



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:50 PM GMT

PDB ID : 3V7M  
Title : Crystal structure of monoclonal human anti-Rhesus D Fc IgG1 T125(YB2/0) in the presence of Zn<sup>2+</sup>  
Authors : Menez, R.; Stura, E.A.; Bourel, D.; Siberil, S.; Jorieux, S.; De Romeuf, C.; Ducancel, F.; Fridman, W.H.; Teillaud, J.L.  
Deposited on : 2011-12-21  
Resolution : 2.02 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 (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

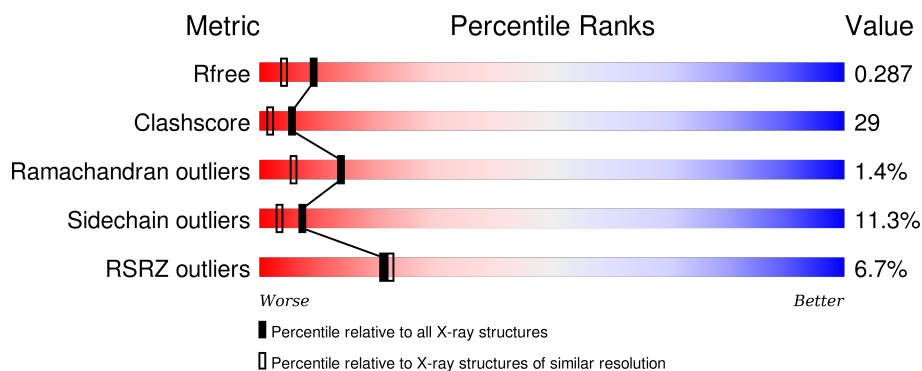
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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	209	<div> <div>7%</div> <div>60%</div> <div>33%</div> <div>8%</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	GAL	A	506	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMD	A	513	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 1935 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	209	Total	C	N	O	S	0	0	0
			1669	1061	281	321	6			

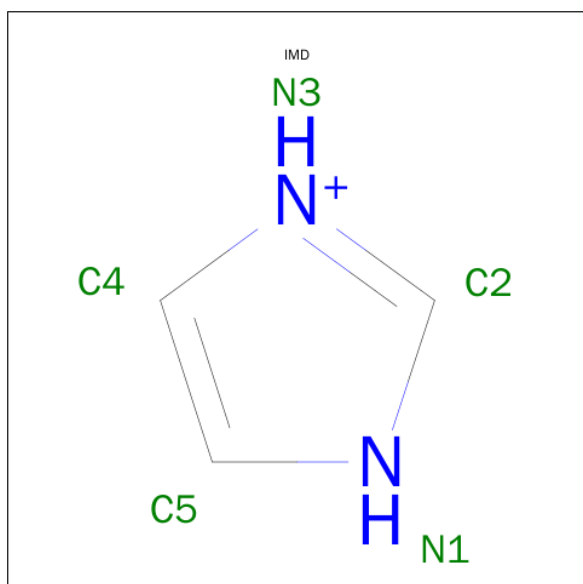
- Molecule 2 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	8	Total	C	N	O	0	0
			100	56	4	40		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

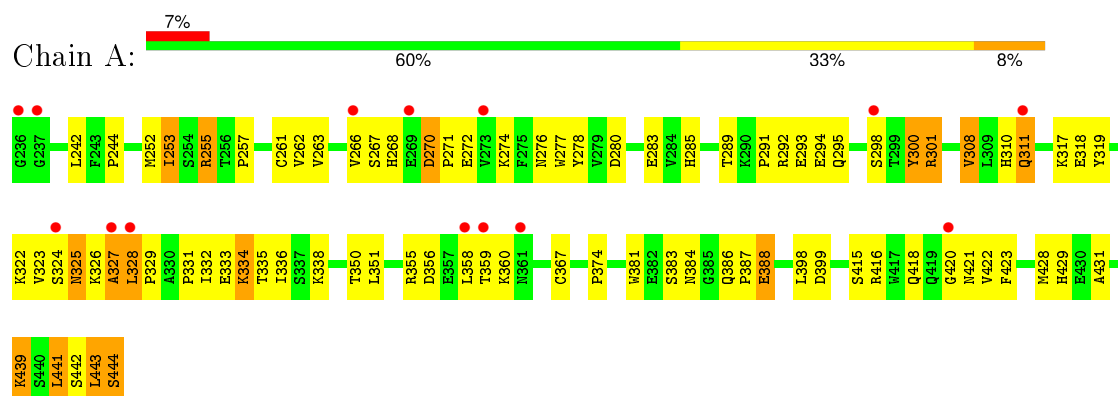
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		

### 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.22Å 147.75Å 75.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.24 – 2.02 35.16 – 2.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.24-2.02) 93.2 (35.16-2.02)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.234 , 0.286 0.238 , 0.287	Depositor DCC
$R_{free}$ test set	882 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.4	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	0 of 17680 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: GOL, ZN, NAG, GAL, MAN, IMD

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	1.09	1/1715 (0.1%)	0.98	2/2335 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	GLN	CB-CG	-6.00	1.36	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	255	ARG	NE-CZ-NH2	5.16	122.88	120.30

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	1669	0	1633	99	0
2	A	100	0	85	2	0
3	A	3	0	0	0	0
4	A	15	0	13	7	0
5	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	142	0	0	18	0
All	All	1935	0	1739	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 29.

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:324:SER:HB2	6:A:742:HOH:O	1.29	1.30
1:A:253:ILE:CD1	1:A:253:ILE:H	1.47	1.20
1:A:386:GLN:CG	1:A:387:PRO:HD2	1.72	1.20
1:A:386:GLN:HG3	6:A:727:HOH:O	1.41	1.17
1:A:253:ILE:HD12	1:A:253:ILE:N	1.59	1.15
1:A:386:GLN:HG2	1:A:387:PRO:CD	1.87	1.03
1:A:415:SER:HA	6:A:654:HOH:O	1.58	1.02
1:A:274:LYS:HB3	6:A:742:HOH:O	1.60	0.99
5:A:515:GOL:H31	6:A:736:HOH:O	1.64	0.98
1:A:271:PRO:HB2	1:A:292:ARG:NH2	1.78	0.98
1:A:253:ILE:HD12	1:A:253:ILE:H	0.78	0.94
1:A:271:PRO:HB2	1:A:292:ARG:HH21	1.36	0.90
1:A:443:LEU:O	1:A:444:SER:HB2	1.69	0.90
1:A:388:GLU:OE2	1:A:423:PHE:HE2	1.57	0.88
1:A:429:HIS:HD2	1:A:431:ALA:H	1.19	0.87
1:A:386:GLN:HG2	1:A:387:PRO:HD2	0.91	0.84
1:A:268:HIS:HD2	6:A:728:HOH:O	1.59	0.84
1:A:270:ASP:HB3	1:A:326:LYS:HG3	1.59	0.83
1:A:388:GLU:OE2	1:A:423:PHE:CE2	2.32	0.82
1:A:429:HIS:CD2	1:A:431:ALA:H	1.96	0.82
2:A:507:MAN:H4	2:A:508:NAG:C1	2.10	0.82
1:A:350:THR:HB	1:A:441:LEU:HG	1.62	0.81
1:A:272:GLU:HA	1:A:292:ARG:HH12	1.46	0.80
1:A:398:LEU:HD23	1:A:399:ASP:N	1.97	0.80
1:A:271:PRO:C	1:A:292:ARG:HH22	1.87	0.77
1:A:398:LEU:HD23	1:A:398:LEU:C	2.05	0.77
1:A:272:GLU:O	1:A:325:ASN:ND2	2.20	0.73
1:A:271:PRO:CB	1:A:292:ARG:NH2	2.54	0.71
1:A:276:ASN:HD22	1:A:322:LYS:HD2	1.56	0.70
1:A:268:HIS:O	1:A:271:PRO:HG3	1.92	0.69
1:A:252:MET:HG3	1:A:428:MET:HE3	1.74	0.69
1:A:263:VAL:HG21	1:A:323:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:CG	1:A:387:PRO:CD	2.61	0.69
1:A:311:GLN:HG2	6:A:689:HOH:O	1.93	0.68
1:A:308:VAL:HG22	1:A:319:TYR:CZ	2.29	0.68
1:A:268:HIS:NE2	1:A:298:SER:O	2.27	0.67
5:A:515:GOL:C3	6:A:736:HOH:O	2.30	0.66
1:A:384:ASN:HB3	6:A:731:HOH:O	1.95	0.65
1:A:310:HIS:CD2	4:A:513:IMD:H2	2.30	0.65
1:A:311:GLN:OE1	1:A:311:GLN:HA	1.96	0.64
1:A:443:LEU:O	1:A:444:SER:CB	2.44	0.64
1:A:311:GLN:OE1	4:A:513:IMD:N3	2.33	0.61
1:A:386:GLN:N	6:A:726:HOH:O	2.34	0.60
1:A:271:PRO:O	1:A:292:ARG:NH2	2.34	0.60
1:A:274:LYS:HE2	6:A:742:HOH:O	2.01	0.60
1:A:267:SER:O	1:A:271:PRO:HB3	2.02	0.59
1:A:252:MET:HG3	1:A:428:MET:CE	2.32	0.59
1:A:294:GLU:N	6:A:741:HOH:O	2.35	0.59
1:A:262:VAL:HG21	6:A:680:HOH:O	2.03	0.58
1:A:398:LEU:CD2	1:A:399:ASP:O	2.51	0.58
1:A:253:ILE:N	1:A:253:ILE:CD1	2.28	0.57
1:A:398:LEU:CD2	1:A:398:LEU:C	2.72	0.56
1:A:374:PRO:O	1:A:429:HIS:HE1	1.88	0.56
1:A:311:GLN:OE1	1:A:311:GLN:CA	2.48	0.56
1:A:318:GLU:HG2	1:A:335:THR:HG21	1.88	0.56
1:A:384:ASN:CB	6:A:731:HOH:O	2.53	0.56
1:A:384:ASN:HD22	1:A:421:ASN:HD22	1.54	0.54
1:A:334:LYS:HA	1:A:334:LYS:HZ2	1.72	0.54
1:A:271:PRO:C	1:A:292:ARG:NH2	2.59	0.54
1:A:333:GLU:O	1:A:334:LYS:NZ	2.40	0.53
1:A:283:GLU:OE2	1:A:285:HIS:HE1	1.92	0.53
1:A:257:PRO:HG2	1:A:308:VAL:HG12	1.91	0.52
1:A:268:HIS:CD2	1:A:298:SER:O	2.63	0.52
1:A:423:PHE:O	1:A:441:LEU:N	2.37	0.52
1:A:244:PRO:HD3	1:A:336:ILE:HD11	1.92	0.50
1:A:359:THR:O	1:A:359:THR:HG22	2.10	0.50
1:A:383:SER:OG	1:A:422:VAL:O	2.25	0.50
4:A:514:IMD:C2	6:A:676:HOH:O	2.60	0.50
1:A:253:ILE:HD11	4:A:514:IMD:H4	1.95	0.49
1:A:420:GLY:HA3	6:A:725:HOH:O	2.12	0.49
1:A:398:LEU:HD23	1:A:399:ASP:O	2.12	0.48
1:A:283:GLU:OE2	1:A:285:HIS:CE1	2.67	0.48
1:A:334:LYS:HA	1:A:334:LYS:NZ	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:C	1:A:420:GLY:H	2.17	0.47
1:A:383:SER:O	1:A:384:ASN:C	2.53	0.47
1:A:266:VAL:CG1	1:A:300:TYR:HB2	2.45	0.47
1:A:285:HIS:HB3	4:A:512:IMD:C2	2.45	0.46
1:A:295:GLN:NE2	1:A:301:ARG:HG2	2.29	0.46
1:A:335:THR:HG22	1:A:336:ILE:N	2.31	0.46
1:A:384:ASN:ND2	1:A:421:ASN:HD22	2.14	0.45
1:A:270:ASP:HB2	1:A:327:ALA:HB2	1.99	0.44
1:A:360:LYS:NZ	6:A:713:HOH:O	2.50	0.44
1:A:418:GLN:C	1:A:420:GLY:N	2.71	0.44
1:A:278:TYR:N	1:A:278:TYR:CD2	2.86	0.44
1:A:318:GLU:HG2	1:A:335:THR:CG2	2.48	0.44
1:A:386:GLN:HB2	6:A:726:HOH:O	2.17	0.43
2:A:507:MAN:C4	2:A:508:NAG:C1	2.84	0.43
1:A:268:HIS:HE1	1:A:294:GLU:OE1	2.01	0.43
1:A:328:LEU:HD11	1:A:332:ILE:HD11	2.00	0.42
1:A:266:VAL:HG12	1:A:300:TYR:O	2.18	0.42
1:A:324:SER:OG	1:A:331:PRO:HB3	2.20	0.42
1:A:285:HIS:HB3	4:A:512:IMD:H2	2.02	0.42
1:A:310:HIS:NE2	4:A:513:IMD:H2	2.34	0.42
1:A:276:ASN:HB2	1:A:322:LYS:HB3	2.02	0.41
1:A:262:VAL:O	1:A:262:VAL:HG23	2.19	0.41
1:A:308:VAL:HG22	1:A:319:TYR:OH	2.18	0.41
1:A:439:LYS:HA	1:A:439:LYS:HD2	1.68	0.41
1:A:388:GLU:OE2	1:A:423:PHE:CD2	2.70	0.41
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.56	0.41
1:A:308:VAL:HG22	1:A:319:TYR:CE2	2.55	0.41
1:A:326:LYS:HG2	1:A:326:LYS:H	1.59	0.41
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.56	0.41
1:A:338:LYS:HB3	1:A:338:LYS:HE3	1.96	0.40
1:A:280:ASP:OD1	1:A:317:LYS:HD3	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	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	14 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ALA
1	A	291	PRO
1	A	329	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	194/194 (100%)	172 (89%)	22 (11%)	7 3

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	253	ILE
1	A	255	ARG
1	A	270	ASP
1	A	289	THR
1	A	293	GLU
1	A	300	TYR
1	A	301	ARG
1	A	308	VAL
1	A	325	ASN
1	A	328	LEU
1	A	334	LYS
1	A	351	LEU
1	A	355	ARG
1	A	358	LEU
1	A	388	GLU

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Mol	Chain	Res	Type
1	A	416	ARG
1	A	439	LYS
1	A	441	LEU
1	A	442	SER
1	A	443	LEU
1	A	444	SER

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	276	ASN
1	A	295	GLN
1	A	342	GLN
1	A	384	ASN
1	A	386	GLN
1	A	389	ASN
1	A	419	GLN
1	A	429	HIS

### 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 ⓘ

8 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	501	1,2	14,14,15	0.63	0	15,19,21	1.20	1 (6%)
2	NAG	A	502	2	14,14,15	0.53	0	15,19,21	2.06	4 (26%)
2	MAN	A	503	2	11,11,12	0.80	0	14,15,17	2.77	5 (35%)
2	MAN	A	504	2	11,11,12	0.78	0	14,15,17	1.58	4 (28%)
2	NAG	A	505	2	14,14,15	0.95	1 (7%)	15,19,21	1.44	3 (20%)
2	GAL	A	506	2	11,11,12	1.04	1 (9%)	14,15,17	0.97	1 (7%)
2	MAN	A	507	2	11,11,12	0.58	0	14,15,17	2.42	6 (42%)
2	NAG	A	508	2	14,14,15	0.83	1 (7%)	15,19,21	2.37	5 (33%)

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	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	MAN	A	503	2	-	0/2/19/22	0/1/1/1
2	MAN	A	504	2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	2	-	0/6/23/26	0/1/1/1
2	GAL	A	506	2	-	0/2/19/22	0/1/1/1
2	MAN	A	507	2	-	0/2/19/22	0/1/1/1
2	NAG	A	508	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	506	GAL	O5-C1	-2.64	1.39	1.43
2	A	505	NAG	O5-C1	-2.49	1.39	1.43
2	A	508	NAG	C1-C2	2.33	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	NAG	C4-C3-C2	-4.44	104.32	111.23
2	A	503	MAN	O3-C3-C2	-4.25	102.31	110.00
2	A	502	NAG	C2-N2-C7	-3.80	118.16	123.04
2	A	504	MAN	O2-C2-C3	-3.33	103.42	110.12
2	A	503	MAN	C2-C3-C4	-2.80	106.29	111.04
2	A	507	MAN	C2-C3-C4	-2.70	106.45	111.04

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	508	NAG	C4-C3-C2	-2.54	107.29	111.23
2	A	508	NAG	C3-C4-C5	-2.50	105.84	110.20
2	A	505	NAG	C1-O5-C5	-2.40	109.20	112.25
2	A	506	GAL	O3-C3-C4	-2.17	105.46	110.34
2	A	508	NAG	O7-C7-C8	-2.15	118.12	122.06
2	A	504	MAN	C6-C5-C4	-2.07	107.91	113.02
2	A	505	NAG	O3-C3-C2	-2.04	105.06	109.11
2	A	504	MAN	C3-C4-C5	2.00	113.68	110.20
2	A	503	MAN	C1-C2-C3	2.15	112.09	109.54
2	A	505	NAG	C3-C4-C5	2.18	114.00	110.20
2	A	507	MAN	O5-C1-C2	2.45	114.83	110.86
2	A	507	MAN	O4-C4-C5	2.51	115.90	109.24
2	A	504	MAN	C1-O5-C5	2.57	115.52	112.25
2	A	502	NAG	O4-C4-C5	2.59	116.09	109.24
2	A	507	MAN	C1-C2-C3	2.60	112.61	109.54
2	A	508	NAG	C3-C2-N2	2.62	116.84	110.56
2	A	507	MAN	O2-C2-C1	2.79	114.80	109.21
2	A	501	NAG	C1-O5-C5	3.40	116.57	112.25
2	A	503	MAN	O5-C1-C2	3.53	116.58	110.86
2	A	502	NAG	C1-O5-C5	3.65	116.88	112.25
2	A	507	MAN	C1-O5-C5	6.18	120.09	112.25
2	A	508	NAG	C1-O5-C5	6.86	120.95	112.25
2	A	503	MAN	C1-O5-C5	7.20	121.39	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	MAN	2	0
2	A	508	NAG	2	0

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	IMD	A	512	3	3,5,5	0.58	0	4,5,5	0.67	0
4	IMD	A	513	3	3,5,5	0.67	0	4,5,5	0.89	0
4	IMD	A	514	3	3,5,5	0.60	0	4,5,5	0.62	0
5	GOL	A	515	-	5,5,5	0.61	0	5,5,5	1.30	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMD	A	512	3	-	0/0/0/0	0/1/1/1
4	IMD	A	513	3	-	0/0/0/0	0/1/1/1
4	IMD	A	514	3	-	0/0/0/0	0/1/1/1
5	GOL	A	515	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	515	GOL	O1-C1-C2	-2.21	99.45	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	512	IMD	2	0
4	A	513	IMD	3	0
4	A	514	IMD	2	0
5	A	515	GOL	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	209/209 (100%)	0.62	14 (6%)	21 22	20, 45, 72, 82	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	SER	5.1
1	A	236	GLY	4.9
1	A	237	GLY	4.5
1	A	358	LEU	3.7
1	A	273	VAL	3.1
1	A	327	ALA	3.0
1	A	359	THR	3.0
1	A	266	VAL	2.8
1	A	269	GLU	2.8
1	A	361	ASN	2.7
1	A	420	GLY	2.6
1	A	311	GLN	2.5
1	A	324	SER	2.5
1	A	328	LEU	2.4

### 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( $\text{\AA}^2$ )	Q<0.9
2	GAL	A	506	11/12	0.90	0.25	4.69	48,50,54,56	11
2	NAG	A	505	14/15	0.91	0.15	0.32	51,54,55,57	0
2	NAG	A	501	14/15	0.83	0.16	-	72,74,76,78	0
2	NAG	A	502	14/15	0.91	0.15	-	61,69,71,71	0
2	MAN	A	507	11/12	0.88	0.27	-	86,91,94,95	0
2	NAG	A	508	14/15	0.61	0.30	-	97,99,100,100	0
2	MAN	A	504	11/12	0.87	0.15	-	53,57,61,63	0
2	MAN	A	503	11/12	0.95	0.09	-	52,68,72,79	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( $\text{\AA}^2$ )	Q<0.9
4	IMD	A	513	5/5	0.85	0.34	2.72	29,30,33,34	5
4	IMD	A	512	5/5	0.97	0.10	-	41,46,50,50	0
5	GOL	A	515	6/6	0.87	0.41	-	28,31,33,33	0
3	ZN	A	509	1/1	0.98	0.12	-	38,38,38,38	0
4	IMD	A	514	5/5	0.98	0.28	-	30,36,37,39	5
3	ZN	A	510	1/1	0.97	0.09	-	63,63,63,63	0
3	ZN	A	511	1/1	0.94	0.10	-	48,48,48,48	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.