



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2023 – 02:02 PM EST

PDB ID : 8DXU  
Title : Fab arms of antibodies GAR03 and 10G4 bound to the receptor binding domain of SARS-CoV-2 in a 1:1:1 complex.  
Authors : Langley, D.B.; Christ, D.  
Deposited on : 2022-08-03  
Resolution : 2.73 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.31.2  
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) : 2.31.2

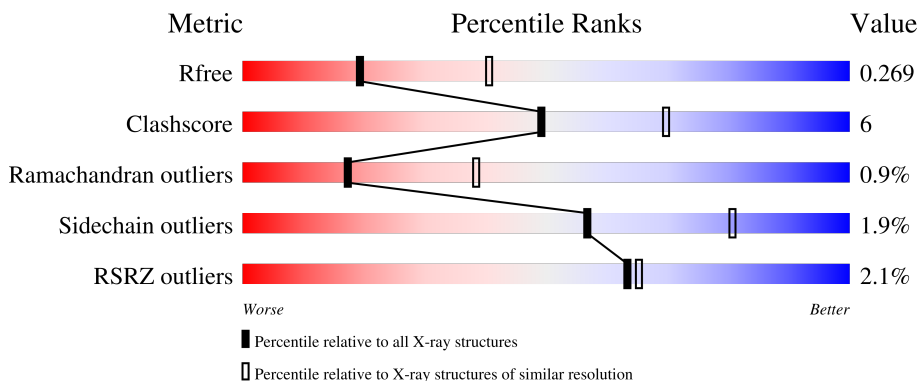
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	R	204	
2	H	228	
3	L	215	
4	A	231	
5	B	215	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7928 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	R	193	1510	964	252	286	8	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	529	GLY	-	expression tag	UNP P0DTC2
R	530	SER	-	expression tag	UNP P0DTC2
R	531	HIS	-	expression tag	UNP P0DTC2
R	532	HIS	-	expression tag	UNP P0DTC2
R	533	HIS	-	expression tag	UNP P0DTC2
R	534	HIS	-	expression tag	UNP P0DTC2
R	535	HIS	-	expression tag	UNP P0DTC2
R	536	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of Fab arm of antibody 10G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1620	1023	272	319	6	0	0	0

- Molecule 3 is a protein called Light chain of Fab arm of antibody 10G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	212	1598	1000	269	323	6	0	0	0

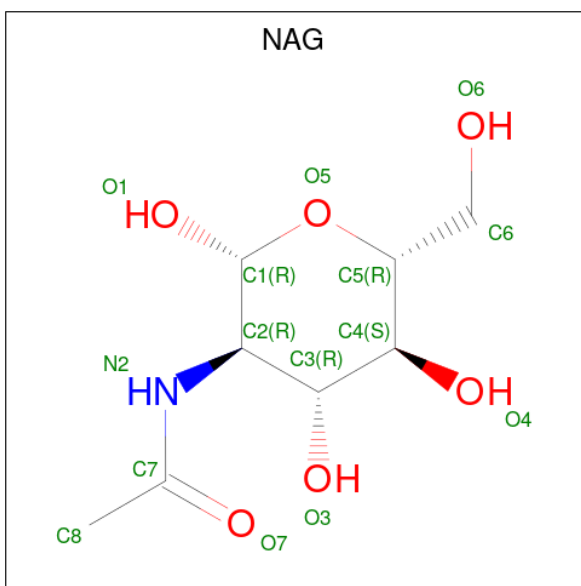
- Molecule 4 is a protein called Heavy chain of Fab arm of antibody GAR03.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	221	1612	1012	265	325	10	0	0	0

- Molecule 5 is a protein called Light chain of Fab arm of antibody GAR03.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	213	1529	953	257	315	4	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	R	1	14	8	1	5	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	R	20	Total O 20 20	0	0
8	H	7	Total O 7 7	0	0
8	L	8	Total O 8 8	0	0

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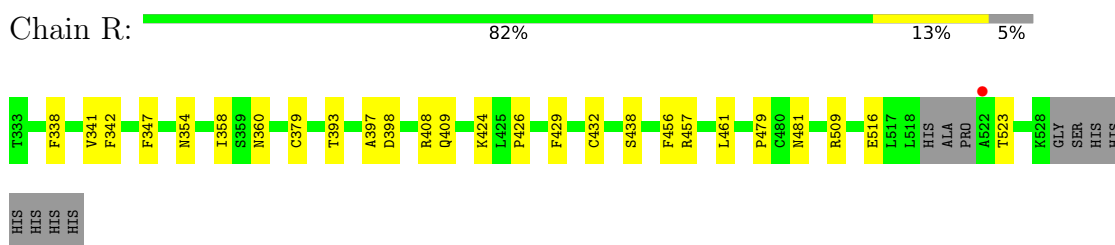
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
8	A	7	Total O 7 7	0	0
8	B	1	Total O 1 1	0	0

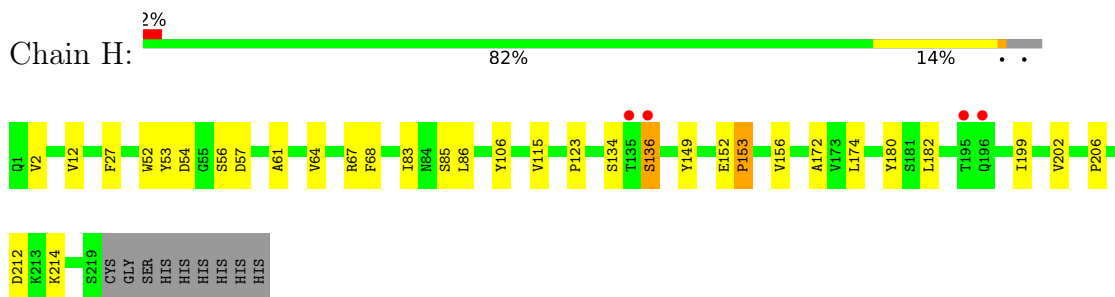
### 3 Residue-property plots [i](#)

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.

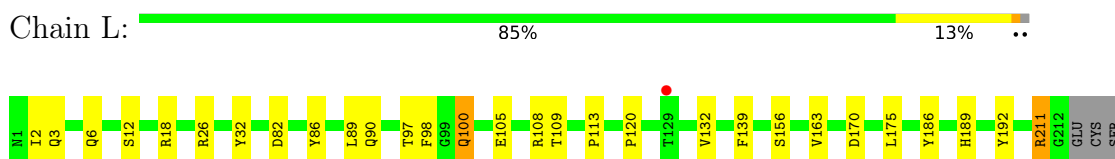
- Molecule 1: Spike protein S1



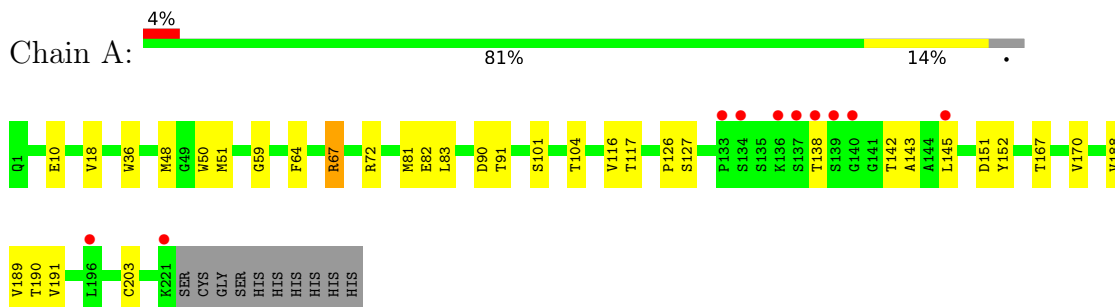
- Molecule 2: Heavy chain of Fab arm of antibody 10G4



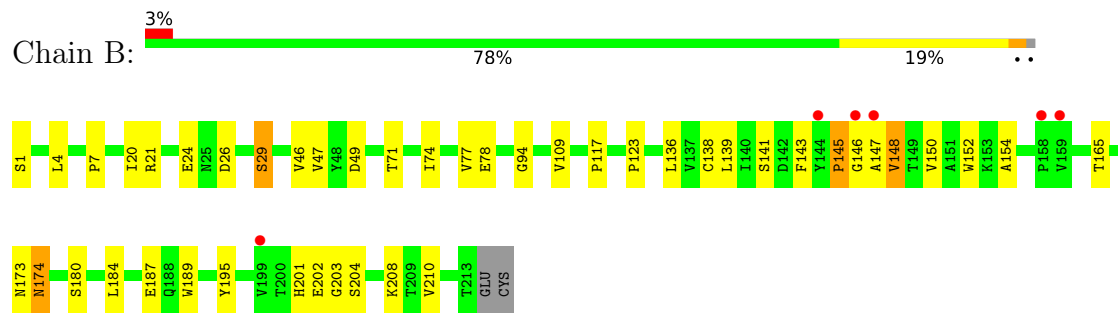
- Molecule 3: Light chain of Fab arm of antibody 10G4



- Molecule 4: Heavy chain of Fab arm of antibody GAR03



## ● Molecule 5: Light chain of Fab arm of antibody GAR03



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.23Å 102.08Å 201.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.55 – 2.73 48.58 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.55-2.73) 99.4 (48.58-2.73)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.11.1-2575	Depositor
R, $R_{free}$	0.223 , 0.269 0.223 , 0.269	Depositor DCC
$R_{free}$ test set	1473 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL

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	R	0.29	0/1550	0.47	0/2109
2	H	0.28	0/1661	0.51	0/2269
3	L	0.28	0/1635	0.49	0/2230
4	A	0.28	0/1651	0.49	0/2256
5	B	0.28	0/1568	0.49	0/2158
All	All	0.28	0/8065	0.49	0/11022

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	152	GLU	Peptide

### 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	R	1510	0	1400	17	0
2	H	1620	0	1544	20	0
3	L	1598	0	1502	15	0
4	A	1612	0	1535	17	0
5	B	1529	0	1404	26	0
6	R	14	0	13	1	0
7	A	2	0	0	0	0
8	A	7	0	0	0	0
8	B	1	0	0	0	0
8	H	7	0	0	0	0
8	L	8	0	0	0	0
8	R	20	0	0	1	0
All	All	7928	0	7398	90	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 6.

All (90) 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)
4:A:104:THR:HG21	5:B:49:ASP:OD1	1.90	0.71
3:L:189:HIS:O	3:L:211:ARG:NH1	2.24	0.69
1:R:456:PHE:HZ	3:L:32:TYR:HH	1.42	0.67
4:A:138:THR:HG22	4:A:143:ALA:HB2	1.78	0.65
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.77	0.65
5:B:46:VAL:HG12	5:B:47:VAL:HG23	1.78	0.65
3:L:108:ARG:NH1	3:L:109:THR:O	2.30	0.64
1:R:342:PHE:HB2	6:R:601:NAG:H82	1.80	0.64
4:A:142:THR:HG22	4:A:190:THR:HG22	1.81	0.63
5:B:123:PRO:HB3	5:B:210:VAL:HG11	1.82	0.61
4:A:91:THR:HG23	4:A:117:THR:HA	1.83	0.61
3:L:186:TYR:O	3:L:192:TYR:OH	2.19	0.60
5:B:7:PRO:HD3	5:B:21:ARG:O	2.03	0.58
3:L:6:GLN:O	3:L:100:GLN:NE2	2.37	0.58
2:H:2:VAL:HG23	2:H:27:PHE:CD1	2.39	0.57
4:A:188:VAL:HG21	5:B:139:LEU:HD13	1.86	0.57
2:H:172:ALA:HB2	2:H:182:LEU:HD23	1.86	0.57
5:B:147:ALA:O	5:B:148:VAL:HG23	2.04	0.56
4:A:142:THR:CG2	4:A:190:THR:HG22	2.36	0.56
1:R:360:ASN:H	1:R:523:THR:HG23	1.71	0.55
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.88	0.55
5:B:201:HIS:O	5:B:204:SER:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:152:TRP:HE1	5:B:180:SER:HG	1.54	0.54
5:B:74:ILE:HG22	5:B:77:VAL:HG22	1.91	0.53
5:B:136:LEU:HD13	5:B:184:LEU:HD23	1.90	0.53
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.91	0.53
3:L:163:VAL:HG22	3:L:175:LEU:HD12	1.91	0.52
5:B:173:ASN:O	5:B:174:ASN:HB2	2.10	0.52
2:H:56:SER:OG	2:H:57:ASP:N	2.43	0.52
4:A:189:VAL:HG22	4:A:191:VAL:HG23	1.92	0.52
4:A:126:PRO:HB3	4:A:152:TYR:HB3	1.91	0.51
5:B:4:LEU:HD23	5:B:24:GLU:HB2	1.92	0.51
3:L:170:ASP:N	3:L:170:ASP:OD1	2.37	0.51
1:R:347:PHE:CD2	1:R:509:ARG:HG2	2.47	0.50
2:H:153:PRO:HD2	2:H:206:PRO:HG2	1.93	0.50
4:A:10:GLU:O	4:A:116:VAL:HA	2.12	0.50
5:B:20:ILE:O	5:B:71:THR:HA	2.11	0.50
1:R:393:THR:HB	1:R:516:GLU:HG2	1.94	0.49
1:R:456:PHE:HZ	3:L:32:TYR:OH	1.95	0.49
2:H:61:ALA:O	2:H:64:VAL:HG12	2.11	0.49
1:R:426:PRO:HD2	1:R:429:PHE:HB2	1.93	0.49
3:L:89:LEU:HD12	3:L:98:PHE:CG	2.48	0.48
2:H:67:ARG:HD2	2:H:85:SER:HB2	1.97	0.46
5:B:77:VAL:HG12	5:B:109:VAL:HG23	1.97	0.46
4:A:18:VAL:O	4:A:82:GLU:HA	2.16	0.46
5:B:201:HIS:O	5:B:203:GLY:N	2.49	0.46
5:B:117:PRO:HA	5:B:143:PHE:HB3	1.97	0.46
5:B:189:TRP:HH2	5:B:210:VAL:HG12	1.82	0.45
1:R:479:PRO:HD3	2:H:53:TYR:CD1	2.51	0.45
2:H:54:ASP:OD1	2:H:56:SER:HB3	2.15	0.45
2:H:12:VAL:O	2:H:115:VAL:HA	2.17	0.45
1:R:438:SER:HB3	1:R:509:ARG:HD2	1.98	0.45
3:L:82:ASP:O	3:L:86:TYR:OH	2.27	0.45
4:A:138:THR:HA	4:A:143:ALA:HA	1.99	0.45
2:H:156:VAL:HG22	2:H:202:VAL:HG22	1.98	0.45
4:A:67:ARG:NH2	4:A:90:ASP:OD2	2.40	0.44
5:B:1:SER:HB3	5:B:94:GLY:HA3	1.99	0.44
2:H:86:LEU:HA	2:H:86:LEU:HD23	1.79	0.44
4:A:167:THR:O	4:A:170:VAL:HG12	2.18	0.44
1:R:379:CYS:HA	1:R:432:CYS:HA	2.00	0.44
1:R:424:LYS:NZ	8:R:704:HOH:O	2.48	0.43
5:B:150:VAL:HG11	5:B:165:THR:HG21	1.99	0.43
1:R:341:VAL:HG11	1:R:397:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:187:GLU:H	5:B:187:GLU:CD	2.22	0.43
1:R:354:ASN:O	1:R:398:ASP:HA	2.18	0.43
3:L:2:ILE:O	3:L:26:ARG:HB3	2.19	0.43
3:L:12:SER:HA	3:L:105:GLU:O	2.19	0.43
4:A:36:TRP:CE2	4:A:81:MET:HB2	2.53	0.43
5:B:145:PRO:HB2	5:B:146:GLY:H	1.72	0.43
3:L:90:GLN:HG3	3:L:97:THR:OG1	2.18	0.43
2:H:67:ARG:C	2:H:68:PHE:HD1	2.22	0.42
2:H:199:ILE:HD13	2:H:214:LYS:HA	2.00	0.42
1:R:360:ASN:H	1:R:523:THR:CG2	2.32	0.42
4:A:50:TRP:NE1	4:A:59:GLY:HA3	2.34	0.42
5:B:78:GLU:O	5:B:109:VAL:HG21	2.20	0.42
2:H:83:ILE:CG2	2:H:86:LEU:HD21	2.49	0.42
1:R:408:ARG:HG3	1:R:409:GLN:N	2.34	0.42
2:H:2:VAL:HG11	2:H:106:TYR:CZ	2.55	0.42
2:H:68:PHE:CZ	2:H:83:ILE:HG23	2.55	0.42
5:B:154:ALA:HB2	5:B:195:TYR:CE2	2.55	0.41
5:B:26:ASP:O	5:B:29:SER:HB3	2.20	0.41
1:R:457:ARG:NH1	1:R:461:LEU:HD12	2.34	0.41
2:H:134:SER:O	2:H:136:SER:N	2.53	0.41
4:A:48:MET:HG2	4:A:64:PHE:CE2	2.55	0.41
5:B:138:CYS:HB2	5:B:152:TRP:CH2	2.55	0.41
2:H:174:LEU:HD13	2:H:180:TYR:CZ	2.56	0.41
1:R:338:PHE:HE1	1:R:358:ILE:HD13	1.86	0.41
3:L:113:PRO:HB3	3:L:139:PHE:HB3	2.02	0.41
4:A:81:MET:HE2	4:A:83:LEU:HB2	2.03	0.40
5:B:77:VAL:CG1	5:B:109:VAL:HG23	2.51	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	R	190/204 (93%)	181 (95%)	9 (5%)	0	100	100
2	H	217/228 (95%)	204 (94%)	11 (5%)	2 (1%)	17	38
3	L	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	15	35
4	A	219/231 (95%)	207 (94%)	11 (5%)	1 (0%)	29	53
5	B	211/215 (98%)	190 (90%)	17 (8%)	4 (2%)	8	18
All	All	1047/1093 (96%)	979 (94%)	59 (6%)	9 (1%)	17	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	153	PRO
5	B	145	PRO
5	B	148	VAL
2	H	136	SER
3	L	211	ARG
5	B	202	GLU
5	B	174	ASN
3	L	3	GLN
4	A	151	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	R	161/176 (92%)	160 (99%)	1 (1%)	86	94
2	H	175/190 (92%)	173 (99%)	2 (1%)	73	89
3	L	176/189 (93%)	173 (98%)	3 (2%)	60	83
4	A	179/197 (91%)	172 (96%)	7 (4%)	32	59
5	B	162/181 (90%)	159 (98%)	3 (2%)	57	81
All	All	853/933 (91%)	837 (98%)	16 (2%)	57	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	481	ASN
2	H	52	TRP
2	H	212	ASP
3	L	18	ARG
3	L	100	GLN
3	L	156	SER
4	A	51	MET
4	A	67	ARG
4	A	72	ARG
4	A	101	SER
4	A	127	SER
4	A	145	LEU
4	A	203	CYS
5	B	29	SER
5	B	141	SER
5	B	208	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	481	ASN
2	H	111	ASN
3	L	199	GLN

### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
6	NAG	R	601	1	14,14,15	0.56	0	17,19,21	1.00	0

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
6	NAG	R	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	601	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	R	193/204 (94%)	-0.24	1 (0%) 91 92	31, 52, 88, 147	0
2	H	219/228 (96%)	-0.17	4 (1%) 68 70	33, 63, 118, 161	0
3	L	212/215 (98%)	-0.17	1 (0%) 91 92	35, 59, 95, 112	0
4	A	221/231 (95%)	-0.01	10 (4%) 33 32	34, 65, 113, 159	0
5	B	213/215 (99%)	0.18	6 (2%) 53 54	35, 74, 111, 141	0
All	All	1058/1093 (96%)	-0.08	22 (2%) 63 65	31, 62, 107, 161	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	522	ALA	5.8
5	B	146	GLY	3.9
4	A	140	GLY	3.7
4	A	137	SER	3.6
5	B	199	VAL	3.4
2	H	195	THR	3.2
4	A	133	PRO	2.7
5	B	144	TYR	2.7
4	A	138	THR	2.6
4	A	136	LYS	2.4
3	L	129	THR	2.4
4	A	196	LEU	2.4
2	H	135	THR	2.3
2	H	136	SER	2.3
4	A	134	SER	2.2
5	B	158	PRO	2.2
4	A	139	SER	2.2
4	A	221	LYS	2.2
2	H	196	GLN	2.2
5	B	159	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	145	LEU	2.1
5	B	147	ALA	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(Å <sup>2</sup> )	Q<0.9
6	NAG	R	601	14/15	0.85	0.27	85,91,96,96	0
7	CL	A	301	1/1	0.91	0.13	67,67,67,67	0
7	CL	A	302	1/1	0.97	0.18	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.