:B:391:TYR:N	2.54	0.40
1:B:439:LYS:HA	1:B:439:LYS:HD3	1.72	0.40
1:A:309:LEU:O	1:A:312:ASP:HB2	2.21	0.40
1:A:309:LEU:O	1:A:312:ASP:N	2.54	0.40
1:A:360:LYS:HB3	1:A:360:LYS:NZ	2.36	0.40
1:B:360:LYS:CE	1:B:361:ASN:H	2.33	0.40
2:B:501:NAG:O6	2:B:502:NAG:N2	2.52	0.40
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.92	0.40
1:A:443:LEU:HA	1:A:443:LEU:HD12	1.85	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	206/208 (99%)	188 (91%)	14 (7%)	4 (2%)	10	22
1	B	206/208 (99%)	189 (92%)	12 (6%)	5 (2%)	7	16
All	All	412/416 (99%)	377 (92%)	26 (6%)	9 (2%)	8	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	ASN
1	A	291	PRO
1	B	253	ALA
1	B	291	PRO
1	A	253	ALA
1	B	296	TYR
1	A	268	HIS
1	B	390	ASN
1	A	266	VAL

### 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	192/192 (100%)	178 (93%)	14 (7%)	17	36
1	B	192/192 (100%)	175 (91%)	17 (9%)	12	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	384/384 (100%)	353 (92%)	31 (8%)	15	30

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	259	VAL
1	A	268	HIS
1	A	289	THR
1	A	326	LYS
1	A	340	LYS
1	A	342	GLN
1	A	344	ARG
1	A	358	LEU
1	A	360	LYS
1	A	389	ASN
1	A	422	VAL
1	A	433	HIS
1	A	438	GLN
1	B	239	SER
1	B	254	SER
1	B	258	GLU
1	B	266	VAL
1	B	270	ASP
1	B	276	ASN
1	B	280	ASP
1	B	282	VAL
1	B	286	ASN
1	B	297	ASN
1	B	300	TYR
1	B	307	THR
1	B	340	LYS
1	B	358	LEU
1	B	360	LYS
1	B	389	ASN
1	B	424	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN

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Mol	Chain	Res	Type
1	A	418	GLN

### 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	$\# Z  > 2$
2	NAG	A	501	1,3	14,14,15	0.37	0	15,19,21	1.23	3 (20%)
3	FUC	A	502	2	10,10,11	0.49	0	13,14,16	1.07	1 (7%)
2	NAG	A	503	4	14,14,15	0.50	0	15,19,21	0.95	0
4	BMA	A	504	2,5	11,11,12	0.59	0	15,15,17	1.16	1 (6%)
5	MAN	A	505	2,4	11,11,12	0.64	0	15,15,17	1.19	1 (6%)
2	NAG	A	506	5	14,14,15	0.49	0	15,19,21	1.90	4 (26%)
5	MAN	A	507	2,4	11,11,12	0.65	0	15,15,17	1.10	1 (6%)
2	NAG	A	508	5	14,14,15	0.60	0	15,19,21	1.44	2 (13%)
2	NAG	B	501	1,3,2	14,14,15	0.39	0	15,19,21	1.92	4 (26%)
2	NAG	B	502	2,4	14,14,15	0.61	0	15,19,21	0.71	0
4	BMA	B	503	2,5	11,11,12	0.50	0	15,15,17	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	B	504	2,4	11,11,12	0.62	0	15,15,17	1.30	2 (13%)
2	NAG	B	505	5	14,14,15	0.63	0	15,19,21	0.91	0
5	MAN	B	506	2,4	11,11,12	0.58	0	15,15,17	1.24	1 (6%)
2	NAG	B	507	5	14,14,15	0.42	0	15,19,21	1.71	1 (6%)
3	FUC	B	508	2	10,10,11	0.59	0	13,14,16	1.30	2 (15%)

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	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	502	2	-	0/0/17/20	0/1/1/1
2	NAG	A	503	4	-	0/6/23/26	0/1/1/1
4	BMA	A	504	2,5	-	0/2/19/22	0/1/1/1
5	MAN	A	505	2,4	-	0/2/19/22	0/1/1/1
2	NAG	A	506	5	-	0/6/23/26	0/1/1/1
5	MAN	A	507	2,4	-	0/2/19/22	0/1/1/1
2	NAG	A	508	5	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1,3,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	502	2,4	-	0/6/23/26	0/1/1/1
4	BMA	B	503	2,5	-	0/2/19/22	0/1/1/1
5	MAN	B	504	2,4	-	0/2/19/22	0/1/1/1
2	NAG	B	505	5	-	0/6/23/26	0/1/1/1
5	MAN	B	506	2,4	-	0/2/19/22	0/1/1/1
2	NAG	B	507	5	-	0/6/23/26	0/1/1/1
3	FUC	B	508	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C4-C3-C2	-3.42	106.03	111.34
5	B	504	MAN	C2-C3-C4	-2.78	106.20	111.05
5	B	504	MAN	O5-C1-C2	-2.76	106.48	110.89
2	B	501	NAG	C2-N2-C7	-2.73	119.56	123.11
2	A	501	NAG	C2-N2-C7	-2.66	119.65	123.11
4	B	503	BMA	O5-C1-C2	-2.64	106.67	110.89
2	A	501	NAG	C6-C5-C4	-2.17	107.56	112.99
2	A	501	NAG	O5-C5-C6	2.05	111.74	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	O4-C4-C5	2.08	114.70	109.23
2	A	506	NAG	O5-C5-C4	2.11	113.64	110.13
3	B	508	FUC	O5-C1-C2	2.16	114.36	110.89
2	A	508	NAG	C4-C3-C2	2.22	114.78	111.34
5	B	506	MAN	O2-C2-C1	2.35	113.94	109.23
5	A	507	MAN	O2-C2-C1	2.35	113.95	109.23
2	A	506	NAG	C3-C4-C5	2.48	114.64	110.23
3	B	508	FUC	C1-C2-C3	2.79	112.93	109.55
3	A	502	FUC	O5-C5-C6	2.84	111.37	106.28
2	A	506	NAG	C2-N2-C7	3.15	127.21	123.11
5	A	505	MAN	C1-C2-C3	3.25	113.48	109.55
4	A	504	BMA	C1-C2-C3	3.54	113.84	109.55
2	A	508	NAG	C1-O5-C5	3.95	117.95	112.14
2	B	501	NAG	C1-O5-C5	4.65	118.98	112.14
2	A	506	NAG	C1-O5-C5	5.14	119.69	112.14
2	B	507	NAG	C1-O5-C5	5.43	120.13	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
3	A	502	FUC	1	0
2	B	501	NAG	2	0
2	B	502	NAG	3	0
2	B	507	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.48	25 (12%) 6 4	39, 86, 163, 197	0
1	B	208/208 (100%)	0.57	26 (12%) 5 4	41, 89, 156, 212	0
All	All	416/416 (100%)	0.53	51 (12%) 5 4	39, 88, 160, 212	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	7.2
1	B	269	GLU	5.5
1	A	298	SER	5.1
1	A	238	PRO	5.0
1	A	331	PRO	4.9
1	A	330	ALA	4.6
1	B	264	VAL	4.5
1	B	328	LEU	4.3
1	A	300	TYR	4.1
1	B	276	ASN	3.9
1	A	266	VAL	3.8
1	B	322	LYS	3.6
1	B	367	CYS	3.3
1	B	366	THR	3.2
1	B	329	PRO	3.2
1	B	278	TYR	3.1
1	A	267	SER	3.1
1	A	327	ALA	3.1
1	B	351	LEU	3.1
1	B	291	PRO	3.1
1	B	331	PRO	3.0
1	A	325	ASN	3.0
1	A	270	ASP	2.9
1	B	286	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	329	PRO	2.7
1	A	291	PRO	2.7
1	A	324	SER	2.7
1	A	326	LYS	2.7
1	B	330	ALA	2.7
1	A	269	GLU	2.7
1	A	264	VAL	2.6
1	B	408	SER	2.6
1	A	285	HIS	2.6
1	A	268	HIS	2.6
1	B	270	ASP	2.5
1	A	263	VAL	2.5
1	B	282	VAL	2.5
1	A	241	PHE	2.4
1	B	274	LYS	2.4
1	A	407	TYR	2.3
1	B	284	VAL	2.3
1	B	359	THR	2.3
1	B	296	TYR	2.2
1	B	266	VAL	2.2
1	B	272	GLU	2.2
1	A	237	GLY	2.1
1	A	271	PRO	2.1
1	B	407	TYR	2.1
1	B	323	VAL	2.1
1	B	239	SER	2.0
1	A	239	SER	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<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	508	14/15	0.83	0.21	0.25	86,109,125,125	0
2	NAG	B	507	14/15	0.81	0.20	-0.14	82,103,109,110	0
2	NAG	A	501	14/15	0.78	0.19	-1.58	133,150,157,161	0
5	MAN	B	506	11/12	0.91	0.13	-	83,103,111,115	0
5	MAN	A	507	11/12	0.85	0.20	-	93,110,117,124	0
2	NAG	B	505	14/15	0.92	0.19	-	115,129,136,139	0
2	NAG	B	502	14/15	0.79	0.30	-	121,153,164,165	0
4	BMA	A	504	11/12	0.90	0.21	-	104,123,139,145	0
5	MAN	A	505	11/12	0.92	0.25	-	120,132,139,148	0
2	NAG	A	506	14/15	0.81	0.29	-	120,139,147,151	0
5	MAN	B	504	11/12	0.95	0.20	-	103,127,134,134	0
3	FUC	B	508	10/11	0.88	0.20	-	126,138,145,146	0
2	NAG	A	503	14/15	0.90	0.19	-	107,121,134,140	0
2	NAG	B	501	14/15	0.80	0.24	-	138,150,162,166	0
4	BMA	B	503	11/12	0.89	0.13	-	110,124,136,139	0
3	FUC	A	502	10/11	0.67	0.35	-	134,148,157,162	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.