wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 02:29 AM 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

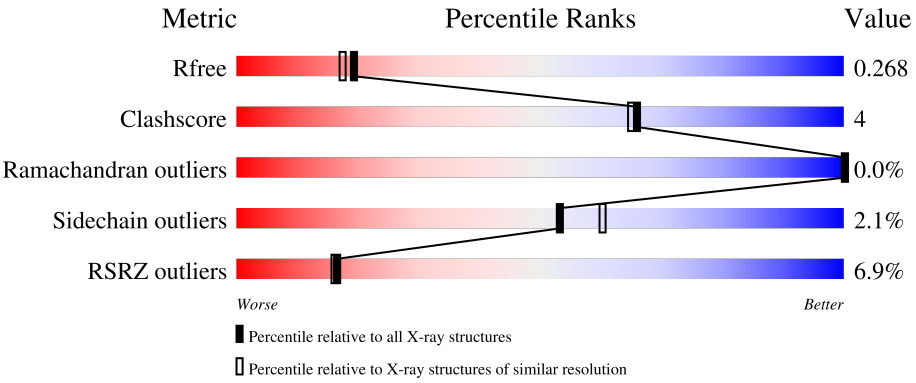
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.25 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 >=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 <=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	6% 90% 8%
1	W	222	10% 87% 9%
2	C	221	7% 85% 14%
2	V	221	5% 90% 10%
3	A	231	9% 77% 7% 16%

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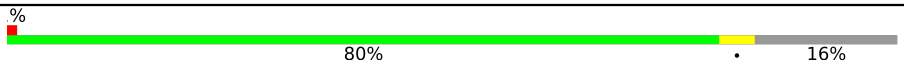
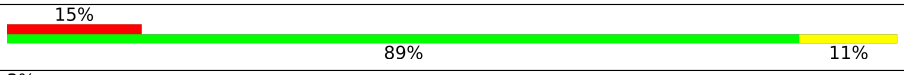
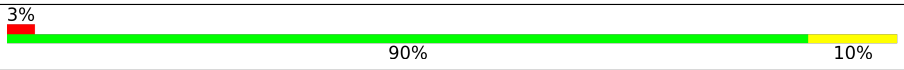
Mol	Chain	Length	Quality of chain
3	Z	231	
4	H	227	
4	X	227	
5	L	216	
5	Y	216	

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

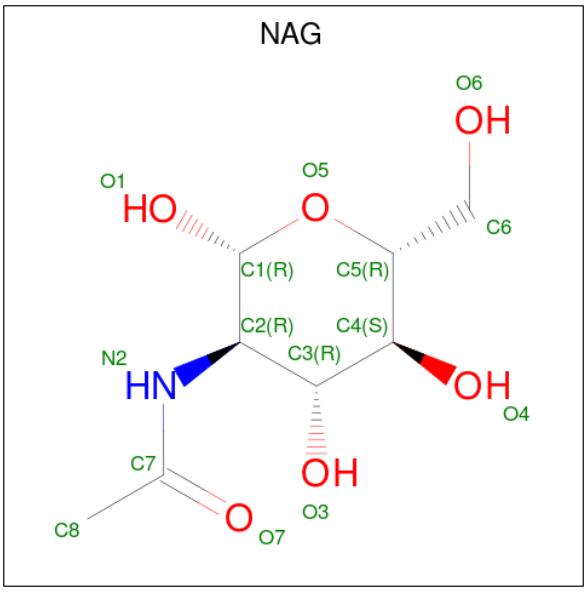
- Molecule 4 is a protein called CV05-163 Fab heavy chain.

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: $C_8H_{15}NO_6$).



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

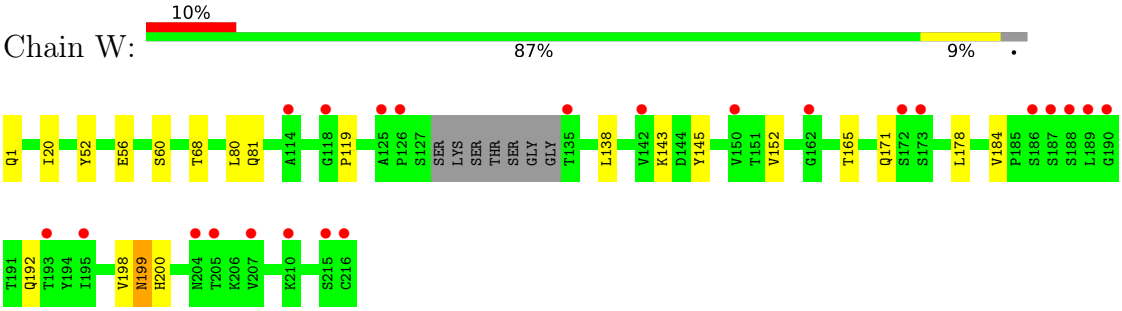
- Molecule 7 is water.

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

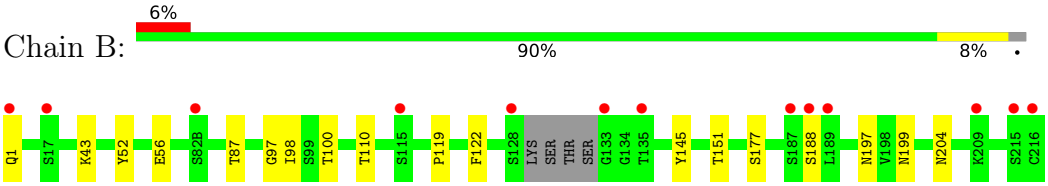
3 Residue-property plots (i)

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.

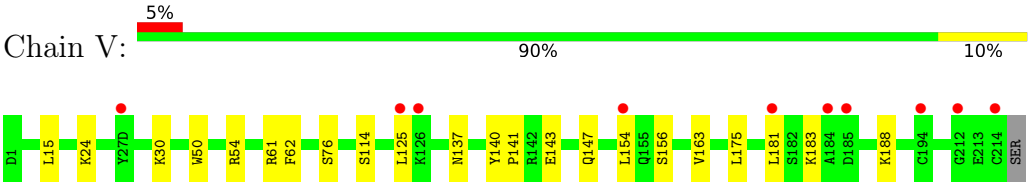
- Molecule 1: CR3022 Fab heavy chain



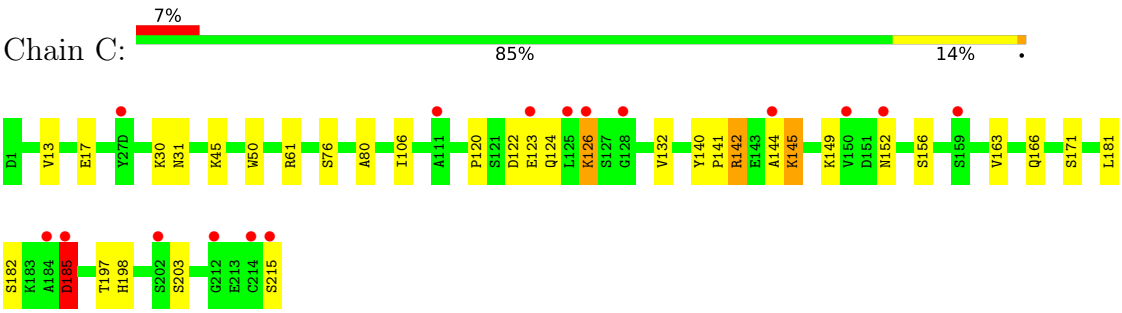
- Molecule 1: CR3022 Fab heavy chain



- Molecule 2: CR3022 Fab light chain

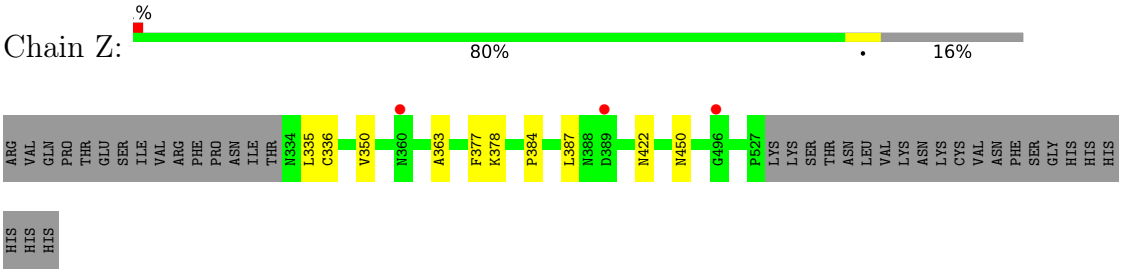


- Molecule 2: CR3022 Fab light chain



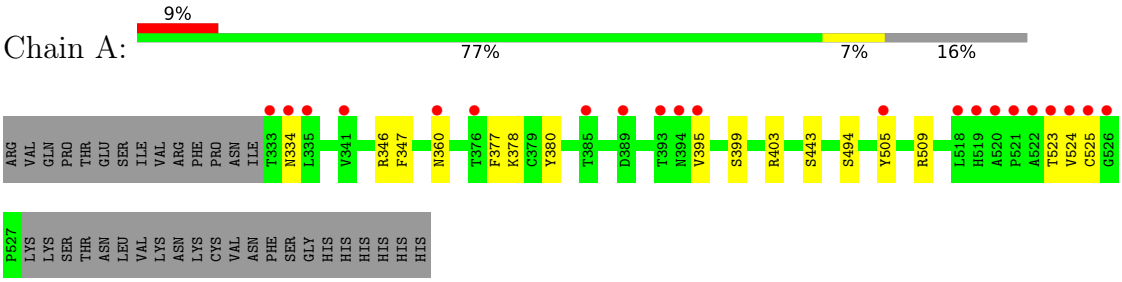
- Molecule 3: Spike protein S1

Chain Z:



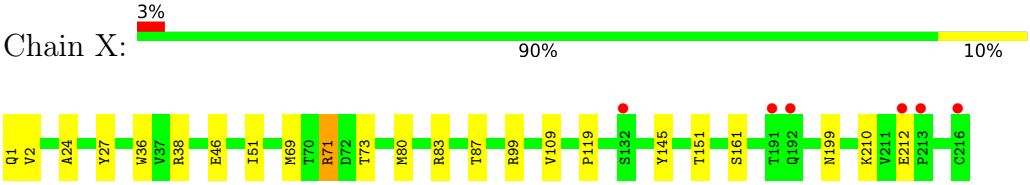
• Molecule 3: Spike protein S1

Chain A:



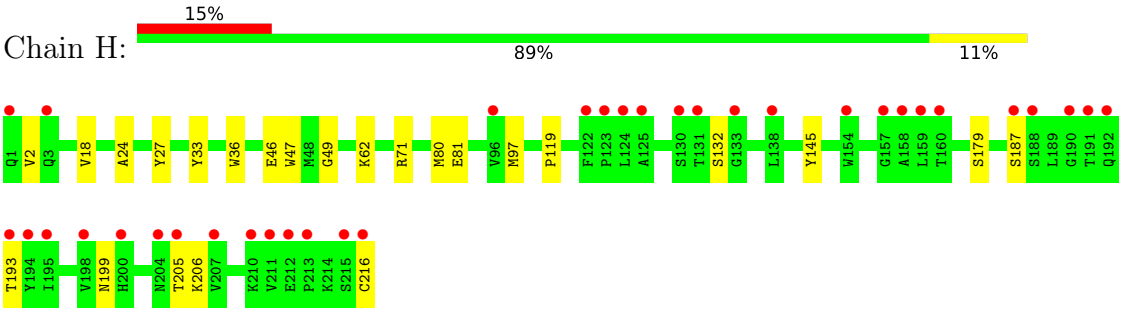
• Molecule 4: CV05-163 Fab heavy chain

Chain X:



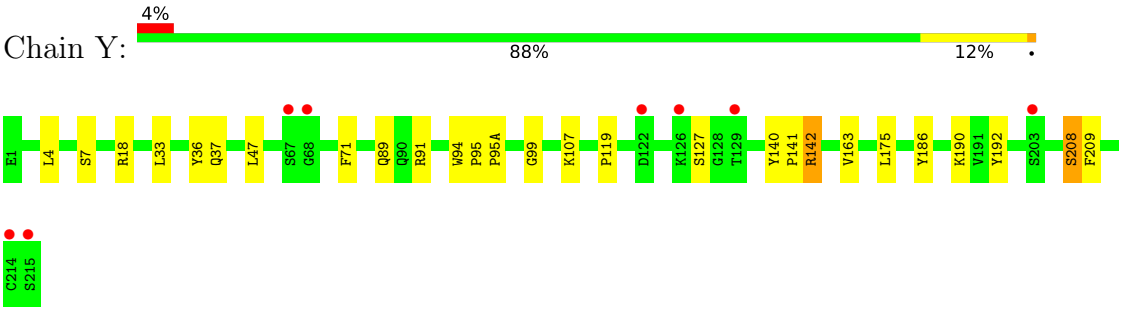
• Molecule 4: CV05-163 Fab heavy chain

Chain H:



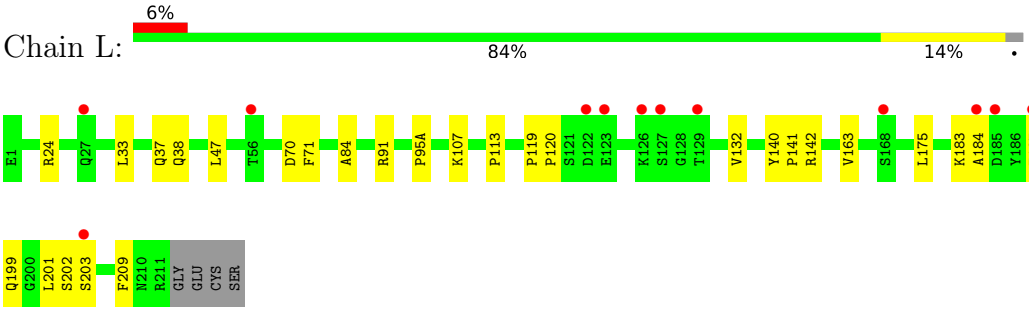
• Molecule 5: CV05-163 Fab light chain

Chain Y:



• Molecule 5: CV05-163 Fab light chain

Chain L:


6%
84%
14%
E1
R24
Q27
L33
Q37
Q38
L47
T56
D70
F71
A84
R91
P95A
K107
P113
P119
P120
S121
D122
E123
K126
S127
G128
T129
V132
Y140
P141
R142
V163
S168
L175
K183
A184
D185
Y186
E187
K188
H189
K190
Q199
G200
L201
S202
S203
F209
N210
R211
GLY
GLU
CYS
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.48 (at 2.25Å)	Xtriage
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^2)	29.1	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17694	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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 (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	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.

The worst 5 of 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

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 (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	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

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	187	SER
3	A	377	PHE
4	H	216	CYS
5	L	202	SER
3	A	443	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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^{th} 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^2)	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

The worst 5 of 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

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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^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.