



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:04 am GMT

PDB ID : 3ZO0  
Title : Mouse IgG2a in complex with mouse TRIM21 PRYSPRY  
Authors : James, L.C.  
Deposited on : 2013-02-19  
Resolution : 1.99 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 : trunk28620  
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) : recalc28949

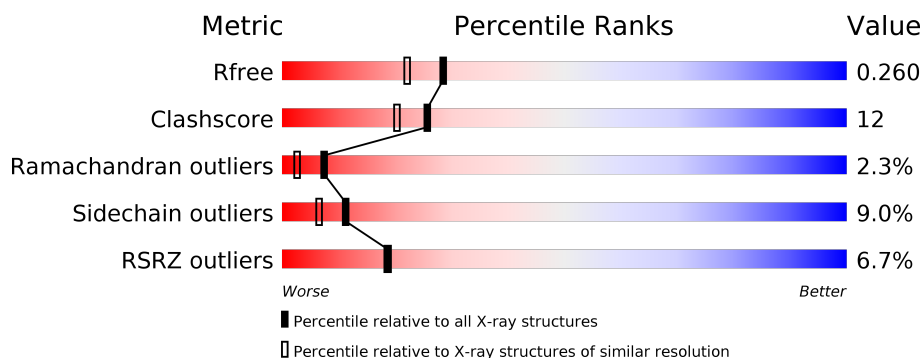
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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>10%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>6%</div> <div>•</div> </div> </div>
2	B	182	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <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
3	NAG	A	1444	X	-	-	-
3	GAL	A	1450	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3405 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, A ALLELE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1673	1059	282	322	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	SER	THR	CONFLICT	UNP P01863

- Molecule 2 is a protein called E3 UBIQUITIN-PROTEIN LIGASE TRIM21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1447	925	250	264	8			

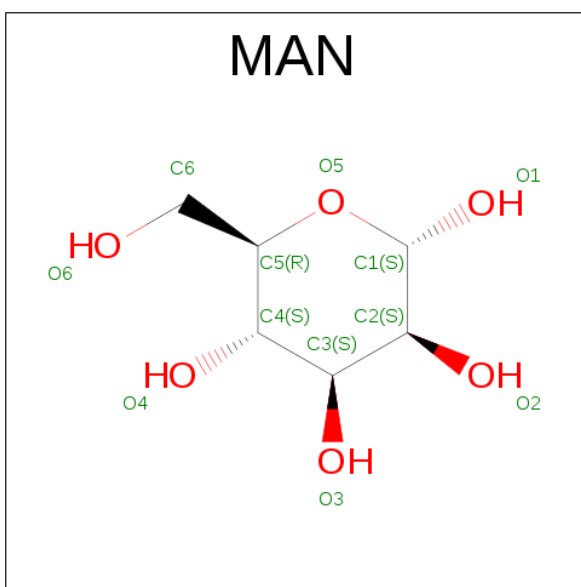
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	EXPRESSION TAG	UNP Q62191
B	8	MET	-	EXPRESSION TAG	UNP Q62191
B	107	LYS	ASP	CONFLICT	UNP Q62191

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

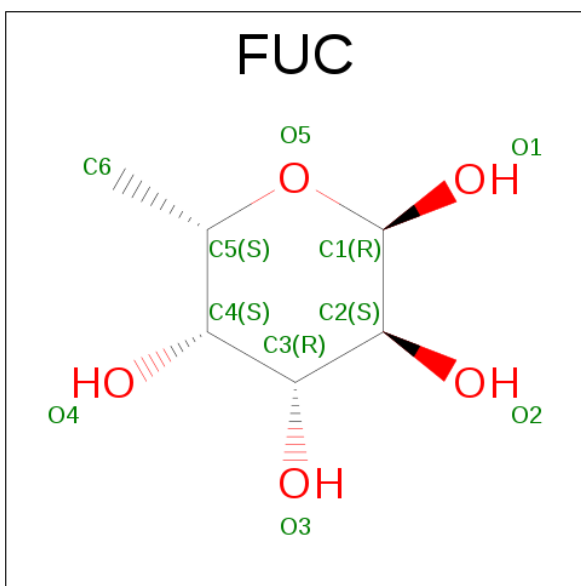
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 4 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (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		

- Molecule 5 is SUGAR (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		

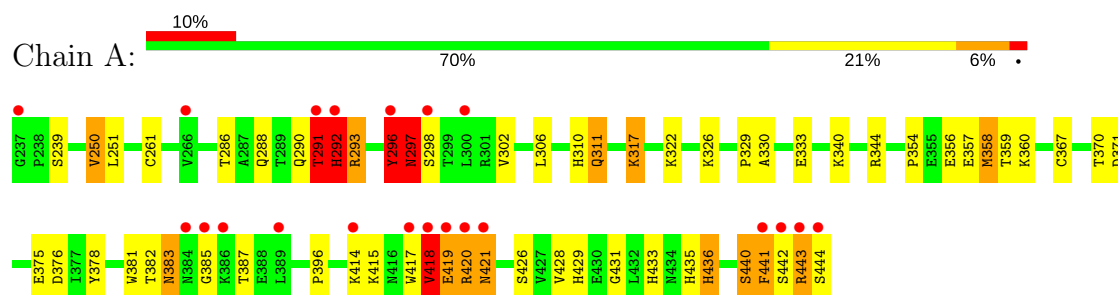
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	94	Total 94	O 94	0	0
6	B	95	Total 95	O 95	0	0

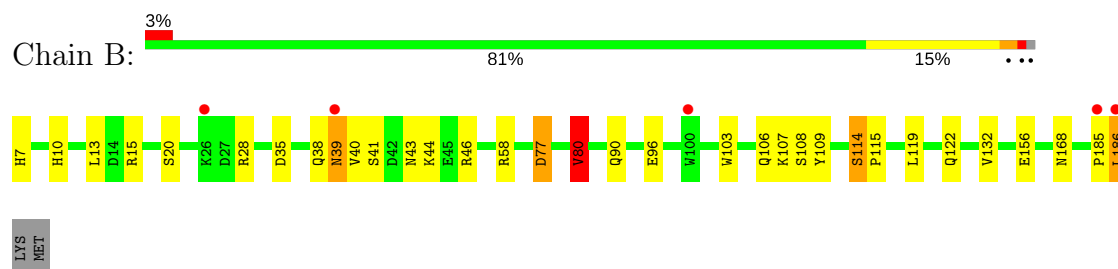
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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-2A CHAIN C REGION, A ALLELE



- Molecule 2: E3 UBIQUITIN-PROTEIN LIGASE TRIM21



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.46Å 186.19Å 124.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.15 – 1.99 44.16 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.15-1.99) 98.0 (44.16-1.99)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.181 , 0.253 0.194 , 0.260	Depositor DCC
$R_{free}$ test set	1798 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MAN, GAL, BMA, NAG, FUC

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	0.89	1/1716 (0.1%)	1.01	6/2336 (0.3%)
2	B	1.00	3/1490 (0.2%)	1.04	6/2025 (0.3%)
All	All	0.94	4/3206 (0.1%)	1.02	12/4361 (0.3%)

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	A	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	96	GLU	CD-OE2	8.62	1.35	1.25
1	A	375	GLU	CD-OE1	5.96	1.32	1.25
2	B	114	SER	CB-OG	-5.81	1.34	1.42
2	B	108	SER	CB-OG	-5.14	1.35	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ASP	CB-CG-OD2	-10.21	109.11	118.30
1	A	297	ASN	CB-CA-C	-8.03	94.34	110.40
1	A	376	ASP	CB-CG-OD1	7.12	124.70	118.30
2	B	77	ASP	CB-CG-OD1	6.37	124.03	118.30
2	B	80	VAL	CB-CA-C	-6.26	99.50	111.40
2	B	40	VAL	N-CA-C	-5.79	95.36	111.00
1	A	261	CYS	CA-CB-SG	-5.37	104.33	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	TYR	N-CA-C	5.32	125.36	111.00
2	B	28	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	B	15	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	B	96	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	A	426	SER	CB-CA-C	-5.00	100.59	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1444	NAG	C1

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	1673	0	1635	49	0
2	B	1447	0	1385	21	0
3	A	75	0	64	7	0
4	A	11	0	10	3	0
5	A	10	0	10	4	0
6	A	94	0	0	8	0
6	B	95	0	0	5	0
All	All	3405	0	3104	75	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 12.

All (75) 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:296:TYR:CD1	1:A:297:ASN:N	2.27	1.03
1:A:250:VAL:O	1:A:310:HIS:HD2	1.58	0.87
2:B:114:SER:HB3	6:B:2061:HOH:O	1.79	0.83
1:A:292:HIS:HB3	1:A:302:VAL:HG22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLN:O	1:A:292:HIS:N	2.19	0.75
3:A:1444:NAG:C6	5:A:1451:FUC:H2	2.18	0.74
1:A:296:TYR:C	1:A:298:SER:H	1.92	0.72
2:B:58:ARG:HD3	6:B:2023:HOH:O	1.89	0.71
3:A:1446:BMA:O3	4:A:1449:MAN:O5	2.09	0.69
1:A:418:VAL:O	1:A:443:ARG:HD2	1.92	0.68
1:A:296:TYR:CG	1:A:297:ASN:N	2.62	0.67
1:A:250:VAL:O	1:A:310:HIS:CD2	2.46	0.67
3:A:1444:NAG:O6	5:A:1451:FUC:H2	1.97	0.65
1:A:429:HIS:HD2	1:A:431:GLY:H	1.43	0.64
1:A:382:THR:HG22	1:A:387:THR:HA	1.79	0.63
1:A:429:HIS:CD2	1:A:431:GLY:H	2.17	0.63
1:A:359:THR:O	1:A:359:THR:HG23	1.99	0.62
3:A:1446:BMA:HO3	4:A:1449:MAN:C5	2.11	0.62
1:A:354:PRO:HD2	1:A:357:GLU:OE1	1.98	0.62
2:B:41:SER:O	2:B:46:ARG:NH1	2.35	0.59
1:A:291:THR:O	1:A:292:HIS:C	2.40	0.59
2:B:107:LYS:HE3	6:B:2057:HOH:O	2.03	0.59
2:B:7:HIS:N	6:B:2001:HOH:O	2.35	0.59
1:A:440:SER:O	1:A:441:PHE:HB3	2.03	0.58
1:A:436:HIS:NE2	6:A:2085:HOH:O	2.20	0.58
1:A:441:PHE:C	1:A:441:PHE:CD1	2.76	0.58
1:A:442:SER:HB2	6:A:2076:HOH:O	2.04	0.57
1:A:296:TYR:CD1	1:A:296:TYR:C	2.79	0.57
1:A:435:HIS:CD2	6:A:2077:HOH:O	2.58	0.56
1:A:378:TYR:CD2	6:A:2064:HOH:O	2.53	0.55
3:A:1444:NAG:C6	5:A:1451:FUC:C2	2.85	0.54
1:A:311:GLN:HE22	2:B:35:ASP:HB3	1.72	0.54
1:A:296:TYR:C	1:A:298:SER:N	2.61	0.54
3:A:1444:NAG:H61	5:A:1451:FUC:C2	2.39	0.52
1:A:370:THR:O	1:A:371:ASP:HB3	2.09	0.51
1:A:433:HIS:HE1	2:B:77:ASP:OD1	1.93	0.51
1:A:382:THR:HG22	1:A:387:THR:HG22	1.93	0.51
1:A:286:THR:HG23	1:A:306:LEU:HD12	1.92	0.51
1:A:421:ASN:O	1:A:442:SER:CB	2.59	0.51
1:A:421:ASN:O	1:A:442:SER:HB3	2.11	0.50
1:A:371:ASP:CG	1:A:371:ASP:O	2.50	0.49
1:A:322:LYS:CG	1:A:333:GLU:HG2	2.42	0.49
1:A:322:LYS:HG2	1:A:333:GLU:HG2	1.94	0.49
1:A:383:ASN:O	1:A:383:ASN:CG	2.51	0.49
1:A:322:LYS:HE2	1:A:333:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:SER:O	2:B:38:GLN:CB	2.61	0.47
2:B:38:GLN:O	2:B:38:GLN:HG3	2.15	0.47
2:B:114:SER:HA	2:B:115:PRO:C	2.35	0.47
2:B:10:HIS:CD2	2:B:186:LEU:HD11	2.50	0.46
1:A:311:GLN:HG2	6:A:2031:HOH:O	2.16	0.46
1:A:417:TRP:CZ3	1:A:442:SER:HA	2.50	0.46
2:B:107:LYS:HE2	2:B:107:LYS:HB2	1.76	0.46
2:B:20:SER:O	2:B:38:GLN:HB3	2.16	0.46
2:B:43:ASN:C	2:B:43:ASN:OD1	2.54	0.46
1:A:326:LYS:HG2	6:A:2040:HOH:O	2.15	0.46
2:B:10:HIS:CD2	2:B:186:LEU:HD21	2.51	0.46
1:A:296:TYR:O	1:A:298:SER:N	2.49	0.45
1:A:359:THR:O	1:A:359:THR:CG2	2.64	0.45
1:A:443:ARG:O	1:A:443:ARG:HG3	2.16	0.44
1:A:329:PRO:O	1:A:330:ALA:HB2	2.16	0.44
1:A:317:LYS:HE2	6:A:2022:HOH:O	2.16	0.44
2:B:38:GLN:O	2:B:39:ASN:HB3	2.18	0.43
2:B:77:ASP:HB2	2:B:168:ASN:HB3	2.00	0.43
1:A:441:PHE:C	1:A:441:PHE:HD1	2.21	0.43
1:A:293:ARG:H	1:A:293:ARG:HG2	1.68	0.43
2:B:90:GLN:HG2	6:B:2021:HOH:O	2.18	0.42
2:B:80:VAL:HG11	2:B:132:VAL:HG21	2.01	0.42
1:A:419:GLU:O	1:A:420:ARG:C	2.58	0.42
3:A:1446:BMA:O3	4:A:1449:MAN:C1	2.68	0.41
2:B:103:TRP:O	2:B:109:TYR:HA	2.21	0.41
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.56	0.41
1:A:358:MET:HA	1:A:358:MET:HE3	2.02	0.41
1:A:251:LEU:HD12	1:A:428:VAL:HG12	2.01	0.41
1:A:291:THR:O	1:A:293:ARG:N	2.54	0.40
6:A:2048:HOH:O	2:B:106:GLN:NE2	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/208 (99%)	190 (92%)	8 (4%)	8 (4%)	3	1
2	B	178/182 (98%)	173 (97%)	4 (2%)	1 (1%)	28	21
All	All	384/390 (98%)	363 (94%)	12 (3%)	9 (2%)	7	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	THR
1	A	297	ASN
1	A	292	HIS
1	A	421	ASN
1	A	420	ARG
1	A	418	VAL
1	A	443	ARG
2	B	185	PRO
1	A	385	GLY

### 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	198/198 (100%)	174 (88%)	24 (12%)	6	3
2	B	158/160 (99%)	150 (95%)	8 (5%)	28	22
All	All	356/358 (99%)	324 (91%)	32 (9%)	11	6

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

Mol	Chain	Res	Type
1	A	239	SER
1	A	250	VAL
1	A	288	GLN
1	A	291	THR

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Mol	Chain	Res	Type
1	A	292	HIS
1	A	293	ARG
1	A	296	TYR
1	A	311	GLN
1	A	317	LYS
1	A	340	LYS
1	A	344	ARG
1	A	356	GLU
1	A	358	MET
1	A	360	LYS
1	A	383	ASN
1	A	396	PRO
1	A	414	LYS
1	A	415	LYS
1	A	418	VAL
1	A	419	GLU
1	A	436	HIS
1	A	440	SER
1	A	441	PHE
1	A	444	SER
2	B	13	LEU
2	B	39	ASN
2	B	44	LYS
2	B	80	VAL
2	B	119	LEU
2	B	122	GLN
2	B	156	GLU
2	B	186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	GLN
1	A	310	HIS
1	A	311	GLN
1	A	325	ASN
1	A	383	ASN
1	A	429	HIS
1	A	433	HIS
1	A	435	HIS
2	B	10	HIS
2	B	39	ASN

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Mol	Chain	Res	Type
2	B	106	GLN
2	B	122	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 ⓘ

6 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	$\# Z  > 2$
3	NAG	A	1444	1,3	14,14,15	1.35	2 (14%)	15,19,21	2.98	5 (33%)
3	NAG	A	1445	3	14,14,15	1.13	3 (21%)	15,19,21	1.20	2 (13%)
3	BMA	A	1446	3	11,11,12	0.91	1 (9%)	13,15,17	1.79	2 (15%)
3	MAN	A	1447	3	11,11,12	1.05	1 (9%)	13,15,17	1.47	3 (23%)
3	NAG	A	1448	3	14,14,15	0.86	0	15,19,21	1.29	1 (6%)
3	GAL	A	1450	3	11,11,12	0.71	0	13,15,17	1.23	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
3	NAG	A	1444	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1445	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	1446	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1447	3	-	0/2/19/22	0/1/1/1
3	NAG	A	1448	3	-	0/6/23/26	0/1/1/1
3	GAL	A	1450	3	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1444	NAG	C2-N2	-2.45	1.42	1.46
3	A	1444	NAG	O5-C1	-2.29	1.40	1.43
3	A	1445	NAG	O5-C1	-2.27	1.40	1.43
3	A	1445	NAG	O7-C7	-2.14	1.18	1.23
3	A	1447	MAN	O5-C1	-2.14	1.40	1.43
3	A	1446	BMA	O5-C1	-2.13	1.40	1.43
3	A	1445	NAG	O5-C5	-2.01	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1444	NAG	O6-C6-C5	-6.55	89.30	111.34
3	A	1444	NAG	C3-C4-C5	-4.08	103.03	110.22
3	A	1444	NAG	C6-C5-C4	-3.51	104.78	113.00
3	A	1447	MAN	C6-C5-C4	-2.90	106.21	113.00
3	A	1448	NAG	O5-C1-C2	-2.89	107.46	111.47
3	A	1446	BMA	O3-C3-C4	-2.59	104.72	110.36
3	A	1447	MAN	O3-C3-C4	-2.24	105.48	110.36
3	A	1445	NAG	O7-C7-C8	-2.23	118.00	122.06
3	A	1447	MAN	C1-O5-C5	2.14	115.12	112.17
3	A	1445	NAG	C1-O5-C5	2.20	115.20	112.17
3	A	1450	GAL	O2-C2-C1	2.98	115.24	109.18
3	A	1444	NAG	O4-C4-C3	3.49	117.95	110.36
3	A	1446	BMA	C1-O5-C5	4.80	118.78	112.17
3	A	1444	NAG	C1-O5-C5	5.81	120.17	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1444	NAG	C1

There are no torsion outliers.

There are no ring outliers.



2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1444	NAG	4	0
3	A	1446	BMA	3	0

## 5.6 Ligand geometry

2 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
4	MAN	A	1449	-	11,11,12	1.15	1 (9%)	13,15,17	3.03	7 (53%)
5	FUC	A	1451	-	9,10,11	1.80	3 (33%)	13,14,16	3.31	8 (61%)

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
4	MAN	A	1449	-	-	0/2/19/22	0/1/1/1
5	FUC	A	1451	-	-	0/0/17/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1451	FUC	O5-C1	-3.08	1.38	1.43
5	A	1451	FUC	C2-C3	-2.94	1.48	1.52
5	A	1451	FUC	O2-C2	-2.85	1.37	1.43
4	A	1449	MAN	C2-C3	2.90	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1451	FUC	O2-C2-C3	-6.62	97.17	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1449	MAN	O2-C2-C1	-5.40	98.19	109.18
5	A	1451	FUC	O2-C2-C1	-4.29	100.45	109.18
5	A	1451	FUC	O5-C1-C2	-4.03	104.47	110.79
4	A	1449	MAN	O5-C1-C2	-3.92	104.64	110.79
4	A	1449	MAN	C3-C4-C5	-2.79	105.30	110.22
5	A	1451	FUC	O4-C4-C3	-2.29	105.38	110.36
5	A	1451	FUC	O5-C5-C4	2.31	113.43	109.62
4	A	1449	MAN	O3-C3-C2	2.66	114.87	110.02
5	A	1451	FUC	C2-C3-C4	2.82	115.79	110.88
5	A	1451	FUC	C3-C4-C5	3.66	115.43	109.68
4	A	1449	MAN	C1-O5-C5	4.06	117.76	112.17
4	A	1449	MAN	O2-C2-C3	4.21	118.44	110.17
4	A	1449	MAN	C1-C2-C3	4.42	115.26	109.65
5	A	1451	FUC	C1-C2-C3	5.35	116.44	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1449	MAN	3	0
5	A	1451	FUC	4	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%)	0.66	21 (10%) 8 8	21, 37, 82, 114	0
2	B	180/182 (98%)	0.45	5 (2%) 53 53	17, 26, 51, 103	0
All	All	388/390 (99%)	0.56	26 (6%) 19 18	17, 31, 71, 114	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	186	LEU	8.1
1	A	420	ARG	5.8
1	A	291	THR	5.8
1	A	418	VAL	5.4
1	A	441	PHE	5.4
1	A	443	ARG	5.3
1	A	444	SER	4.9
1	A	292	HIS	4.7
1	A	417	TRP	4.4
1	A	296	TYR	4.2
1	A	419	GLU	3.9
2	B	185	PRO	3.8
1	A	385	GLY	3.5
1	A	298	SER	3.4
1	A	389	LEU	3.3
1	A	442	SER	3.2
1	A	421	ASN	3.1
1	A	300	LEU	2.9
1	A	386	LYS	2.5
1	A	266	VAL	2.4
1	A	414	LYS	2.3
1	A	237	GLY	2.2
1	A	384	ASN	2.2
2	B	39	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	26	LYS	2.1
2	B	100	TRP	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<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
3	GAL	A	1450	11/12	0.85	0.19	4.94	34,42,50,50	0
3	NAG	A	1444	14/15	0.92	0.16	-0.71	29,35,39,40	0
3	NAG	A	1448	14/15	0.95	0.07	-1.38	27,32,36,38	0
3	BMA	A	1446	11/12	0.91	0.10	-	23,27,31,32	0
3	NAG	A	1445	14/15	0.96	0.10	-	26,29,33,37	0
3	MAN	A	1447	11/12	0.96	0.07	-	23,32,34,50	0

## 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
4	MAN	A	1449	11/12	0.86	0.13	-	31,34,39,40	0
5	FUC	A	1451	10/11	0.74	0.21	-	33,50,57,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.