



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2021 – 01:39 PM EDT

PDB ID : 7LOP  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies CV05-163 and CR3022  
Authors : Yuan, M.; Zhu, X.; Wilson, I.A.  
Deposited on : 2021-02-10  
Resolution : 2.25 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 : 2.23.1  
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) : 2.23.1

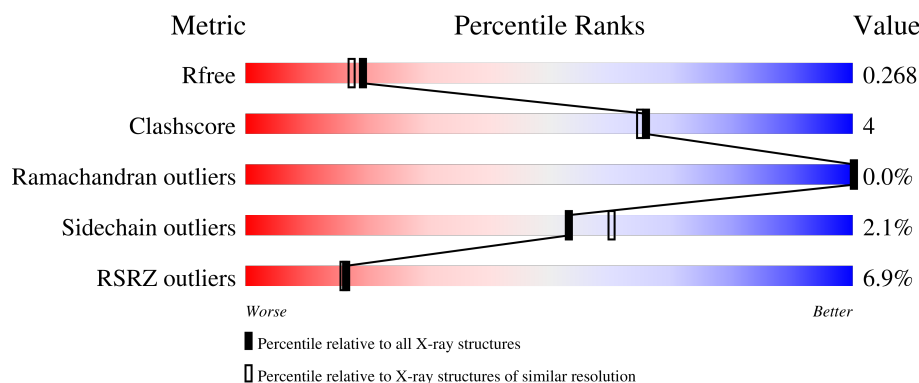
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	B	222	<div> <div>6%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	W	222	<div> <div>10%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
2	C	221	<div> <div>7%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	V	221	<div> <div>5%</div> <div>90%</div> <div>10%</div> <div>.</div> </div>
3	A	231	<div> <div>9%</div> <div>77%</div> <div>7%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Z	231	<div><div></div><div>%</div><div>80%</div><div>16%</div><div>.</div></div>
4	H	227	<div><div>15%</div><div></div><div>89%</div><div>11%</div></div>
4	X	227	<div><div>3%</div><div></div><div>90%</div><div>10%</div></div>
5	L	216	<div><div>6%</div><div></div><div>84%</div><div>14%</div><div>.</div></div>
5	Y	216	<div><div>4%</div><div></div><div>88%</div><div>12%</div><div>.</div></div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17694 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 CR3022 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	215	Total	C	N	O	S	0	0	0
			1604	1020	260	315	9			
1	B	218	Total	C	N	O	S	0	0	0
			1619	1027	263	320	9			

- Molecule 2 is a protein called CR3022 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	220	Total	C	N	O	S	0	0	0
			1709	1073	283	348	5			
2	C	221	Total	C	N	O	S	0	0	0
			1716	1076	284	351	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	194	Total	C	N	O	S	0	1	0
			1547	991	260	288	8			
3	A	195	Total	C	N	O	S	0	1	0
			1554	995	261	290	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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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

- Molecule 4 is a protein called CV05-163 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	227	Total	C	N	O	S	0	0	0
			1698	1068	289	330	11			
4	H	227	Total	C	N	O	S	0	0	0
			1698	1068	289	330	11			

- Molecule 5 is a protein called CV05-163 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Y	216	Total	C	N	O	S	0	0	0
			1655	1034	281	335	5			
5	L	212	Total	C	N	O	S	0	0	0
			1629	1021	277	327	4			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

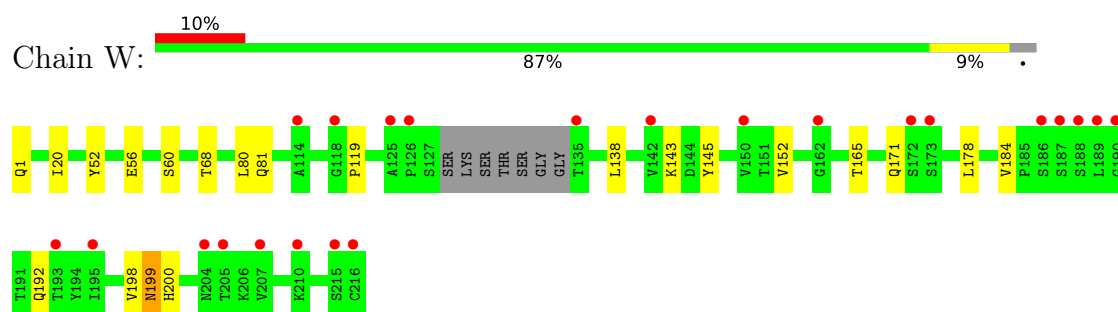
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	W	120	Total	O	0	0
			120	120		
7	V	127	Total	O	0	0
			127	127		
7	B	139	Total	O	0	0
			139	139		
7	C	109	Total	O	0	0
			109	109		
7	Z	125	Total	O	0	0
			125	125		
7	X	132	Total	O	0	0
			132	132		
7	Y	143	Total	O	0	0
			143	143		
7	H	119	Total	O	0	0
			119	119		
7	L	123	Total	O	0	0
			123	123		
7	A	100	Total	O	0	0
			100	100		

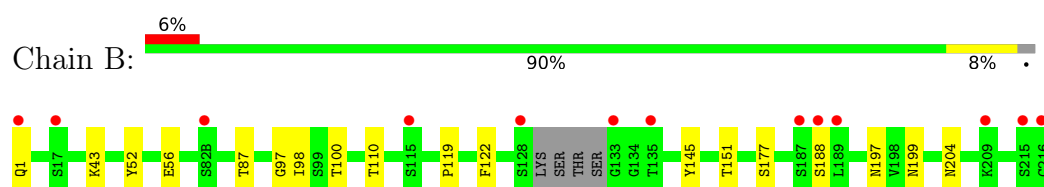
### 3 Residue-property plots [i](#)

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.

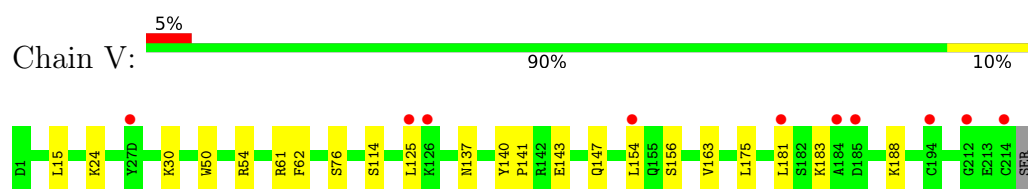
- Molecule 1: CR3022 Fab heavy chain



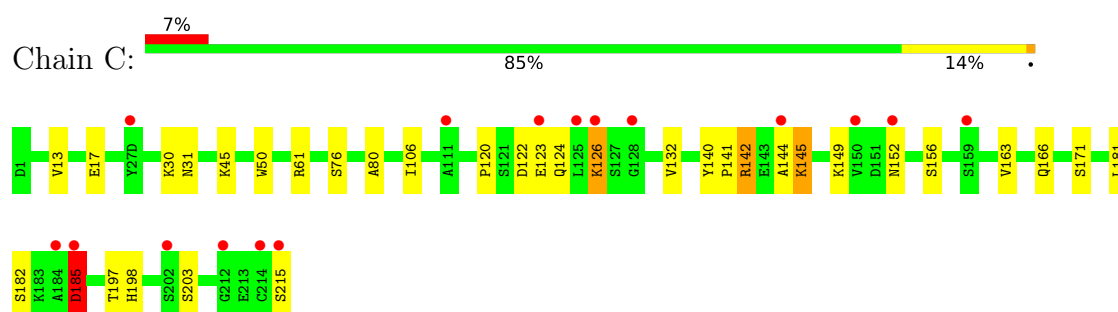
- Molecule 1: CR3022 Fab heavy chain



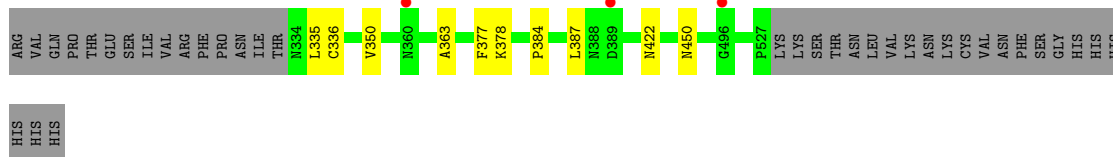
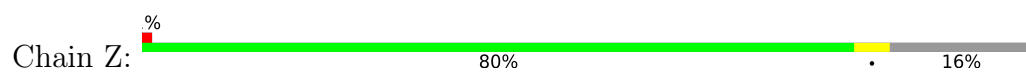
- Molecule 2: CR3022 Fab light chain



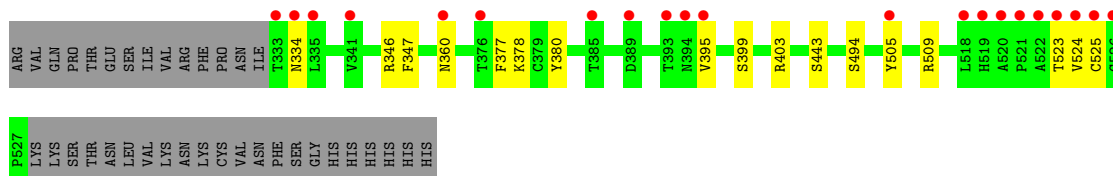
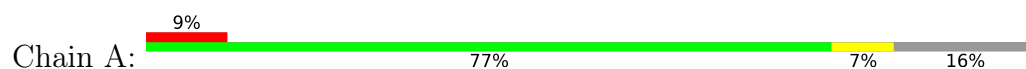
- Molecule 2: CR3022 Fab light chain



- Molecule 3: Spike protein S1



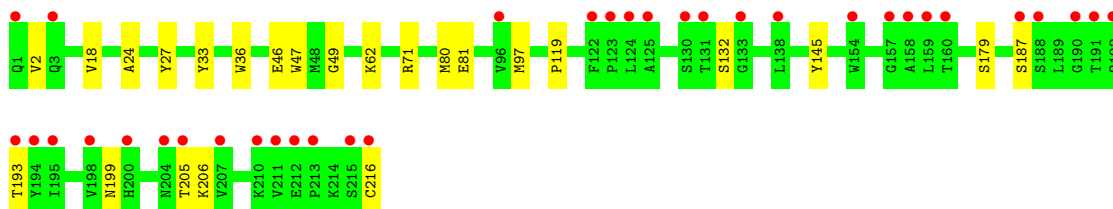
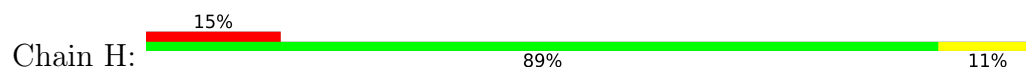
- Molecule 3: Spike protein S1



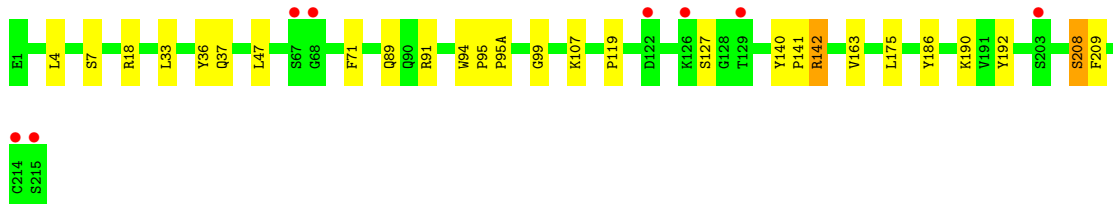
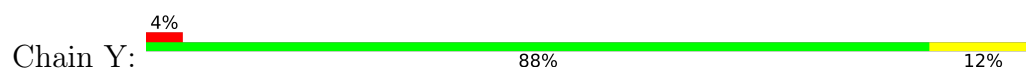
- Molecule 4: CV05-163 Fab heavy chain



- Molecule 4: CV05-163 Fab heavy chain

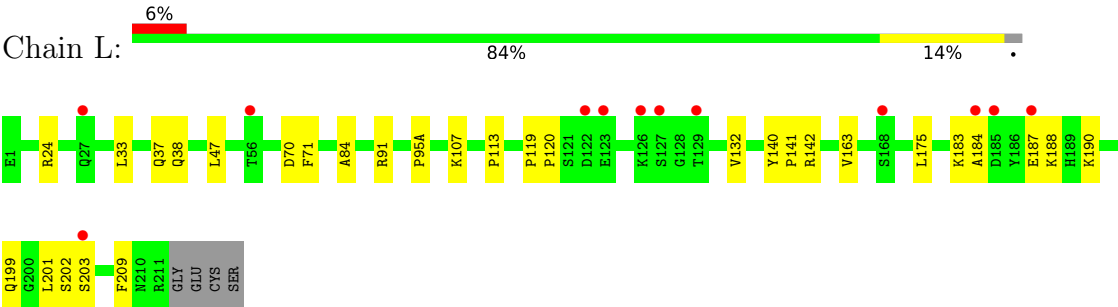


- Molecule 5: CV05-163 Fab light chain



- Molecule 5: CV05-163 Fab light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.00Å 132.88Å 111.33Å 90.00° 100.68° 90.00°	Depositor
Resolution (Å)	49.39 – 2.25 49.39 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.39-2.25) 98.6 (49.39-2.25)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.220 , 0.268 0.220 , 0.268	Depositor DCC
$R_{free}$ test set	5783 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.429	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.9	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	17694	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4927e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	B	0.28	0/1660	0.52	0/2259
1	W	0.26	0/1645	0.49	0/2241
2	C	0.30	0/1754	0.59	4/2383 (0.2%)
2	V	0.25	0/1747	0.46	0/2375
3	A	0.27	0/1598	0.47	0/2175
3	Z	0.27	0/1591	0.44	0/2165
4	H	0.26	0/1740	0.50	0/2370
4	X	0.26	0/1740	0.50	0/2370
5	L	0.28	0/1666	0.49	0/2267
5	Y	0.25	0/1692	0.46	0/2300
All	All	0.27	0/16833	0.49	4/22905 (0.0%)

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
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	145	LYS	CD-CE-NZ	-8.12	93.03	111.70
2	C	185	ASP	CB-CG-OD2	6.42	124.08	118.30
2	C	185	ASP	CB-CG-OD1	-6.06	112.85	118.30
2	C	126	LYS	CD-CE-NZ	-5.07	100.04	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	SER	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	B	1619	0	1591	11	0
1	W	1604	0	1580	12	0
2	C	1716	0	1658	24	0
2	V	1709	0	1653	12	0
3	A	1554	0	1471	12	0
3	Z	1547	0	1464	6	0
4	H	1698	0	1671	14	0
4	X	1698	0	1670	13	0
5	L	1629	0	1588	16	0
5	Y	1655	0	1606	15	0
6	A	14	0	13	0	0
6	Z	14	0	13	0	0
7	A	100	0	0	1	0
7	B	139	0	0	4	0
7	C	109	0	0	2	0
7	H	119	0	0	1	0
7	L	123	0	0	3	0
7	V	127	0	0	2	0
7	W	120	0	0	2	0
7	X	132	0	0	1	0
7	Y	143	0	0	2	0
7	Z	125	0	0	1	0
All	All	17694	0	15978	129	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 4.

All (129) 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)
5:L:183:LYS:HG2	5:L:187:GLU:OE2	1.70	0.89
2:C:149:LYS:NZ	2:C:152:ASN:O	2.13	0.81
3:A:403:ARG:HH21	3:A:505:TYR:HB3	1.46	0.81
2:C:122:ASP:O	2:C:126:LYS:HB2	1.87	0.75
2:C:149:LYS:HE3	2:C:152:ASN:OD1	1.88	0.74
2:V:125:LEU:O	2:V:183:LYS:CE	2.39	0.71
1:B:1:GLN:NE2	7:B:301:HOH:O	2.20	0.70
7:B:301:HOH:O	5:Y:18:ARG:NH1	2.23	0.69
5:Y:127:SER:OG	7:Y:301:HOH:O	2.08	0.69
2:C:149:LYS:HG2	2:C:152:ASN:HA	1.76	0.68
3:A:403:ARG:HE	3:A:505:TYR:HA	1.59	0.67
4:H:46:GLU:OE1	4:H:62:LYS:NZ	2.27	0.67
5:L:183:LYS:CG	5:L:187:GLU:OE2	2.42	0.67
5:L:113:PRO:O	7:L:301:HOH:O	2.11	0.67
4:X:69:MET:SD	7:X:401:HOH:O	2.51	0.67
4:H:193:THR:O	7:H:301:HOH:O	2.12	0.67
2:C:182:SER:OG	2:C:185:ASP:HB2	1.94	0.67
2:V:125:LEU:O	2:V:183:LYS:HE2	1.95	0.66
4:X:38:ARG:HG2	4:X:46:GLU:HG3	1.78	0.65
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.78	0.64
2:C:149:LYS:HZ1	2:C:152:ASN:C	2.01	0.63
4:X:119:PRO:HB3	4:X:145:TYR:HB3	1.81	0.62
2:C:120:PRO:HD3	2:C:132:VAL:HG22	1.82	0.62
2:C:45:LYS:NZ	7:C:305:HOH:O	2.29	0.60
2:V:163:VAL:HG22	2:V:175:LEU:HD12	1.83	0.60
2:C:149:LYS:NZ	2:C:152:ASN:C	2.55	0.60
3:A:395:VAL:HG23	3:A:524:VAL:HG21	1.84	0.60
1:W:56:GLU:OE2	3:Z:378:LYS:NZ	2.35	0.59
1:W:152:VAL:HG22	1:W:198:VAL:HG22	1.85	0.58
3:A:403:ARG:NH2	3:A:505:TYR:HB3	2.16	0.57
2:C:142:ARG:CZ	2:C:163:VAL:HG21	2.37	0.55
2:V:24:LYS:NZ	7:V:304:HOH:O	2.34	0.55
1:B:56:GLU:OE2	3:A:378:LYS:NZ	2.39	0.55
1:B:122:PHE:CE1	2:C:124:GLN:HG3	2.41	0.55
5:Y:142:ARG:NH2	5:Y:163:VAL:HG21	2.23	0.54
3:A:360:ASN:HA	3:A:523:THR:HB	1.89	0.54
3:A:403:ARG:HH21	3:A:505:TYR:CB	2.18	0.54
2:V:125:LEU:HD22	2:V:183:LYS:HG3	1.89	0.53
1:W:199:ASN:HD22	1:W:200:HIS:N	2.07	0.53
4:H:205:THR:C	4:H:206:LYS:HD3	2.29	0.53
5:L:120:PRO:HD3	5:L:132:VAL:HG22	1.90	0.53
2:C:61:ARG:HB2	2:C:76:SER:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1:GLN:NE2	7:W:307:HOH:O	2.39	0.52
2:C:80:ALA:HA	2:C:106:ILE:HD11	1.91	0.52
1:W:119:PRO:HB3	1:W:145:TYR:HB3	1.92	0.52
2:C:30:LYS:NZ	7:C:310:HOH:O	2.43	0.52
1:W:52:TYR:CD2	3:Z:378:LYS:HD3	2.45	0.52
3:Z:450:ASN:ND2	7:Z:701:HOH:O	2.27	0.52
5:Y:37:GLN:HB2	5:Y:47:LEU:HD11	1.92	0.52
1:B:98:ILE:HG22	3:A:380:TYR:HA	1.91	0.51
4:H:199:ASN:HB3	4:H:206:LYS:NZ	2.27	0.50
5:L:184:ALA:O	5:L:188:LYS:HG3	2.12	0.49
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.95	0.49
2:V:30:LYS:HG2	2:V:50:TRP:CD2	2.48	0.49
1:W:20:ILE:HD11	1:W:80:LEU:HD23	1.95	0.48
1:W:138:LEU:HD23	1:W:184:VAL:HG21	1.94	0.48
4:H:36:TRP:CE2	4:H:80:MET:HB2	2.48	0.48
1:W:165:THR:HG23	1:W:178:LEU:HD21	1.96	0.48
2:V:54:ARG:NH1	2:V:62:PHE:O	2.38	0.48
2:C:122:ASP:O	2:C:126:LYS:CB	2.58	0.48
4:X:51:ILE:HB	4:X:69:MET:HE2	1.95	0.48
3:Z:350:VAL:HG22	3:Z:422:ASN:HB3	1.96	0.48
1:W:143:LYS:NZ	1:W:171:GLN:OE1	2.47	0.47
2:C:123:GLU:O	2:C:126:LYS:HB3	2.14	0.47
4:X:36:TRP:CE2	4:X:80:MET:HB2	2.49	0.47
1:B:119:PRO:HB3	1:B:145:TYR:HB3	1.96	0.47
1:B:204:ASN:ND2	7:B:317:HOH:O	2.47	0.47
3:A:525:CYS:SG	7:A:779:HOH:O	2.61	0.47
3:Z:384:PRO:HA	3:Z:387:LEU:HG	1.97	0.47
4:H:2:VAL:HG13	4:H:27:TYR:CD1	2.49	0.47
2:V:61:ARG:HB2	2:V:76:SER:O	2.15	0.47
5:Y:4:LEU:HB2	5:Y:99:GLY:HA2	1.97	0.46
2:C:30:LYS:HG2	2:C:50:TRP:CD2	2.51	0.46
5:Y:91:ARG:HD2	5:Y:95(A):PRO:O	2.16	0.46
4:H:24:ALA:HB1	4:H:27:TYR:CE1	2.50	0.45
4:H:205:THR:O	4:H:206:LYS:HD3	2.16	0.45
5:L:119:PRO:HB3	5:L:209:PHE:CE1	2.52	0.45
2:V:30:LYS:NZ	7:V:317:HOH:O	2.49	0.45
5:Y:163:VAL:HG22	5:Y:175:LEU:HD12	1.99	0.45
1:B:52:TYR:CD2	3:A:378:LYS:HD3	2.51	0.45
4:X:71:ARG:HD3	4:X:73:THR:HG23	1.97	0.45
1:W:68:THR:HB	1:W:81:GLN:HG2	1.98	0.45
4:X:210:LYS:NZ	4:X:212:GLU:OE2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:201:LEU:HD21	7:L:301:HOH:O	2.17	0.44
3:Z:336:CYS:SG	3:Z:363:ALA:HB2	2.58	0.44
3:A:347:PHE:CE2	3:A:509:ARG:HB3	2.53	0.44
2:C:13:VAL:HG13	2:C:17:GLU:HB2	2.00	0.44
2:C:145:LYS:HB2	2:C:197:THR:HB	2.00	0.44
4:X:210:LYS:HB3	4:X:210:LYS:HE3	1.92	0.43
2:C:149:LYS:HE3	2:C:152:ASN:CG	2.38	0.43
5:L:24:ARG:HH12	5:L:70:ASP:HB2	1.83	0.43
4:X:24:ALA:HB1	4:X:27:TYR:CE1	2.53	0.43
5:L:38:GLN:O	5:L:84:ALA:HB1	2.18	0.43
2:V:114:SER:HB2	2:V:137:ASN:HB3	2.01	0.43
4:X:87:THR:HA	4:X:109:VAL:O	2.19	0.43
5:Y:94:TRP:HA	5:Y:95:PRO:HA	1.91	0.43
5:Y:140:TYR:CG	5:Y:141:PRO:HA	2.54	0.43
2:C:144:ALA:HB2	2:C:198:HIS:HD2	1.84	0.42
5:Y:107:LYS:HA	5:Y:140:TYR:OH	2.19	0.42
4:H:18:VAL:O	4:H:81:GLU:HA	2.19	0.42
4:H:33:TYR:CE2	4:H:97:MET:HG2	2.54	0.42
4:H:199:ASN:CG	4:H:206:LYS:HD2	2.39	0.42
5:Y:119:PRO:HB3	5:Y:209:PHE:CE1	2.54	0.42
5:L:91:ARG:HD2	5:L:95(A):PRO:O	2.19	0.42
1:B:87:THR:HG23	1:B:110:THR:HA	2.02	0.42
4:X:151:THR:OG1	4:X:199:ASN:HB2	2.20	0.42
2:V:140:TYR:CG	2:V:141:PRO:HA	2.55	0.42
2:V:147:GLN:HG2	2:V:154:LEU:HD11	2.01	0.42
5:L:107:LYS:HA	5:L:140:TYR:OH	2.20	0.42
1:B:43:LYS:NZ	7:B:321:HOH:O	2.52	0.42
5:Y:33:LEU:HG	5:Y:71:PHE:CG	2.55	0.42
2:C:166:GLN:HG2	2:C:171:SER:HA	2.02	0.41
1:B:151:THR:OG1	1:B:199:ASN:HB3	2.20	0.41
5:L:163:VAL:HG22	5:L:175:LEU:HD12	2.02	0.41
5:L:140:TYR:CG	5:L:141:PRO:HA	2.54	0.41
5:L:199:GLN:NE2	7:L:309:HOH:O	2.40	0.41
2:C:31:ASN:O	2:C:50:TRP:HA	2.21	0.41
4:H:199:ASN:CB	4:H:206:LYS:HD2	2.50	0.41
4:X:1:GLN:HB3	4:X:2:VAL:H	1.72	0.41
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.56	0.41
5:Y:36:TYR:HE1	5:Y:89:GLN:HB3	1.86	0.41
1:B:97:GLY:O	1:B:100:THR:OG1	2.23	0.41
5:Y:186:TYR:HA	5:Y:192:TYR:OH	2.21	0.41
4:X:2:VAL:HG13	4:X:27:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:192:GLN:OE1	7:W:301:HOH:O	2.22	0.40
2:C:140:TYR:CG	2:C:141:PRO:HA	2.56	0.40
5:L:33:LEU:HG	5:L:71:PHE:CG	2.56	0.40
3:A:403:ARG:NH2	3:A:505:TYR:O	2.54	0.40
5:Y:208:SER:O	7:Y:302:HOH:O	2.21	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	B	214/222 (96%)	209 (98%)	5 (2%)	0	100	100
1	W	211/222 (95%)	206 (98%)	5 (2%)	0	100	100
2	C	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
2	V	218/221 (99%)	212 (97%)	6 (3%)	0	100	100
3	A	194/231 (84%)	188 (97%)	5 (3%)	1 (0%)	29	28
3	Z	193/231 (84%)	187 (97%)	6 (3%)	0	100	100
4	H	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
4	X	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
5	L	210/216 (97%)	204 (97%)	6 (3%)	0	100	100
5	Y	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
All	All	2123/2234 (95%)	2061 (97%)	61 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	334	ASN



### 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	B	183/187 (98%)	181 (99%)	2 (1%)	73	80
1	W	182/187 (97%)	180 (99%)	2 (1%)	73	80
2	C	196/196 (100%)	190 (97%)	6 (3%)	40	46
2	V	195/196 (100%)	190 (97%)	5 (3%)	46	52
3	A	169/203 (83%)	164 (97%)	5 (3%)	41	47
3	Z	168/203 (83%)	166 (99%)	2 (1%)	71	78
4	H	190/190 (100%)	185 (97%)	5 (3%)	46	52
4	X	190/190 (100%)	186 (98%)	4 (2%)	53	60
5	L	184/187 (98%)	180 (98%)	4 (2%)	52	59
5	Y	187/187 (100%)	183 (98%)	4 (2%)	53	60
All	All	1844/1926 (96%)	1805 (98%)	39 (2%)	53	60

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	60	SER
1	W	199	ASN
2	V	15	LEU
2	V	143	GLU
2	V	156	SER
2	V	181	LEU
2	V	188	LYS
1	B	177	SER
1	B	197	ASN
2	C	142	ARG
2	C	156	SER
2	C	181	LEU
2	C	185	ASP
2	C	203	SER
2	C	215	SER
3	Z	335	LEU

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Mol	Chain	Res	Type
3	Z	377	PHE
4	X	71	ARG
4	X	83	ARG
4	X	99	ARG
4	X	161	SER
5	Y	7	SER
5	Y	142	ARG
5	Y	190	LYS
5	Y	208	SER
4	H	71	ARG
4	H	132	SER
4	H	179	SER
4	H	187	SER
4	H	216	CYS
5	L	142	ARG
5	L	190	LYS
5	L	202	SER
5	L	203	SER
3	A	346	ARG
3	A	377	PHE
3	A	399	SER
3	A	443	SER
3	A	494	SER

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

Mol	Chain	Res	Type
1	W	199	ASN
2	V	42	GLN
5	L	199	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [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	$\# Z  > 2$
6	NAG	A	601	3	14,14,15	0.33	0	17,19,21	0.54	0
6	NAG	Z	601	3	14,14,15	0.37	0	17,19,21	0.53	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	A	601	3	-	2/6/23/26	0/1/1/1
6	NAG	Z	601	3	-	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
6	A	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	Z	601	NAG	O5-C5-C6-O6
6	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	B	218/222 (98%)	0.67	13 (5%) 21 21	23, 35, 58, 118	0
1	W	215/222 (96%)	0.87	23 (10%) 6 5	21, 39, 74, 137	0
2	C	221/221 (100%)	0.79	16 (7%) 15 14	24, 37, 67, 101	0
2	V	220/221 (99%)	0.66	10 (4%) 33 33	17, 36, 68, 90	0
3	A	195/231 (84%)	0.76	21 (10%) 5 5	25, 36, 64, 101	0
3	Z	194/231 (83%)	0.50	3 (1%) 73 74	19, 31, 49, 65	0
4	H	227/227 (100%)	0.86	35 (15%) 2 1	21, 37, 76, 114	0
4	X	227/227 (100%)	0.43	6 (2%) 56 57	16, 32, 55, 100	0
5	L	212/216 (98%)	0.54	12 (5%) 23 23	20, 36, 60, 87	0
5	Y	216/216 (100%)	0.41	8 (3%) 41 41	19, 32, 54, 83	0
All	All	2145/2234 (96%)	0.65	147 (6%) 16 16	16, 35, 67, 137	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	216	CYS	12.1
5	Y	214	CYS	9.1
1	B	216	CYS	9.0
4	X	216	CYS	8.2
2	C	215	SER	7.9
1	W	188	SER	7.6
1	B	188	SER	7.1
3	A	522	ALA	6.2
4	H	193	THR	6.0
4	H	216	CYS	5.9
3	A	520	ALA	5.5
4	H	192	GLN	5.3
4	H	190	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
4	H	130	SER	5.0
4	X	191	THR	4.9
5	L	126	LYS	4.7
2	V	154	LEU	4.6
1	W	173	SER	4.5
2	C	126	LYS	4.4
4	H	205	THR	4.4
2	V	125	LEU	4.3
3	A	521	PRO	4.2
5	L	122	ASP	4.1
4	H	191	THR	4.1
4	H	159	LEU	4.1
5	L	129	THR	4.1
4	H	215	SER	4.0
1	W	207	VAL	3.9
2	V	126	LYS	3.9
3	A	518	LEU	3.9
4	H	187	SER	3.9
2	V	212	GLY	3.8
3	A	333	THR	3.7
3	A	525	CYS	3.7
5	Y	215	SER	3.7
2	V	184	ALA	3.6
1	B	187	SER	3.6
1	W	215	SER	3.4
1	W	210	LYS	3.4
2	C	185	ASP	3.3
2	V	214	CYS	3.3
2	C	212	GLY	3.3
5	Y	129	THR	3.2
1	B	128	SER	3.2
1	W	189	LEU	3.2
1	B	133	GLY	3.2
2	C	128	GLY	3.2
4	H	158	ALA	3.2
4	H	188	SER	3.2
4	H	133	GLY	3.1
5	L	187	GLU	3.1
3	A	334	ASN	3.1
5	Y	126	LYS	3.1
1	W	114	ALA	3.1
4	H	212	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
3	Z	389	ASP	3.1
1	W	193	THR	3.1
5	L	27	GLN	3.0
4	H	211	VAL	3.0
4	H	123	PRO	3.0
1	W	118	GLY	2.9
3	A	360	ASN	2.9
1	W	195	ILE	2.9
3	A	393	THR	2.9
5	Y	68	GLY	2.8
4	H	198	VAL	2.8
5	Y	122	ASP	2.8
4	H	1	GLN	2.8
1	W	187	SER	2.8
3	A	523	THR	2.8
4	H	131	THR	2.8
2	C	125	LEU	2.8
5	L	203	SER	2.8
3	A	519	HIS	2.8
3	Z	496	GLY	2.7
1	B	115	SER	2.7
2	C	27(D)	TYR	2.7
2	C	214	CYS	2.7
2	C	202	SER	2.7
5	L	184	ALA	2.6
3	A	335	LEU	2.6
1	B	1	GLN	2.6
2	C	152	ASN	2.6
1	W	190	GLY	2.6
4	H	213	PRO	2.5
2	C	150	VAL	2.5
4	H	157	GLY	2.5
5	L	56	THR	2.5
2	V	181	LEU	2.5
3	A	389	ASP	2.5
1	W	204	ASN	2.5
4	H	122	PHE	2.5
2	V	27(D)	TYR	2.5
3	A	385	THR	2.5
1	W	125	ALA	2.5
4	H	154	TRP	2.4
2	V	185	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	184	ALA	2.4
4	H	204	ASN	2.4
2	C	144	ALA	2.4
4	H	194	TYR	2.4
4	X	212	GLU	2.4
1	B	189	LEU	2.4
1	W	150	VAL	2.4
4	H	195	ILE	2.4
4	H	125	ALA	2.4
3	A	394	ASN	2.4
4	H	160	THR	2.3
1	W	172	SER	2.3
3	A	524	VAL	2.3
1	B	135	THR	2.3
4	X	132	SER	2.3
5	L	168	SER	2.3
3	A	341	VAL	2.3
4	H	138	LEU	2.3
5	L	123	GLU	2.3
4	X	192	GLN	2.3
5	L	185	ASP	2.2
3	A	395	VAL	2.2
4	H	96	VAL	2.2
5	L	127	SER	2.2
2	C	111	ALA	2.2
4	H	210	LYS	2.2
1	B	215	SER	2.2
1	W	135	THR	2.2
3	A	376	THR	2.2
1	B	209	LYS	2.2
1	W	162	GLY	2.2
3	A	526	GLY	2.2
4	H	3	GLN	2.2
4	H	207	VAL	2.1
5	Y	203	SER	2.1
1	W	142	VAL	2.1
4	X	213	PRO	2.1
1	W	126	PRO	2.1
1	B	17	SER	2.1
1	B	82(B)	SER	2.1
2	C	123	GLU	2.1
3	Z	360	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	W	186	SER	2.1
3	A	505	TYR	2.1
5	Y	67	SER	2.1
4	H	200	HIS	2.1
2	C	159	SER	2.0
2	V	194	CYS	2.0
4	H	124	LEU	2.0
1	W	205	THR	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
6	NAG	A	601	14/15	0.81	0.17	46,53,56,60	0
6	NAG	Z	601	14/15	0.86	0.15	36,45,49,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.