



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:02 AM BST

PDB ID : 3IF1  
Title : Crystal structure of 237mAb in complex with a GalNAc  
Authors : Brooks, C.L.; Evans, S.V.; Borisova, S.N.  
Deposited on : 2009-07-23  
Resolution : 2.39 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

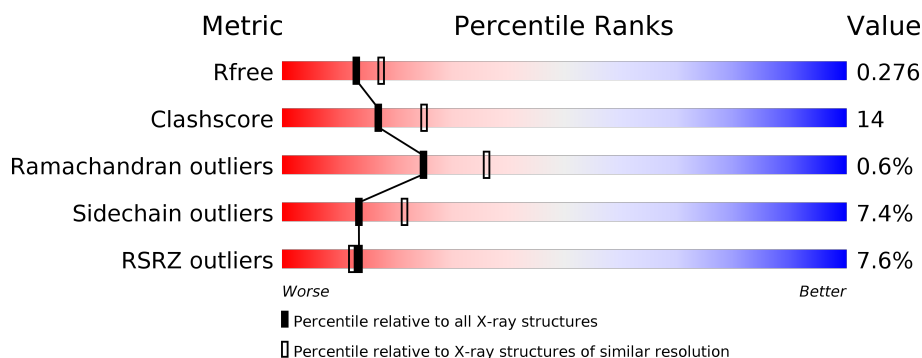
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. 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	215	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
1	C	215	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>.</div> </div> </div>
2	B	217	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>30%</div> <div>5%</div> <div>.</div> </div> </div>
2	D	217	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>.</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NGA	B	1(A)	X	-	-	-
5	NGA	D	213	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6981 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 Immunoglobulin light chain (IgG2a).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1659	1036	282	336	5			
1	C	215	Total	C	N	O	S	0	0	0
			1659	1036	282	336	5			

- Molecule 2 is a protein called Immunoglobulin heavy chain (IgG2a).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1600	1006	272	314	8			
2	D	210	Total	C	N	O	S	0	0	0
			1600	1006	272	314	8			

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

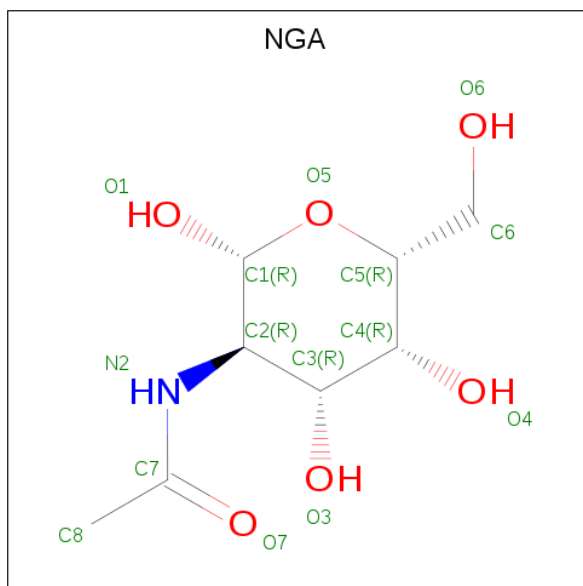
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	3	Total	Mg	0	0
			3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA)

(formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			15	8	1	6		
5	D	1	Total	C	N	O	0	0
			15	8	1	6		

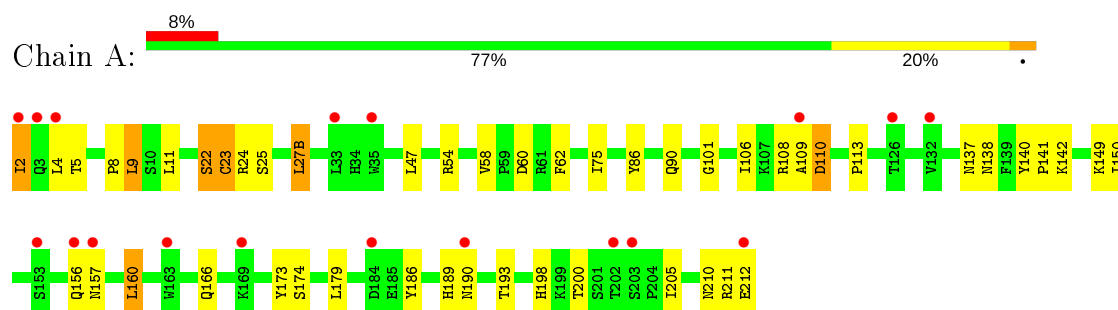
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	115	Total	O	0	0
			115	115		
6	C	92	Total	O	0	0
			92	92		
6	D	93	Total	O	0	0
			93	93		

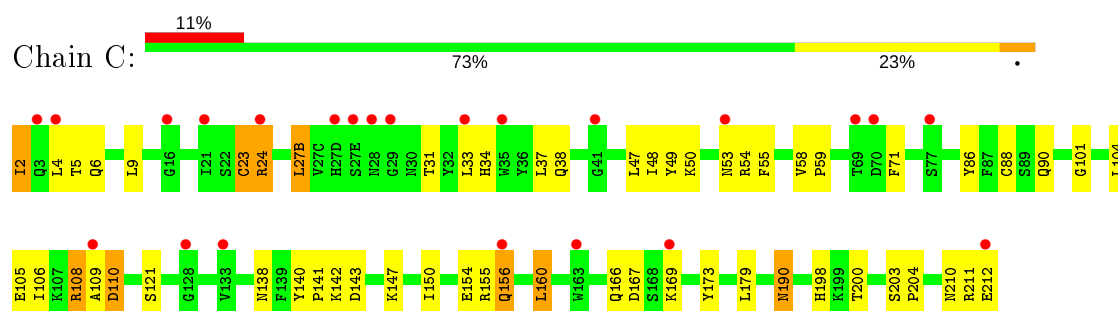
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

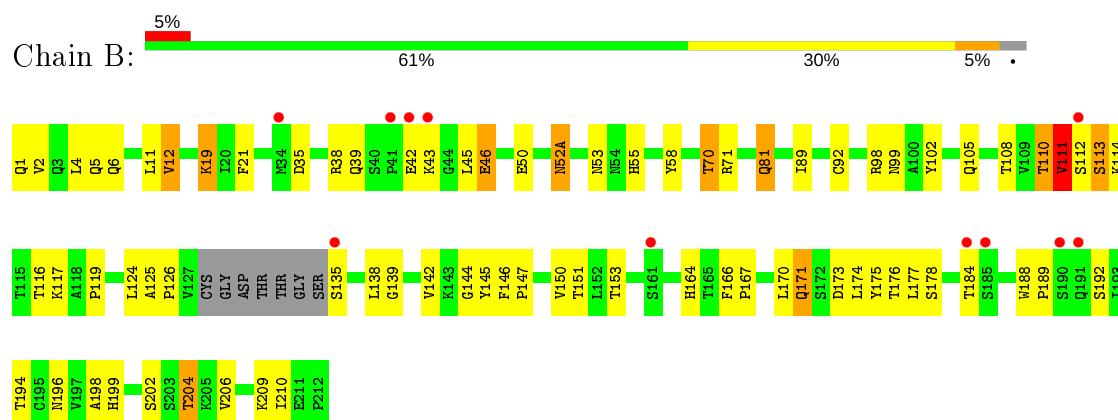
- Molecule 1: Immunoglobulin light chain (IgG2a)



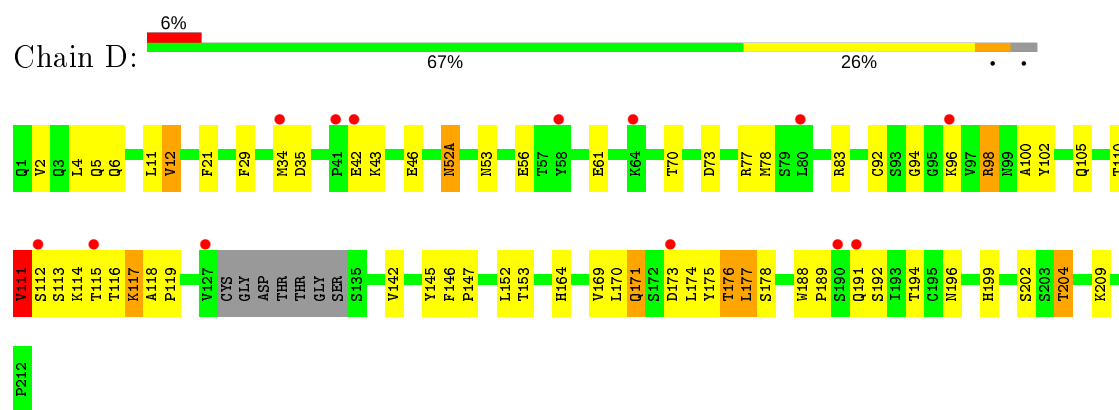
- Molecule 1: Immunoglobulin light chain (IgG2a)



- Molecule 2: Immunoglobulin heavy chain (IgG2a)



- Molecule 2: Immunoglobulin heavy chain (IgG2a)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.35Å 38.42Å 95.99Å 90.00° 109.11° 90.00°	Depositor
Resolution (Å)	19.93 – 2.39 19.93 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.93-2.39) 99.0 (19.93-2.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.38Å)	Xtriage
Refinement program	PHENIX 1.4 _4	Depositor
R, $R_{free}$	0.224 , 0.285 0.215 , 0.276	Depositor DCC
$R_{free}$ test set	1938 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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: MG, ZN, NGA

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	0.26	0/1697	0.46	0/2303
1	C	0.25	0/1697	0.44	0/2303
2	B	0.26	0/1638	0.49	0/2228
2	D	0.26	0/1638	0.48	0/2228
All	All	0.26	0/6670	0.47	0/9062

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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	111	VAL	Peptide
2	D	111	VAL	Peptide

## 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	1659	0	1601	32	0
1	C	1659	0	1601	45	0
2	B	1600	0	1563	58	0
2	D	1600	0	1563	53	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	C	3	0	0	0	0
5	B	15	0	14	1	0
5	D	15	0	14	0	0
6	A	123	0	0	3	0
6	B	115	0	0	1	0
6	C	92	0	0	3	0
6	D	93	0	0	4	0
All	All	6981	0	6356	181	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 14.

All (181) 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)
2:B:11:LEU:HD11	2:B:112:SER:HB3	1.19	1.14
2:D:6:GLN:HE21	2:D:92:CYS:H	1.09	1.00
2:B:11:LEU:HD11	2:B:112:SER:CB	1.99	0.94
2:B:11:LEU:CD1	2:B:112:SER:HB3	1.97	0.93
2:B:6:GLN:HE21	2:B:92:CYS:H	1.01	0.93
2:D:11:LEU:HD11	2:D:112:SER:HB3	1.55	0.88
1:C:109:ALA:O	1:C:110:ASP:HB2	1.80	0.81
2:D:11:LEU:HD11	2:D:112:SER:CB	2.12	0.80
1:A:109:ALA:O	1:A:110:ASP:HB2	1.82	0.79
2:D:153:THR:HG22	2:D:196:ASN:HB2	1.66	0.77
2:D:6:GLN:NE2	2:D:92:CYS:H	1.83	0.76
2:B:153:THR:HG22	2:B:196:ASN:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:HD3	6:C:217:HOH:O	1.86	0.75
1:A:211:ARG:O	1:A:212:GLU:HG2	1.86	0.73
2:B:199:HIS:HD2	2:B:202:SER:OG	1.75	0.70
2:D:11:LEU:CD1	2:D:112:SER:HB3	2.21	0.70
2:B:6:GLN:NE2	2:B:92:CYS:H	1.85	0.69
2:B:6:GLN:HE21	2:B:92:CYS:N	1.84	0.69
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.74	0.69
1:C:190:ASN:HB2	1:C:211:ARG:HB2	1.73	0.69
1:C:4:LEU:HD11	1:C:90:GLN:HG3	1.74	0.69
1:A:106:ILE:H	1:A:166:GLN:HE22	1.41	0.68
2:D:35:ASP:OD2	2:D:98:ARG:HD2	1.95	0.66
2:B:35:ASP:OD2	2:B:98:ARG:HD2	1.95	0.66
2:D:147:PRO:O	2:D:199:HIS:HE1	1.78	0.65
1:C:50:LYS:HB2	1:C:53:ASN:HD22	1.60	0.65
2:D:83:ARG:O	2:D:111:VAL:HG11	1.97	0.65
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.79	0.64
2:B:144:GLY:HA2	2:B:174:LEU:HG	1.79	0.64
2:B:135:SER:HB2	2:B:184:THR:HA	1.79	0.64
1:A:9:LEU:HD22	2:D:77:ARG:HD2	1.80	0.64
1:C:110:ASP:N	6:C:217:HOH:O	2.30	0.64
1:C:6:GLN:HG2	1:C:23:CYS:HB2	1.81	0.63
1:C:106:ILE:H	1:C:166:GLN:HE22	1.45	0.62
2:B:11:LEU:HB2	2:B:147:PRO:HG3	1.80	0.62
2:D:199:HIS:HD2	2:D:202:SER:OG	1.82	0.62
2:D:177:LEU:HD13	2:D:178:SER:N	2.14	0.62
1:A:113:PRO:HG2	1:A:205:ILE:HD12	1.82	0.62
2:B:147:PRO:O	2:B:199:HIS:HE1	1.83	0.61
2:D:188:TRP:CG	2:D:189:PRO:HA	2.36	0.61
2:B:202:SER:OG	2:B:204:THR:HG23	2.02	0.59
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.83	0.59
2:B:43:LYS:HD3	2:B:46:GLU:CD	2.22	0.59
2:B:188:TRP:CG	2:B:189:PRO:HA	2.37	0.59
1:C:211:ARG:O	1:C:212:GLU:HG2	2.02	0.58
1:C:4:LEU:HD11	1:C:90:GLN:CG	2.33	0.58
1:A:109:ALA:O	1:A:110:ASP:CB	2.51	0.58
2:B:114:LYS:HD3	2:B:173:ASP:HA	1.86	0.58
2:D:115:THR:HG22	6:D:229:HOH:O	2.03	0.58
1:A:157:ASN:HB2	6:A:317:HOH:O	2.03	0.58
2:B:177:LEU:HD13	2:B:178:SER:N	2.18	0.57
2:B:188:TRP:CD1	2:B:189:PRO:HA	2.40	0.57
2:B:112:SER:OG	2:B:113:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HE3	2:B:81:GLN:NE2	2.20	0.56
2:D:142:VAL:HB	2:D:177:LEU:HB3	1.85	0.56
2:D:115:THR:HG23	2:D:117:LYS:HD2	1.88	0.55
2:D:53:ASN:O	2:D:56:GLU:HG3	2.06	0.55
1:C:198:HIS:HD2	1:C:200:THR:OG1	1.90	0.55
2:D:114:LYS:HD2	2:D:146:PHE:CE2	2.42	0.55
1:A:4:LEU:HD11	1:A:90:GLN:HG3	1.89	0.54
2:B:50:GLU:HG2	2:B:58:TYR:HB2	1.89	0.54
2:D:5:GLN:NE2	2:D:105:GLN:HE22	2.06	0.54
2:D:114:LYS:HD2	2:D:146:PHE:CZ	2.42	0.54
1:A:138:ASN:HD21	2:B:164:HIS:CE1	2.26	0.53
1:C:142:LYS:HB3	1:C:173:TYR:CE1	2.43	0.53
2:D:43:LYS:HD3	2:D:46:GLU:OE1	2.08	0.53
2:B:43:LYS:HD3	2:B:46:GLU:OE1	2.08	0.53
2:D:192:SER:HB2	2:D:209:LYS:HE3	1.90	0.53
2:D:6:GLN:HE21	2:D:92:CYS:N	1.91	0.53
1:C:160:LEU:HD12	2:D:176:THR:HG23	1.92	0.52
1:C:55:PHE:CZ	2:D:100:ALA:HB1	2.44	0.52
1:A:198:HIS:HD2	1:A:200:THR:OG1	1.93	0.52
1:A:106:ILE:H	1:A:166:GLN:NE2	2.07	0.52
1:A:211:ARG:O	1:A:212:GLU:CG	2.57	0.51
1:C:147:LYS:HE3	1:C:154:GLU:OE1	2.11	0.51
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.92	0.51
2:D:96:LYS:HG3	6:D:342:HOH:O	2.10	0.51
2:D:12:VAL:O	2:D:111:VAL:HA	2.11	0.50
2:B:12:VAL:O	2:B:111:VAL:HA	2.12	0.50
2:B:171:GLN:HG3	2:B:171:GLN:O	2.11	0.50
2:D:170:LEU:HD12	2:D:171:GLN:N	2.27	0.50
2:B:166:PHE:O	2:B:177:LEU:HD22	2.12	0.50
2:B:170:LEU:HB2	2:B:175:TYR:CE2	2.47	0.49
2:B:55:HIS:CD2	2:B:71:ARG:HD3	2.47	0.49
2:D:114:LYS:HB2	2:D:146:PHE:CE1	2.48	0.49
2:D:202:SER:OG	2:D:204:THR:HG23	2.13	0.49
1:C:54:ARG:HG2	1:C:58:VAL:HB	1.95	0.49
2:B:138:LEU:HG	2:B:210:ILE:HG21	1.95	0.48
2:D:112:SER:OG	2:D:113:SER:N	2.45	0.48
2:D:29:PHE:HD2	2:D:73:ASP:HA	1.78	0.48
1:C:138:ASN:HD21	2:D:164:HIS:CE1	2.32	0.48
2:B:19:LYS:HD2	2:B:21:PHE:CZ	2.49	0.48
2:B:192:SER:HB2	2:B:209:LYS:HE3	1.94	0.48
2:B:19:LYS:HD3	2:B:21:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HD11	1:A:27(B):LEU:HD11	1.96	0.47
1:A:189:HIS:O	1:A:211:ARG:HD3	2.14	0.47
1:C:2:ILE:HD13	1:C:90:GLN:HG2	1.96	0.47
1:C:47:LEU:HA	1:C:58:VAL:HG21	1.97	0.47
2:B:114:LYS:HD2	2:B:146:PHE:CZ	2.50	0.47
2:B:114:LYS:HB2	2:B:146:PHE:CE1	2.49	0.46
2:B:153:THR:HG23	2:B:196:ASN:OD1	2.14	0.46
2:B:2:VAL:HG21	2:B:102:TYR:CZ	2.50	0.46
1:C:160:LEU:HD13	2:D:169:VAL:HB	1.97	0.46
1:A:86:TYR:O	1:A:101:GLY:HA2	2.15	0.46
2:D:176:THR:HG21	6:D:296:HOH:O	2.15	0.46
2:D:188:TRP:CD1	2:D:189:PRO:HA	2.50	0.46
2:B:114:LYS:HE3	2:B:173:ASP:OD2	2.14	0.46
1:C:167:ASP:OD2	1:C:169:LYS:HB2	2.16	0.46
2:B:2:VAL:HG11	2:B:102:TYR:CG	2.50	0.46
2:B:5:GLN:NE2	2:B:105:GLN:NE2	2.63	0.46
1:A:186:TYR:CZ	1:A:211:ARG:HD2	2.51	0.46
1:C:54:ARG:HD3	1:C:59:PRO:O	2.15	0.46
1:C:190:ASN:O	1:C:210:ASN:HA	2.16	0.45
2:B:112:SER:O	2:B:113:SER:CB	2.64	0.45
1:A:142:LYS:HB3	1:A:173:TYR:CE1	2.52	0.45
1:C:27(B):LEU:HB3	1:C:31:THR:HG23	1.98	0.45
2:B:5:GLN:NE2	2:B:105:GLN:HE22	2.14	0.45
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.99	0.45
2:B:153:THR:CG2	2:B:196:ASN:HB2	2.44	0.45
1:C:37:LEU:HD12	1:C:38:GLN:N	2.32	0.45
2:B:38:ARG:HA	2:B:89:ILE:O	2.16	0.45
1:C:141:PRO:O	1:C:198:HIS:HE1	2.00	0.45
2:D:52(A):ASN:HB2	2:D:53:ASN:HD22	1.82	0.45
2:D:34:MET:SD	2:D:94:GLY:HA3	2.57	0.45
2:B:98:ARG:NH2	5:B:1(A):NGA:O3	2.50	0.44
1:C:147:LYS:HE3	1:C:154:GLU:CD	2.38	0.44
2:D:114:LYS:HE3	2:D:173:ASP:OD2	2.18	0.44
1:C:104:LEU:HD23	1:C:104:LEU:C	2.38	0.44
1:C:34:HIS:O	1:C:88:CYS:HA	2.17	0.44
2:D:152:LEU:HD23	2:D:153:THR:N	2.32	0.44
1:A:190:ASN:O	1:A:210:ASN:HA	2.18	0.43
1:A:2:ILE:HD11	1:A:25:SER:HB2	1.98	0.43
2:B:70:THR:HB	6:B:214:HOH:O	2.17	0.43
2:B:81:GLN:HB2	2:B:81:GLN:HE21	1.62	0.43
1:A:54:ARG:HD3	1:A:60:ASP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LEU:HD23	1:C:105:GLU:N	2.32	0.43
2:D:171:GLN:O	2:D:171:GLN:HG3	2.18	0.43
2:D:52(A):ASN:HB3	2:D:53:ASN:H	1.83	0.43
1:A:149:LYS:HB2	1:A:193:THR:HB	2.00	0.43
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.99	0.43
1:C:33:LEU:C	1:C:34:HIS:HD2	2.21	0.43
2:D:118:ALA:HB1	2:D:204:THR:HG21	1.99	0.43
1:C:156:GLN:HB3	1:C:156:GLN:HE21	1.63	0.43
2:D:2:VAL:HG11	2:D:102:TYR:CG	2.53	0.43
1:C:86:TYR:O	1:C:101:GLY:HA2	2.19	0.43
1:C:121:SER:HB2	6:C:384:HOH:O	2.19	0.43
2:B:142:VAL:HB	2:B:177:LEU:HB3	2.00	0.43
1:C:49:TYR:O	1:C:53:ASN:HB2	2.19	0.43
2:D:191:GLN:HB3	2:D:191:GLN:HE21	1.68	0.43
1:A:160:LEU:HD22	1:A:160:LEU:HA	1.90	0.42
2:B:124:LEU:HB2	2:B:139:GLY:CA	2.48	0.42
2:D:170:LEU:HB2	2:D:175:TYR:CE2	2.54	0.42
2:D:29:PHE:CD2	2:D:73:ASP:HA	2.54	0.42
1:A:8:PRO:HB3	2:D:21:PHE:HE2	1.84	0.42
2:B:52(A):ASN:HB2	2:B:53:ASN:HD22	1.84	0.42
2:B:151:THR:OG1	2:B:198:ALA:HB3	2.20	0.42
2:B:166:PHE:HA	2:B:167:PRO:HD3	1.87	0.42
1:A:140:TYR:CG	1:A:141:PRO:HA	2.55	0.42
1:A:22:SER:HB3	6:A:290:HOH:O	2.20	0.42
2:B:145:TYR:CE1	2:B:150:VAL:HG13	2.54	0.42
2:B:108:THR:HG22	2:B:110:THR:HG22	2.01	0.42
1:C:4:LEU:HA	1:C:24:ARG:O	2.19	0.42
2:D:176:THR:HG22	6:D:248:HOH:O	2.18	0.42
1:C:5:THR:O	1:C:23:CYS:HA	2.20	0.42
1:C:34:HIS:CD2	1:C:34:HIS:N	2.87	0.42
1:C:160:LEU:HA	1:C:160:LEU:HD22	1.88	0.41
1:C:34:HIS:HA	1:C:48:ILE:O	2.20	0.41
1:A:137:ASN:HD22	1:A:174:SER:HB3	1.84	0.41
2:B:125:ALA:HA	2:B:126:PRO:HD3	1.90	0.41
2:B:98:ARG:HG3	2:B:99:ASN:ND2	2.36	0.41
1:A:2:ILE:N	6:A:243:HOH:O	2.53	0.41
1:C:27(B):LEU:HD22	1:C:71:PHE:CE1	2.56	0.41
1:A:106:ILE:N	1:A:166:GLN:HE22	2.12	0.41
1:C:140:TYR:CG	1:C:141:PRO:HA	2.56	0.41
1:A:62:PHE:CD1	1:A:75:ILE:HG12	2.56	0.40
2:D:152:LEU:C	2:D:152:LEU:HD23	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:O	1:A:23:CYS:HA	2.21	0.40
2:D:112:SER:O	2:D:113:SER:CB	2.69	0.40
2:D:118:ALA:CB	2:D:204:THR:HG21	2.52	0.40
1:C:50:LYS:CB	1:C:53:ASN:HD22	2.31	0.40
1:C:203:SER:HB2	1:C:204:PRO:HD2	2.03	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	213/215 (99%)	207 (97%)	5 (2%)	1 (0%)	29	41
1	C	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	29	41
2	B	206/217 (95%)	200 (97%)	4 (2%)	2 (1%)	15	23
2	D	206/217 (95%)	198 (96%)	7 (3%)	1 (0%)	29	41
All	All	838/864 (97%)	810 (97%)	23 (3%)	5 (1%)	25	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
2	B	52(A)	ASN
2	B	113	SER
2	D	52(A)	ASN
1	C	110	ASP

### 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	193/193 (100%)	183 (95%)	10 (5%)	23	38
1	C	193/193 (100%)	182 (94%)	11 (6%)	20	33
2	B	180/185 (97%)	163 (91%)	17 (9%)	8	13
2	D	180/185 (97%)	163 (91%)	17 (9%)	8	13
All	All	746/756 (99%)	691 (93%)	55 (7%)	13	22

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	9	LEU
1	A	11	LEU
1	A	22	SER
1	A	23	CYS
1	A	24	ARG
1	A	27(B)	LEU
1	A	108	ARG
1	A	156	GLN
1	A	160	LEU
2	B	1	GLN
2	B	4	LEU
2	B	12	VAL
2	B	19	LYS
2	B	42	GLU
2	B	46	GLU
2	B	70	THR
2	B	81	GLN
2	B	110	THR
2	B	111	VAL
2	B	116	THR
2	B	117	LYS
2	B	171	GLN
2	B	176	THR
2	B	194	THR
2	B	204	THR
2	B	206	VAL
1	C	2	ILE

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Mol	Chain	Res	Type
1	C	9	LEU
1	C	23	CYS
1	C	24	ARG
1	C	27(B)	LEU
1	C	108	ARG
1	C	143	ASP
1	C	155	ARG
1	C	156	GLN
1	C	160	LEU
1	C	190	ASN
2	D	4	LEU
2	D	12	VAL
2	D	42	GLU
2	D	61	GLU
2	D	70	THR
2	D	78	MET
2	D	98	ARG
2	D	110	THR
2	D	111	VAL
2	D	116	THR
2	D	117	LYS
2	D	171	GLN
2	D	174	LEU
2	D	176	THR
2	D	177	LEU
2	D	194	THR
2	D	204	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	137	ASN
1	A	138	ASN
1	A	156	GLN
1	A	157	ASN
1	A	161	ASN
1	A	166	GLN
1	A	198	HIS
2	B	1	GLN
2	B	13	GLN
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	81	GLN
2	B	99	ASN
2	B	105	GLN
2	B	191	GLN
2	B	199	HIS
1	C	34	HIS
1	C	53	ASN
1	C	137	ASN
1	C	138	ASN
1	C	156	GLN
1	C	157	ASN
1	C	161	ASN
1	C	166	GLN
1	C	198	HIS
1	C	210	ASN
2	D	1	GLN
2	D	5	GLN
2	D	53	ASN
2	D	99	ASN
2	D	171	GLN
2	D	191	GLN
2	D	199	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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
5	NGA	B	1(A)	-	15,15,15	1.60	3 (20%)	21,21,21	2.18	8 (38%)
5	NGA	D	213	-	15,15,15	1.55	3 (20%)	21,21,21	2.19	6 (28%)

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
5	NGA	B	1(A)	-	1/1/6/7	1/6/26/26	0/1/1/1
5	NGA	D	213	-	1/1/6/7	1/6/26/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1(A)	NGA	C1-C2	-3.53	1.48	1.52
5	D	213	NGA	C1-C2	-3.35	1.48	1.52
5	B	1(A)	NGA	C2-N2	-3.21	1.40	1.45
5	D	213	NGA	C2-N2	-3.15	1.40	1.45
5	D	213	NGA	O1-C1	-2.32	1.32	1.39
5	B	1(A)	NGA	O1-C1	-2.29	1.32	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	213	NGA	O1-C1-C2	6.32	122.34	109.22
5	B	1(A)	NGA	O1-C1-C2	6.12	121.94	109.22
5	D	213	NGA	C1-C2-N2	-3.92	106.18	110.73
5	B	1(A)	NGA	C1-C2-N2	-3.56	106.60	110.73
5	D	213	NGA	O3-C3-C2	-3.30	102.99	109.66
5	B	1(A)	NGA	O3-C3-C2	-3.28	103.04	109.66
5	B	1(A)	NGA	C4-C3-C2	-3.16	105.72	110.34
5	D	213	NGA	C4-C3-C2	-3.07	105.84	110.34
5	B	1(A)	NGA	O5-C1-C2	-2.79	106.71	109.52
5	B	1(A)	NGA	C1-C2-C3	-2.49	107.14	110.54
5	B	1(A)	NGA	C6-C5-C4	2.37	118.55	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	213	NGA	O6-C6-C5	-2.34	103.25	111.29
5	B	1(A)	NGA	O6-C6-C5	-2.25	103.57	111.29
5	D	213	NGA	C6-C5-C4	2.22	118.21	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1(A)	NGA	C1
5	D	213	NGA	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	213	NGA	O5-C5-C6-O6
5	B	1(A)	NGA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1(A)	NGA	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	215/215 (100%)	0.50	18 (8%) 11 10	16, 28, 43, 61	0
1	C	215/215 (100%)	0.67	23 (10%) 6 5	20, 34, 49, 60	0
2	B	210/217 (96%)	0.43	11 (5%) 27 26	15, 26, 42, 52	0
2	D	210/217 (96%)	0.54	13 (6%) 20 19	21, 30, 46, 57	0
All	All	850/864 (98%)	0.53	65 (7%) 13 12	15, 29, 46, 61	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	ALA	5.2
1	C	212	GLU	4.5
2	D	112	SER	4.5
1	A	169	LYS	4.0
1	A	212	GLU	3.7
2	B	43	LYS	3.7
1	C	4	LEU	3.6
1	A	203	SER	3.5
1	A	202	THR	3.4
1	C	3	GLN	3.2
1	C	163	TRP	3.2
2	B	185	SER	3.1
2	D	96	LYS	3.1
1	A	3	GLN	3.1
1	C	33	LEU	3.0
2	D	190	SER	3.0
1	C	169	LYS	2.9
1	A	163	TRP	2.9
2	D	42	GLU	2.9
1	A	109	ALA	2.8
1	A	156	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	41	PRO	2.7
1	C	16	GLY	2.7
1	C	77	SER	2.7
1	C	133	VAL	2.7
1	A	184	ASP	2.6
1	C	27(D)	HIS	2.6
2	D	191	GLN	2.6
2	B	42	GLU	2.6
2	B	135	SER	2.6
1	A	157	ASN	2.6
1	A	126	THR	2.5
2	D	115	THR	2.5
2	D	127	VAL	2.5
2	B	112	SER	2.5
1	A	190	ASN	2.5
1	C	128	GLY	2.5
2	B	184	THR	2.4
1	A	4	LEU	2.4
1	C	70	ASP	2.3
1	C	27(E)	SER	2.3
1	A	33	LEU	2.3
1	C	21	ILE	2.3
1	A	2	ILE	2.3
2	D	173	ASP	2.3
2	B	191	GLN	2.3
1	C	24	ARG	2.2
2	D	80	LEU	2.2
2	D	34	MET	2.2
1	C	53	ASN	2.2
1	A	153	SER	2.2
1	C	156	GLN	2.1
2	B	190	SER	2.1
2	D	64	LYS	2.1
2	D	58	TYR	2.1
1	C	69	THR	2.1
1	C	29	GLY	2.1
2	B	41	PRO	2.1
1	C	28	ASN	2.0
1	C	41	GLY	2.0
1	C	35	TRP	2.0
2	B	34	MET	2.0
1	A	132	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	35	TRP	2.0
2	B	161	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	1	1/1	0.75	0.28	37,37,37,37	0
4	MG	C	214	1/1	0.85	0.31	34,34,34,34	0
4	MG	C	1	1/1	0.86	0.25	36,36,36,36	0
5	NGA	B	1(A)	15/15	0.90	0.25	24,26,34,34	0
4	MG	C	213	1/1	0.92	0.15	38,38,38,38	0
4	MG	A	214	1/1	0.92	0.26	19,19,19,19	0
5	NGA	D	213	15/15	0.92	0.22	36,46,54,54	0
3	ZN	A	222	1/1	0.98	0.08	39,39,39,39	0
3	ZN	A	213	1/1	0.98	0.03	42,42,42,42	0
3	ZN	A	215	1/1	0.98	0.04	42,42,42,42	0
3	ZN	C	218	1/1	0.99	0.05	30,30,30,30	0
3	ZN	D	221	1/1	0.99	0.07	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.