



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:51 PM BST

PDB ID : 6XC2  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody CC12.1  
Authors : Yuan, M.; Liu, H.; Wu, N.C.; Zhu, X.; Wilson, I.A.  
Deposited on : 2020-06-08  
Resolution : 3.11 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 : 2.14.4.dev1  
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) : 2.14.4.dev1

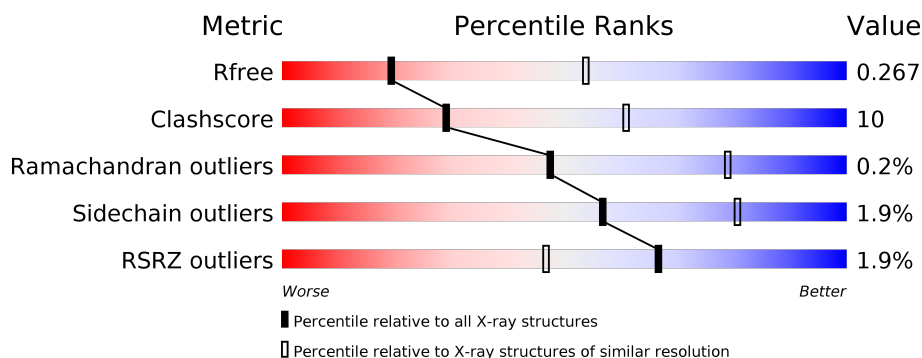
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	231	<div> <div>2%</div> <div>63% 20% 16%</div> </div>
1	Z	231	<div> <div>2%</div> <div>66% 17% 16%</div> </div>
2	L	217	<div> <div>%</div> <div>79% 18% ..</div> </div>
2	Y	217	<div> <div>2%</div> <div>75% 24% .</div> </div>
3	H	220	<div> <div>%</div> <div>75% 20% ..</div> </div>
3	X	220	<div> <div>2%</div> <div>75% 21% ..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9584 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
1	A	193	Total	C	N	O	S	0	0	0
			1537	987	256	286	8			
1	Z	193	Total	C	N	O	S	0	0	0
			1537	987	256	286	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
Z	542	SER	-	expression tag	UNP P0DTC2
Z	543	GLY	-	expression tag	UNP P0DTC2
Z	544	HIS	-	expression tag	UNP P0DTC2
Z	545	HIS	-	expression tag	UNP P0DTC2
Z	546	HIS	-	expression tag	UNP P0DTC2
Z	547	HIS	-	expression tag	UNP P0DTC2
Z	548	HIS	-	expression tag	UNP P0DTC2
Z	549	HIS	-	expression tag	UNP P0DTC2

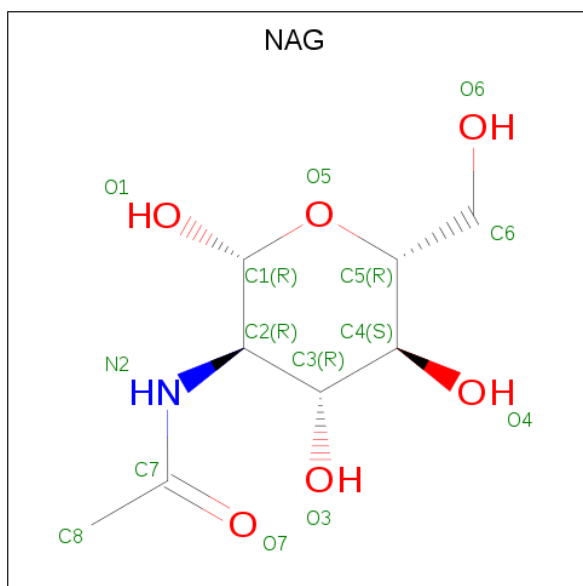
- Molecule 2 is a protein called CC12.1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1650	1041	273	331	5			
2	Y	215	Total	C	N	O	S	0	0	0
			1650	1041	273	331	5			

- Molecule 3 is a protein called CC12.1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1591	1001	266	318	6			
3	X	215	Total	C	N	O	S	0	0	0
			1591	1001	266	318	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

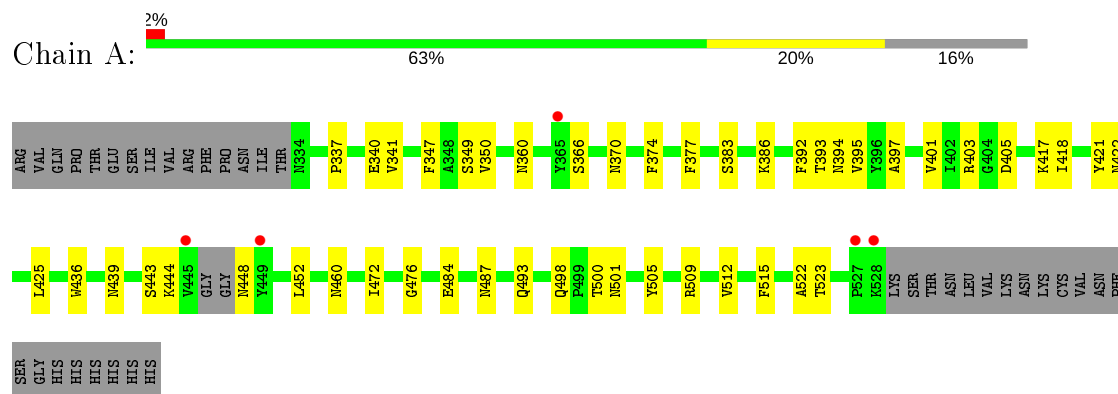


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	Z	1	Total	C	N	O	0	0
			14	8	1	5		

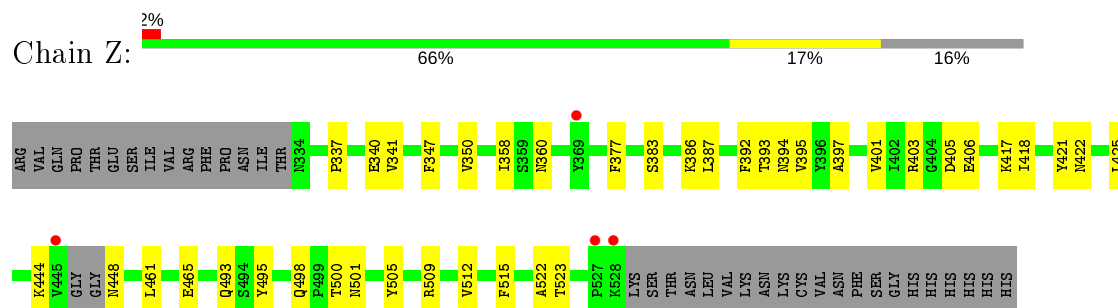
### 3 Residue-property plots [i](#)

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.

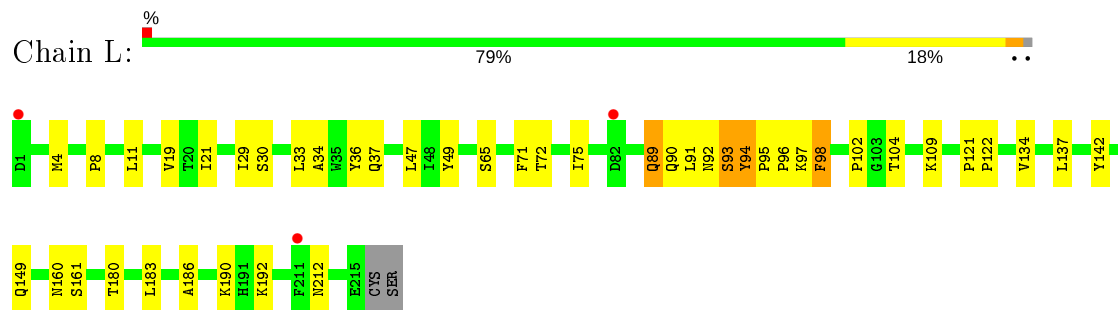
#### • Molecule 1: Spike protein S1



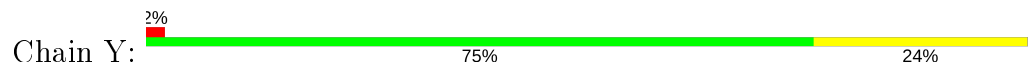
#### • Molecule 1: Spike protein S1

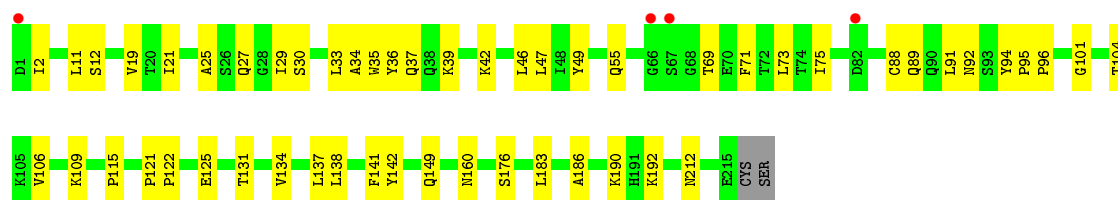


#### • Molecule 2: CC12.1 light chain

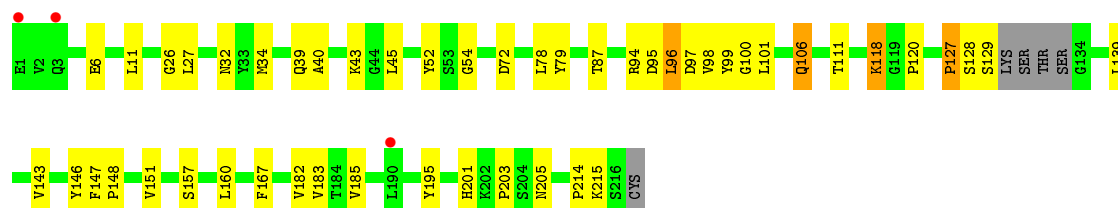
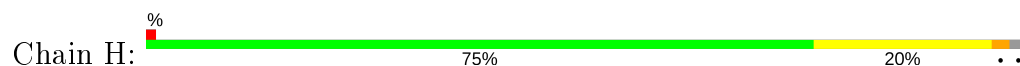


#### • Molecule 2: CC12.1 light chain

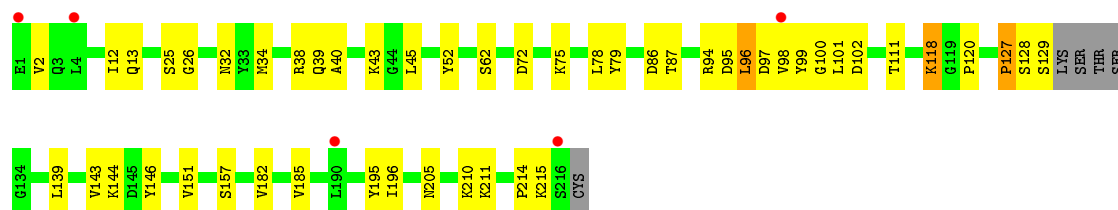
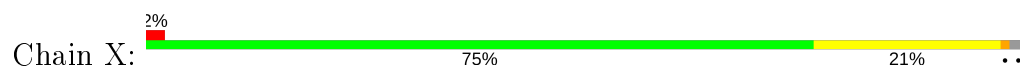




• Molecule 3: CC12.1 heavy chain



• Molecule 3: CC12.1 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.70Å 143.49Å 81.47Å 90.00° 118.68° 90.00°	Depositor
Resolution (Å)	40.34 – 3.11 40.34 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.3 (40.34-3.11) 88.3 (40.34-3.11)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.213 , 0.267 0.213 , 0.267	Depositor DCC
$R_{free}$ test set	1289 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 24.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h-l,k,h 0.004 for l,k,-h-l 0.417 for h,-k,-h-l 0.019 for -h-l,-k,l 0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: NAG

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	0.28	0/1580	0.46	0/2149
1	Z	0.28	0/1580	0.46	0/2149
2	L	0.29	0/1688	0.49	0/2293
2	Y	0.30	0/1688	0.50	0/2293
3	H	0.29	0/1625	0.52	0/2214
3	X	0.29	0/1625	0.53	0/2214
All	All	0.29	0/9786	0.49	0/13312

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	L	0	2
2	Y	0	1
3	H	0	2
3	X	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	127	PRO	Peptide
3	H	96	LEU	Peptide
2	L	29	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	L	93	SER	Peptide
3	X	127	PRO	Peptide
3	X	96	LEU	Peptide
2	Y	29	ILE	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	1537	0	1458	36	0
1	Z	1537	0	1458	32	0
2	L	1650	0	1615	34	0
2	Y	1650	0	1615	42	0
3	H	1591	0	1565	36	0
3	X	1591	0	1565	34	0
4	A	14	0	13	0	0
4	Z	14	0	13	0	0
All	All	9584	0	9302	182	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 10.

All (182) 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:Y:36:TYR:CE1	2:Y:89:GLN:OE1	2.08	1.07
2:Y:36:TYR:CZ	2:Y:89:GLN:OE1	2.23	0.90
2:Y:12:SER:OG	2:Y:142:TYR:OH	1.94	0.84
2:Y:36:TYR:OH	2:Y:89:GLN:OE1	2.00	0.79
3:X:127:PRO:HG3	3:X:139:LEU:HB3	1.64	0.79
1:Z:383:SER:HB2	1:Z:386:LYS:HG3	1.65	0.78
1:Z:501:ASN:ND2	2:Y:30:SER:OG	2.15	0.77
1:A:383:SER:HB2	1:A:386:LYS:HG3	1.66	0.77
3:X:96:LEU:HB3	3:X:99:TYR:HB2	1.65	0.77
3:H:96:LEU:HB3	3:H:99:TYR:HB2	1.67	0.76
3:H:127:PRO:HG3	3:H:139:LEU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:95:PRO:HB2	2:L:96:PRO:HD3	1.69	0.74
3:H:6:GLU:O	3:H:106:GLN:NE2	2.22	0.73
3:X:128:SER:HB3	3:X:215:LYS:HB2	1.70	0.73
1:A:360:ASN:H	1:A:523:THR:HB	1.54	0.73
1:A:366:SER:O	1:A:370:ASN:HB3	1.88	0.72
2:Y:36:TYR:HE1	2:Y:89:GLN:OE1	1.69	0.71
3:X:2:VAL:HA	3:X:26:GLY:HA3	1.72	0.71
3:H:87:THR:HG23	3:H:111:THR:HA	1.73	0.71
1:A:403:ARG:NH1	1:A:405:ASP:OD1	2.25	0.70
1:Z:444:LYS:O	1:Z:448:ASN:N	2.26	0.69
3:X:87:THR:HG23	3:X:111:THR:HA	1.75	0.69
1:Z:360:ASN:H	1:Z:523:THR:HB	1.57	0.68
2:Y:91:LEU:HG	3:X:98:VAL:HA	1.76	0.68
3:H:34:MET:HB3	3:H:78:LEU:HD22	1.76	0.67
1:Z:403:ARG:NH1	1:Z:405:ASP:OD1	2.27	0.67
2:Y:94:TYR:HB3	2:Y:95:PRO:HD3	1.77	0.67
3:H:127:PRO:HD2	3:H:214:PRO:HA	1.75	0.67
2:Y:37:GLN:HB2	2:Y:47:LEU:HD11	1.75	0.67
1:A:444:LYS:O	1:A:448:ASN:N	2.28	0.67
2:L:122:PRO:HD3	2:L:134:VAL:HG22	1.78	0.65
3:X:127:PRO:HD2	3:X:214:PRO:HA	1.79	0.65
3:H:32:ASN:OD1	3:H:94:ARG:NH1	2.26	0.65
2:L:33:LEU:HD22	2:L:71:PHE:HD1	1.61	0.65
1:Z:405:ASP:HB3	2:Y:94:TYR:HB2	1.77	0.64
2:Y:34:ALA:HB3	2:Y:89:GLN:HG2	1.78	0.64
1:Z:498:GLN:NE2	2:Y:30:SER:HB3	2.13	0.64
1:A:501:ASN:OD1	2:L:30:SER:OG	2.13	0.64
1:A:405:ASP:HB3	2:L:94:TYR:HB2	1.80	0.64
3:H:128:SER:HB3	3:H:215:LYS:HB2	1.79	0.63
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.79	0.63
1:A:498:GLN:NE2	2:L:30:SER:HB3	2.13	0.63
1:A:403:ARG:HH21	2:L:92:ASN:HB3	1.64	0.62
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.79	0.62
3:X:39:GLN:HB2	3:X:45:LEU:HD23	1.81	0.62
3:X:32:ASN:OD1	3:X:94:ARG:NH1	2.32	0.61
1:Z:403:ARG:NH2	2:Y:92:ASN:O	2.33	0.61
2:L:89:GLN:NE2	2:L:98:PHE:HB3	2.16	0.61
1:A:403:ARG:HD2	1:A:505:TYR:HA	1.84	0.60
2:Y:95:PRO:HB2	2:Y:96:PRO:HD3	1.82	0.60
3:X:34:MET:HB3	3:X:78:LEU:HD22	1.84	0.60
2:L:19:VAL:HG22	2:L:75:ILE:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:403:ARG:HD2	1:Z:505:TYR:HA	1.83	0.59
1:Z:493:GLN:HE22	3:X:98:VAL:HG12	1.68	0.58
2:L:121:PRO:HG2	3:H:215:LYS:HE2	1.85	0.58
2:Y:19:VAL:HG22	2:Y:75:ILE:HB	1.84	0.58
2:Y:55:GLN:HE22	3:X:102:ASP:HB2	1.70	0.57
2:Y:122:PRO:HD3	2:Y:134:VAL:HG22	1.86	0.57
2:L:34:ALA:HB3	2:L:89:GLN:HG2	1.85	0.57
3:X:96:LEU:O	3:X:99:TYR:N	2.38	0.57
1:A:403:ARG:NH2	2:L:92:ASN:HB3	2.18	0.57
2:Y:55:GLN:NE2	3:X:102:ASP:HB2	2.20	0.56
1:Z:403:ARG:HH21	2:Y:92:ASN:HB3	1.69	0.56
1:Z:498:GLN:OE1	1:Z:500:THR:OG1	2.23	0.56
3:H:11:LEU:HD22	3:H:148:PRO:HG3	1.88	0.54
1:A:393:THR:HA	1:A:522:ALA:HA	1.90	0.54
1:A:425:LEU:HD21	1:A:512:VAL:HG11	1.90	0.53
3:H:96:LEU:O	3:H:99:TYR:N	2.41	0.53
2:L:33:LEU:HB2	2:L:71:PHE:HE1	1.74	0.53
1:A:487:ASN:ND2	3:H:26:GLY:O	2.41	0.53
2:Y:39:LYS:HB2	2:Y:42:LYS:HG2	1.90	0.52
2:L:91:LEU:HG	3:H:98:VAL:HA	1.91	0.52
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.91	0.52
3:X:143:VAL:HG11	3:X:151:VAL:HG11	1.90	0.52
1:A:498:GLN:OE1	1:A:500:THR:OG1	2.28	0.52
2:L:33:LEU:HB2	2:L:71:PHE:CE1	2.45	0.52
2:Y:11:LEU:HD22	2:Y:106:VAL:HG13	1.91	0.52
2:Y:2:ILE:HD13	2:Y:27:GLN:HG2	1.91	0.51
2:L:36:TYR:HE1	2:L:89:GLN:HG2	1.76	0.51
3:X:40:ALA:HB3	3:X:43:LYS:HB2	1.93	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.92	0.50
3:X:96:LEU:HB2	3:X:100:GLY:O	2.12	0.50
1:Z:350:VAL:HG11	1:Z:418:ILE:HD12	1.93	0.50
1:Z:341:VAL:HG11	1:Z:397:ALA:HB1	1.94	0.49
1:Z:401:VAL:HG22	1:Z:509:ARG:HG2	1.93	0.49
3:H:143:VAL:HG11	3:H:151:VAL:HG11	1.93	0.49
2:Y:121:PRO:HG2	3:X:215:LYS:HE2	1.93	0.49
1:Z:498:GLN:HE21	2:Y:30:SER:HB3	1.75	0.49
1:A:448:ASN:HD22	1:A:448:ASN:N	2.11	0.49
1:Z:418:ILE:HA	1:Z:422:ASN:HB2	1.94	0.49
1:A:374:PHE:HD1	1:A:436:TRP:HB3	1.77	0.48
1:Z:393:THR:HA	1:Z:522:ALA:HA	1.95	0.48
3:X:72:ASP:HB2	3:X:79:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:109:LYS:HA	2:Y:142:TYR:OH	2.13	0.48
2:Y:25:ALA:O	2:Y:69:THR:OG1	2.27	0.48
1:Z:350:VAL:HG22	1:Z:422:ASN:HB3	1.96	0.48
1:A:498:GLN:HE21	2:L:30:SER:HB3	1.78	0.48
2:L:8:PRO:HG2	2:L:11:LEU:HB2	1.95	0.47
2:L:90:GLN:CD	2:L:93:SER:HB3	2.34	0.47
2:Y:21:ILE:HG12	2:Y:104:THR:HG21	1.96	0.47
1:A:341:VAL:HG11	1:A:397:ALA:HB1	1.96	0.47
3:H:96:LEU:HB2	3:H:100:GLY:O	2.14	0.47
2:L:137:LEU:HD13	3:H:182:VAL:HG21	1.95	0.47
1:A:337:PRO:HB2	1:A:340:GLU:HG2	1.96	0.47
3:H:160:LEU:HD21	3:H:183:VAL:HG21	1.97	0.47
1:Z:448:ASN:N	1:Z:448:ASN:HD22	2.11	0.47
2:L:49:TYR:HB2	3:H:98:VAL:O	2.15	0.46
3:H:95:ASP:HA	3:H:101:LEU:HD13	1.97	0.46
1:Z:337:PRO:HB2	1:Z:340:GLU:HG2	1.96	0.46
3:X:128:SER:O	3:X:129:SER:HB3	2.16	0.46
1:Z:395:VAL:HG22	1:Z:515:PHE:HD1	1.81	0.46
2:L:33:LEU:HG	2:L:34:ALA:N	2.30	0.46
2:Y:115:PRO:CA	2:Y:141:PHE:HB3	2.47	0.45
1:Z:347:PHE:HB3	1:Z:401:VAL:HG23	1.98	0.45
2:Y:33:LEU:HD22	2:Y:71:PHE:CG	2.52	0.45
3:H:185:VAL:HG11	3:H:195:TYR:CE1	2.52	0.45
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.97	0.45
1:A:349:SER:HB3	1:A:452:LEU:O	2.16	0.45
2:L:109:LYS:HA	2:L:142:TYR:OH	2.17	0.45
1:Z:405:ASP:CB	2:Y:94:TYR:HB2	2.46	0.45
3:H:118:LYS:HB2	3:H:118:LYS:HE2	1.83	0.45
3:X:120:PRO:HB3	3:X:146:TYR:HB3	1.97	0.45
3:X:38:ARG:NH2	3:X:62:SER:OG	2.50	0.45
1:Z:421:TYR:OH	3:X:52:TYR:HB3	2.17	0.45
1:Z:392:PHE:CD1	1:Z:515:PHE:HB3	2.52	0.44
1:A:417:LYS:HG2	1:A:417:LYS:H	1.66	0.44
2:Y:115:PRO:HA	2:Y:141:PHE:HB3	1.99	0.44
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.53	0.44
2:Y:186:ALA:O	2:Y:190:LYS:HG3	2.18	0.44
1:A:366:SER:O	1:A:370:ASN:CB	2.61	0.44
1:A:476:GLY:HA2	3:H:27:LEU:HA	1.98	0.44
3:H:72:ASP:HB2	3:H:79:TYR:HE2	1.83	0.44
2:L:21:ILE:HG12	2:L:104:THR:HG21	1.99	0.44
1:A:493:GLN:HE22	3:H:98:VAL:HG12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLN:H	1:A:501:ASN:ND2	2.16	0.44
1:A:347:PHE:HB3	1:A:401:VAL:HG23	2.00	0.44
3:X:12:ILE:HG22	3:X:13:GLN:O	2.18	0.44
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.83	0.44
1:Z:461:LEU:HD22	1:Z:465:GLU:HB3	1.99	0.44
3:X:185:VAL:HG11	3:X:195:TYR:CE1	2.53	0.43
3:H:128:SER:O	3:H:129:SER:HB3	2.17	0.43
2:L:65:SER:OG	2:L:72:THR:OG1	2.36	0.43
3:X:95:ASP:HA	3:X:101:LEU:HD13	2.00	0.43
3:H:6:GLU:H	3:H:106:GLN:HE21	1.66	0.43
3:X:196:ILE:HG12	3:X:211:LYS:HA	2.00	0.43
2:Y:160:ASN:OD1	2:Y:160:ASN:N	2.52	0.43
3:X:72:ASP:OD2	3:X:75:LYS:NZ	2.45	0.43
1:Z:425:LEU:HD21	1:Z:512:VAL:HG11	2.01	0.43
2:L:161:SER:HA	2:L:180:THR:O	2.18	0.43
2:Y:49:TYR:HB2	3:X:98:VAL:O	2.19	0.42
2:Y:35:TRP:CD2	2:Y:73:LEU:HB2	2.54	0.42
2:Y:88:CYS:O	2:Y:101:GLY:N	2.49	0.42
1:A:439:ASN:O	1:A:443:SER:HB2	2.20	0.42
2:Y:131:THR:HG21	3:X:144:LYS:HE2	2.02	0.42
2:Y:36:TYR:CZ	2:Y:46:LEU:HD13	2.54	0.42
2:L:97:LYS:HD2	2:L:97:LYS:HA	1.80	0.42
1:A:350:VAL:HG11	1:A:418:ILE:HD12	2.00	0.42
2:Y:138:LEU:O	2:Y:176:SER:HA	2.20	0.42
3:H:120:PRO:HB3	3:H:146:TYR:HB3	2.01	0.42
2:L:93:SER:O	2:L:96:PRO:HD2	2.19	0.42
2:Y:125:GLU:OE2	3:X:210:LYS:NZ	2.40	0.41
3:H:96:LEU:HD23	3:H:96:LEU:HA	1.94	0.41
2:L:186:ALA:O	2:L:190:LYS:HG3	2.20	0.41
3:X:118:LYS:HB2	3:X:118:LYS:HE2	1.83	0.41
3:X:38:ARG:NH1	3:X:86:ASP:OD1	2.51	0.41
1:Z:417:LYS:H	1:Z:417:LYS:HG2	1.64	0.41
2:L:4:MET:O	2:L:102:PRO:HD3	2.20	0.41
1:A:460:ASN:OD1	3:H:54:GLY:HA3	2.21	0.41
2:Y:192:LYS:HD2	2:Y:212:ASN:HB3	2.02	0.41
1:Z:418:ILE:HA	1:Z:422:ASN:HD22	1.85	0.41
2:L:160:ASN:OD1	2:L:160:ASN:N	2.52	0.41
2:L:192:LYS:HD2	2:L:212:ASN:HB3	2.02	0.41
3:H:147:PHE:HA	3:H:148:PRO:HA	1.86	0.41
3:H:201:HIS:CD2	3:H:203:PRO:HD2	2.55	0.41
1:Z:406:GLU:OE1	1:Z:495:TYR:OH	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:TYR:OH	3:H:52:TYR:HB3	2.20	0.41
2:Y:137:LEU:HD13	3:X:182:VAL:HG21	2.01	0.41
2:L:93:SER:O	2:L:96:PRO:O	2.38	0.41
3:H:167:PHE:HE1	3:H:182:VAL:HG22	1.86	0.40
1:Z:358:ILE:HB	1:Z:395:VAL:HB	2.02	0.40
1:A:472:ILE:HD12	1:A:484:GLU:HG2	2.04	0.40
3:H:106:GLN:HG3	3:H:106:GLN:H	1.58	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	189/231 (82%)	176 (93%)	13 (7%)	0	100	100
1	Z	189/231 (82%)	174 (92%)	15 (8%)	0	100	100
2	L	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
2	Y	213/217 (98%)	201 (94%)	12 (6%)	0	100	100
3	H	211/220 (96%)	204 (97%)	6 (3%)	1 (0%)	29	63
3	X	211/220 (96%)	203 (96%)	7 (3%)	1 (0%)	29	63
All	All	1226/1336 (92%)	1162 (95%)	62 (5%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	97	ASP
3	X	97	ASP

### 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	168/203 (83%)	166 (99%)	2 (1%)	71	87
1	Z	168/203 (83%)	165 (98%)	3 (2%)	59	82
2	L	188/190 (99%)	183 (97%)	5 (3%)	44	73
2	Y	188/190 (99%)	186 (99%)	2 (1%)	73	88
3	H	180/185 (97%)	176 (98%)	4 (2%)	52	77
3	X	180/185 (97%)	176 (98%)	4 (2%)	52	77
All	All	1072/1156 (93%)	1052 (98%)	20 (2%)	57	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	PHE
1	A	394	ASN
2	L	89	GLN
2	L	94	TYR
2	L	98	PHE
2	L	149	GLN
2	L	183	LEU
3	H	106	GLN
3	H	118	LYS
3	H	157	SER
3	H	205	ASN
1	Z	377	PHE
1	Z	387	LEU
1	Z	394	ASN
2	Y	149	GLN
2	Y	183	LEU
3	X	25	SER
3	X	118	LYS
3	X	157	SER
3	X	205	ASN

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	498	GLN
1	Z	501	ASN

### 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](#)

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	NAG	A	601	1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	Z	601	1	14,14,15	0.25	0	17,19,21	0.43	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
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Z	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	Z	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	Z	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	193/231 (83%)	0.50	5 (2%)	56 33	51, 73, 106, 122	0
1	Z	193/231 (83%)	0.53	4 (2%)	63 43	51, 74, 103, 113	0
2	L	215/217 (99%)	0.45	3 (1%)	75 58	49, 69, 89, 112	0
2	Y	215/217 (99%)	0.47	4 (1%)	66 47	47, 71, 90, 102	0
3	H	215/220 (97%)	0.37	3 (1%)	75 58	45, 61, 91, 123	0
3	X	215/220 (97%)	0.41	5 (2%)	60 39	43, 64, 90, 120	0
All	All	1246/1336 (93%)	0.45	24 (1%)	66 47	43, 69, 94, 123	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	216	SER	5.4
2	L	1	ASP	3.9
1	Z	445	VAL	3.6
1	A	445	VAL	3.3
1	A	528	LYS	3.3
1	Z	527	PRO	3.1
3	X	1	GLU	2.8
2	Y	66	GLY	2.8
3	H	3	GLN	2.7
1	A	365	TYR	2.6
3	H	190	LEU	2.5
2	Y	1	ASP	2.5
1	A	527	PRO	2.3
3	X	4	LEU	2.3
2	Y	67	SER	2.3
2	Y	82	ASP	2.2
1	Z	369	TYR	2.2
1	Z	528	LYS	2.2
3	X	190	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	1	GLU	2.1
3	X	98	VAL	2.1
1	A	449	TYR	2.1
2	L	211	PHE	2.1
2	L	82	ASP	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	NAG	A	601	14/15	0.82	0.26	88,98,106,111	0
4	NAG	Z	601	14/15	0.84	0.22	85,92,109,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.