



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2022 – 06:15 PM JST

PDB ID : 7EW5
Title : immune complex of HPV6 L1 pentamer and neutralizing antibody 13H5
Authors : Wang, Z.P.; Wang, D.N.; Gu, Y.; Li, S.W.
Deposited on : 2021-05-24
Resolution : 3.61 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

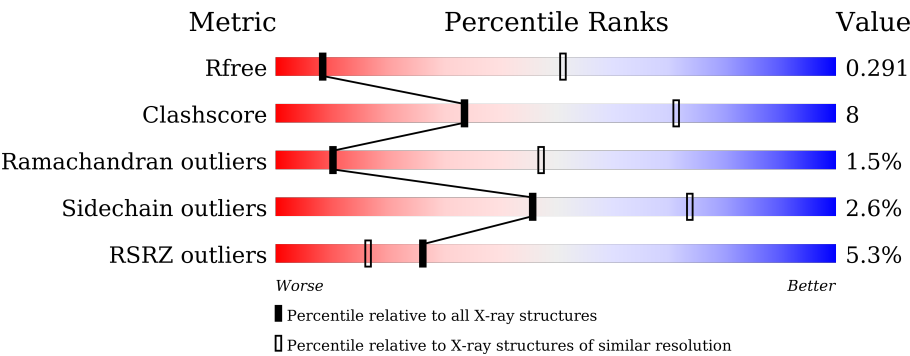
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.61 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.





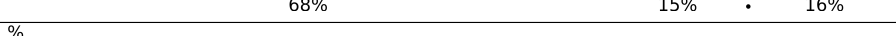


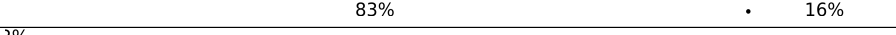

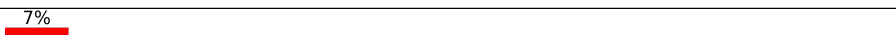


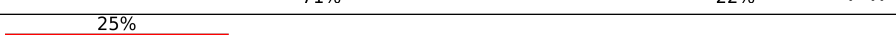


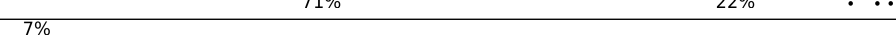


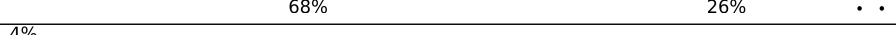







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 $\leq 5\%$. 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	496	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%14%•16%</div></div>
1	D	496	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%15%16%</div></div>
1	G	496	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>68%15%•16%</div></div>
1	J	496	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%14%•16%</div></div>
1	M	496	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>67%16%•16%</div></div>
1	P	496	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%14%•16%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	S	496	
1	V	496	
1	Y	496	
1	b	496	
2	B	221	
2	E	221	
2	H	221	
2	K	221	
2	N	221	
2	Q	221	
2	T	221	
2	W	221	
2	Z	221	
2	g	221	
3	C	214	
3	F	214	
3	I	214	
3	L	214	
3	O	214	
3	R	214	
3	U	214	
3	X	214	
3	a	214	
3	j	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 65550 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	D	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	G	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	J	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	M	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	P	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	S	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	V	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	Y	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	b	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q9W9C6
A	376	VAL	MET	conflict	UNP Q9W9C6
D	-2	MET	-	initiating methionine	UNP Q9W9C6
D	376	VAL	MET	conflict	UNP Q9W9C6
G	-2	MET	-	initiating methionine	UNP Q9W9C6
G	376	VAL	MET	conflict	UNP Q9W9C6
J	-2	MET	-	initiating methionine	UNP Q9W9C6
J	376	VAL	MET	conflict	UNP Q9W9C6
M	-2	MET	-	initiating methionine	UNP Q9W9C6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	376	VAL	MET	conflict	UNP Q9W9C6
P	-2	MET	-	initiating methionine	UNP Q9W9C6
P	376	VAL	MET	conflict	UNP Q9W9C6
S	-2	MET	-	initiating methionine	UNP Q9W9C6
S	376	VAL	MET	conflict	UNP Q9W9C6
V	-2	MET	-	initiating methionine	UNP Q9W9C6
V	376	VAL	MET	conflict	UNP Q9W9C6
Y	-2	MET	-	initiating methionine	UNP Q9W9C6
Y	376	VAL	MET	conflict	UNP Q9W9C6
b	-2	MET	-	initiating methionine	UNP Q9W9C6
b	376	VAL	MET	conflict	UNP Q9W9C6

- Molecule 2 is a protein called Heavy chain of 13H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	E	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	H	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	K	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	N	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	g	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	Q	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	T	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	W	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	Z	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			

- Molecule 3 is a protein called Light chain of 13H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	F	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			

Continued on next page...

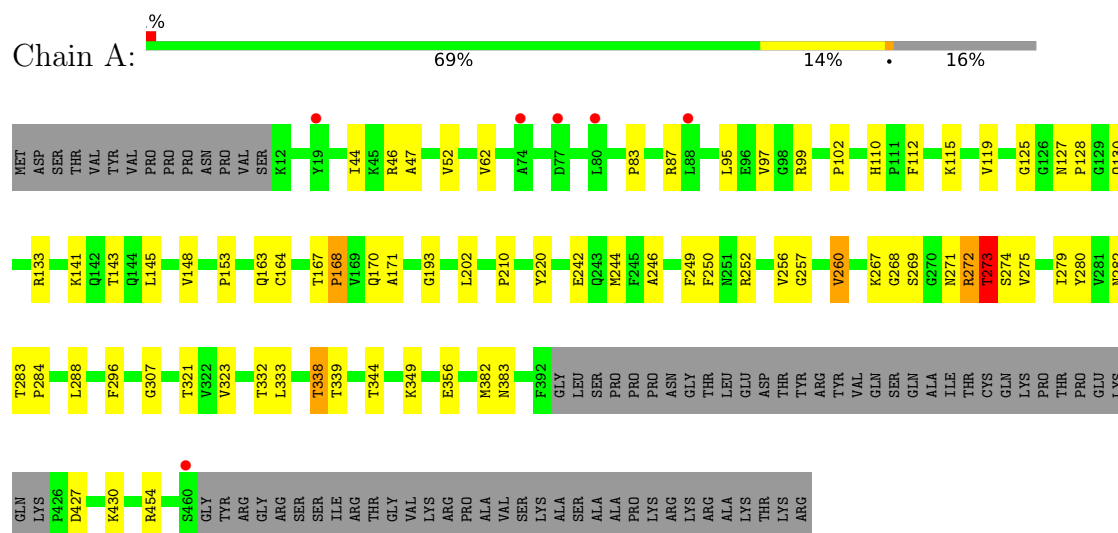
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	L	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	O	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	j	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	R	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	U	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	X	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	a	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			

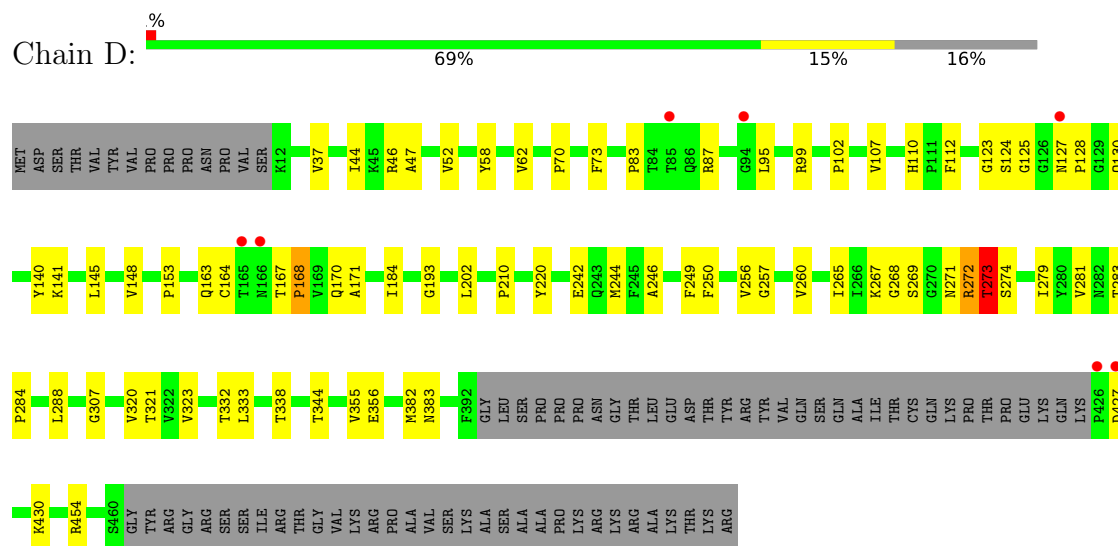
3 Residue-property plots [i](#)

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: Major capsid protein L1

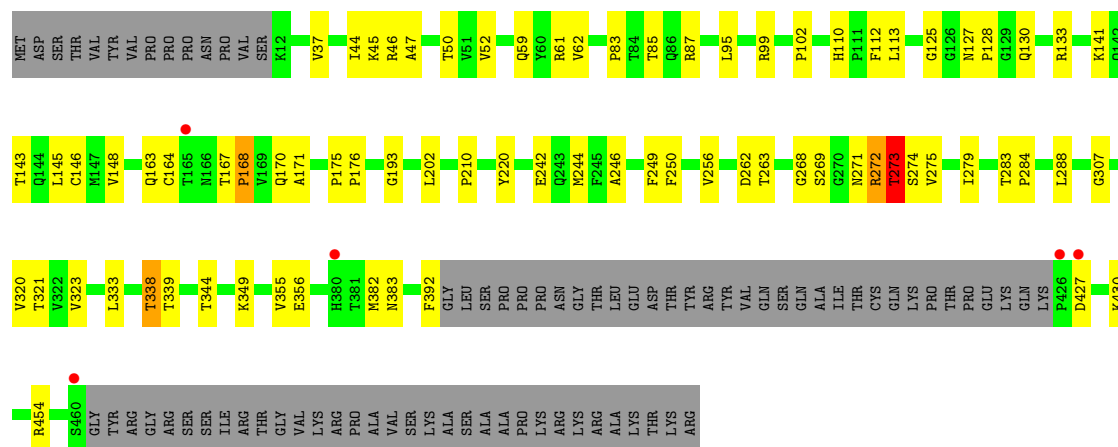


• Molecule 1: Major capsid protein L1



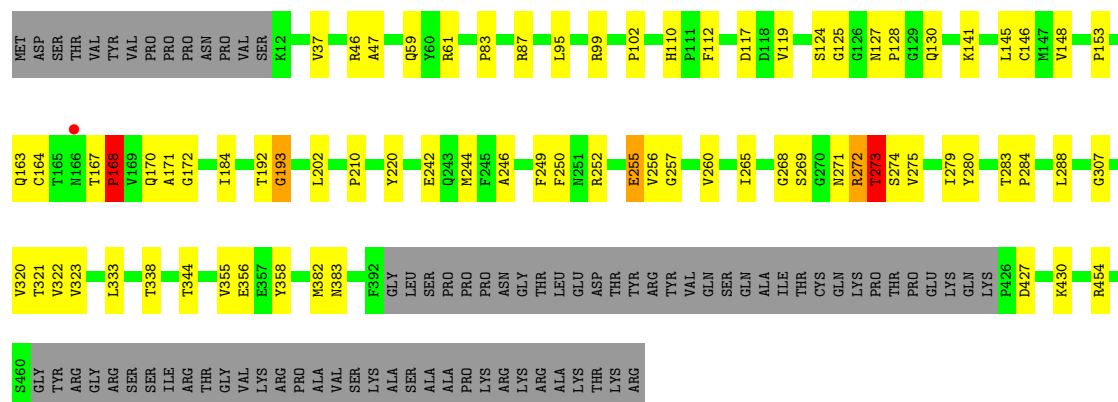
• Molecule 1: Major capsid protein L1





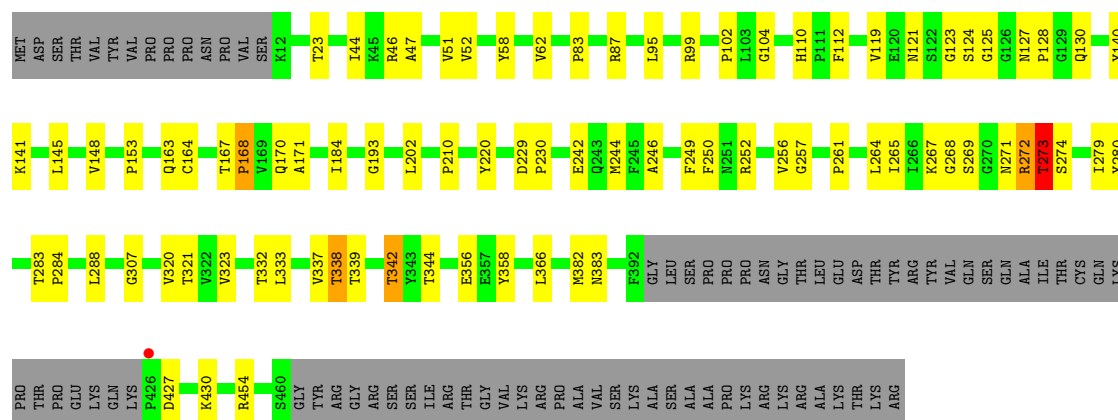
• Molecule 1: Major capsid protein L1

Chain J: 69% 14% 16%



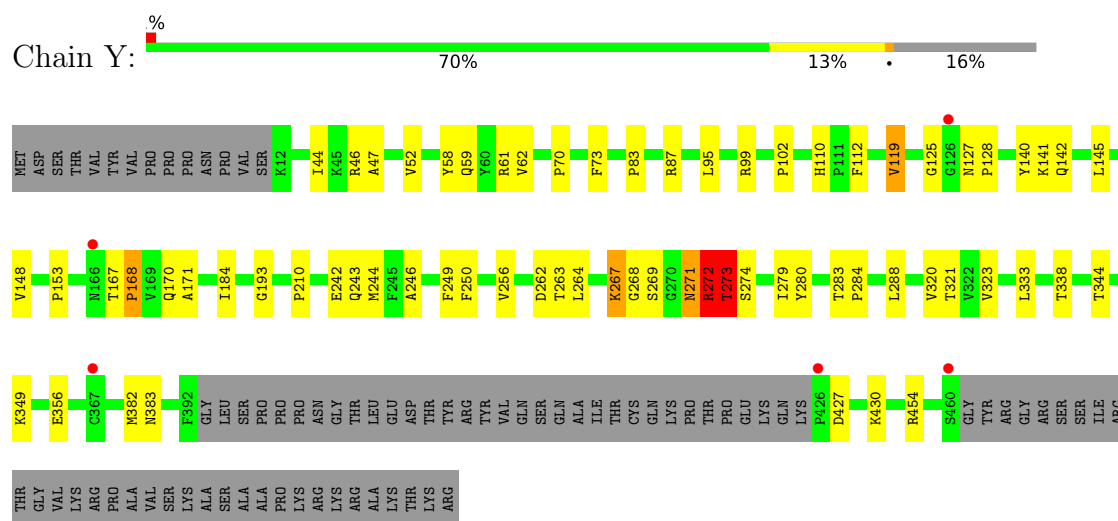
• Molecule 1: Major capsid protein L1

Chain M: 67% 16% 16%

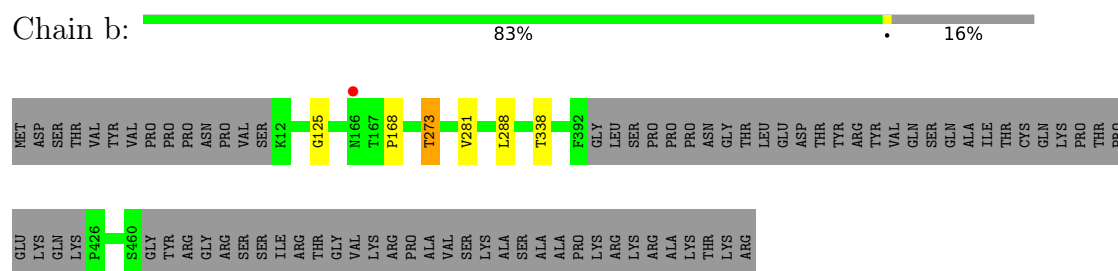


• Molecule 1: Major capsid protein L1

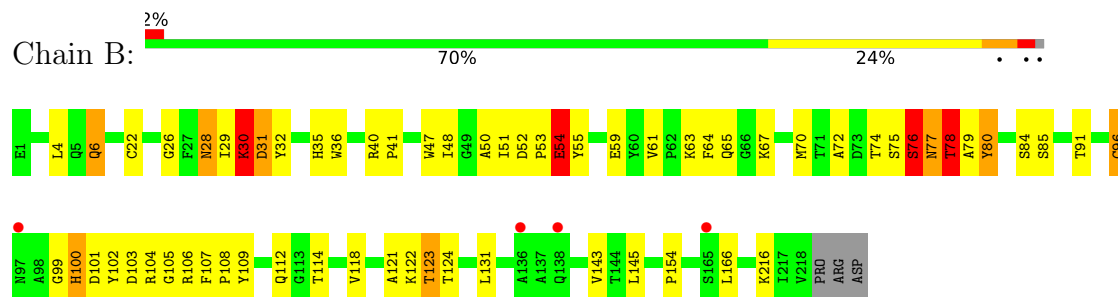
Chain P: 2% 69% 14% 16%



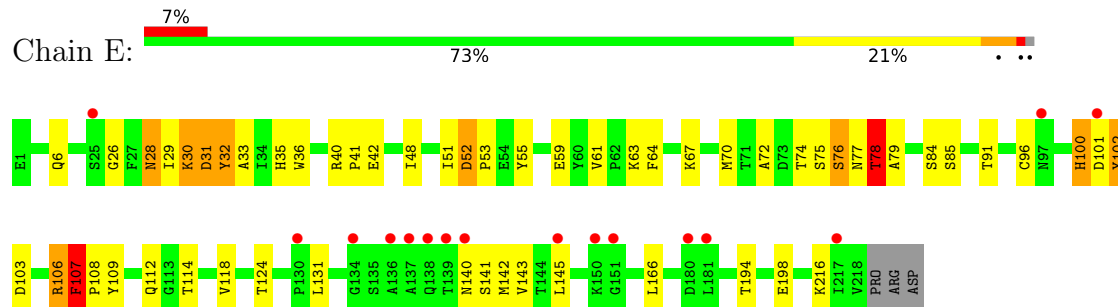
- Molecule 1: Major capsid protein L1



- Molecule 2: Heavy chain of 13H5

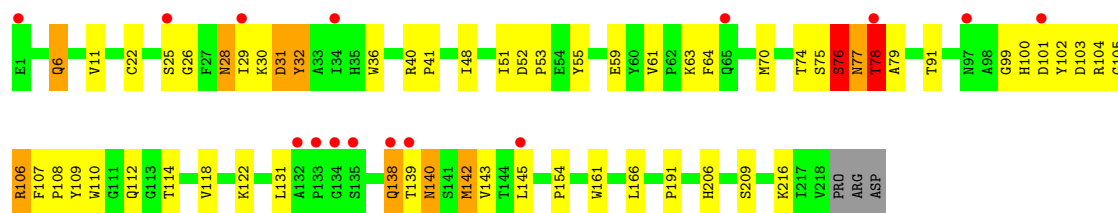


- Molecule 2: Heavy chain of 13H5

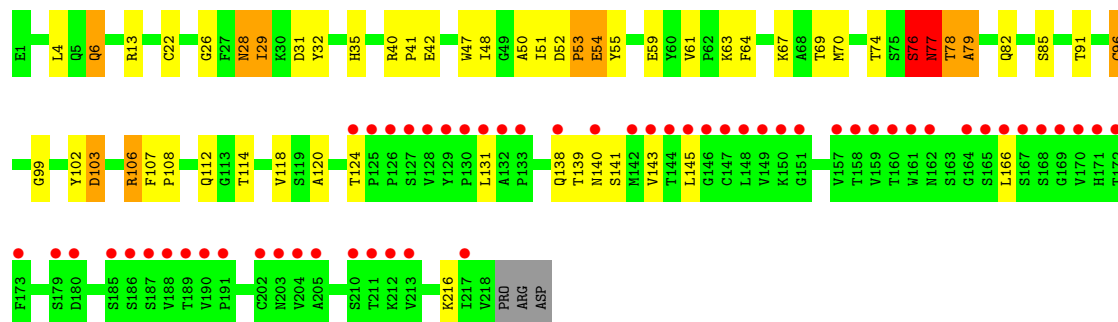
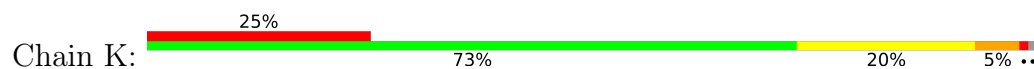


- Molecule 2: Heavy chain of 13H5

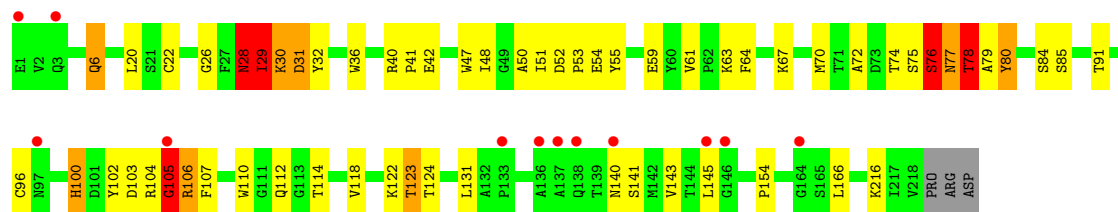




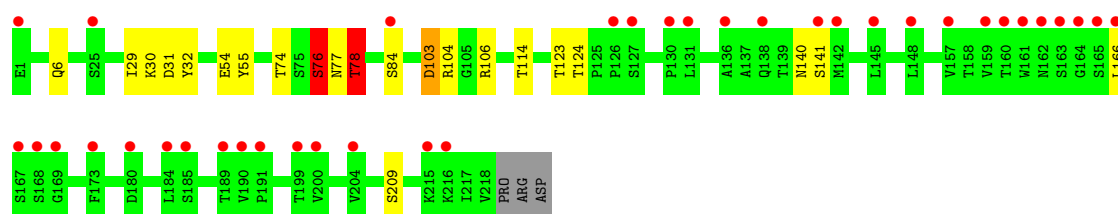
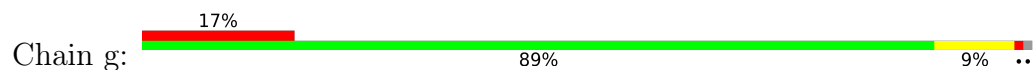
• Molecule 2: Heavy chain of 13H5



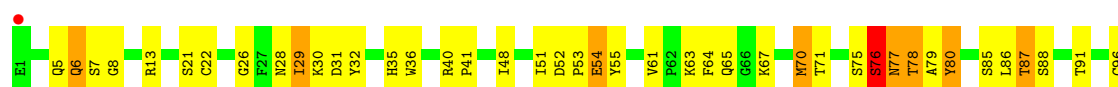
• Molecule 2: Heavy chain of 13H5

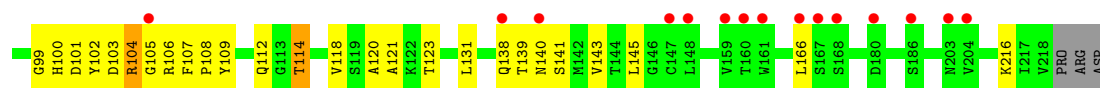


• Molecule 2: Heavy chain of 13H5

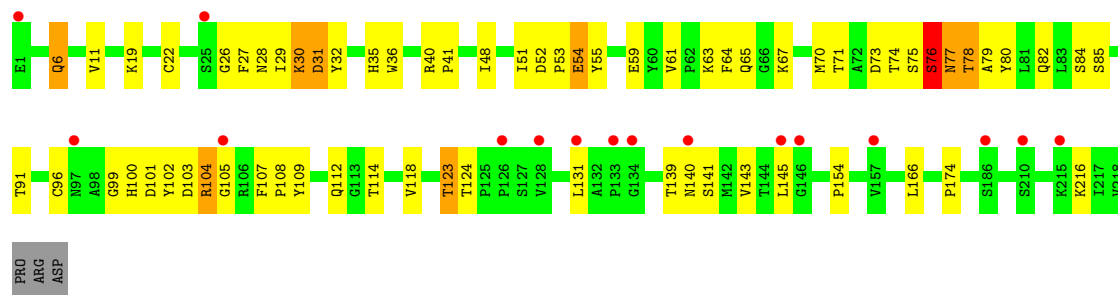


• Molecule 2: Heavy chain of 13H5

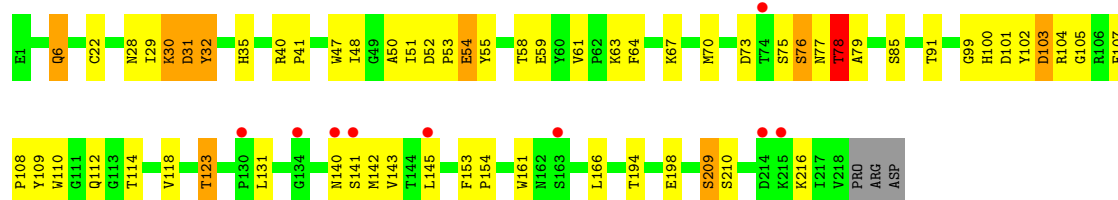




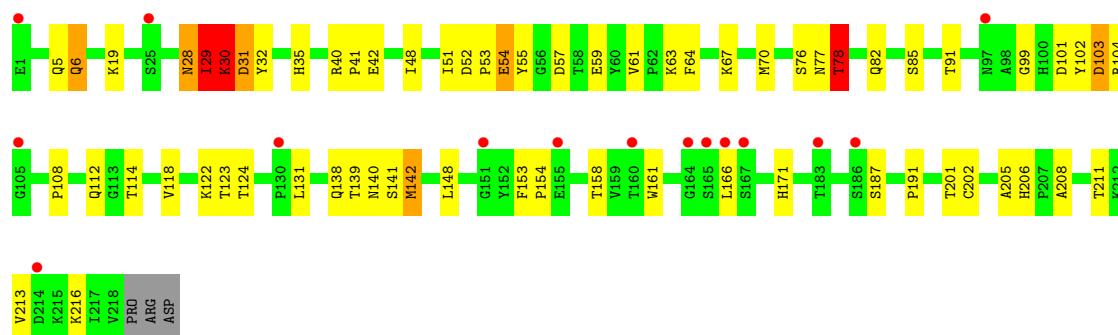
• Molecule 2: Heavy chain of 13H5



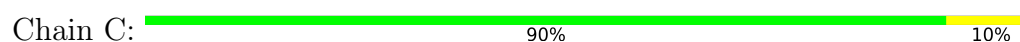
• Molecule 2: Heavy chain of 13H5



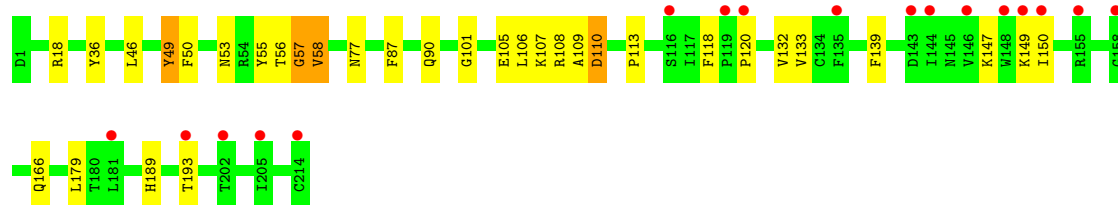
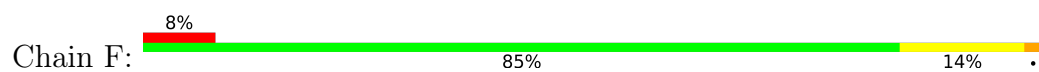
• Molecule 2: Heavy chain of 13H5



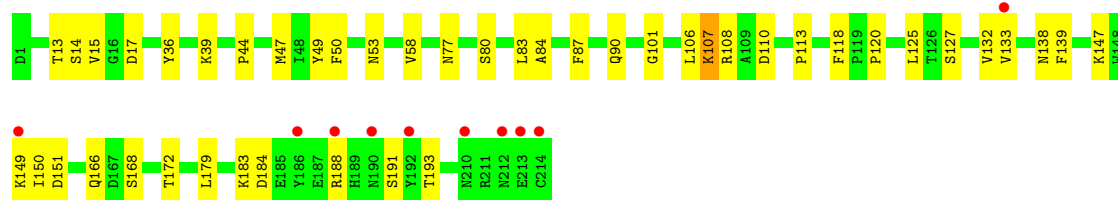
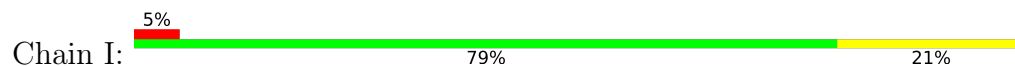
• Molecule 3: Light chain of 13H5



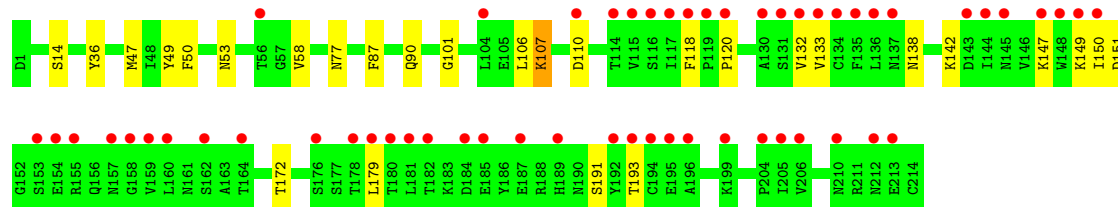
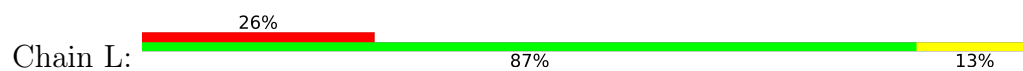
• Molecule 3: Light chain of 13H5



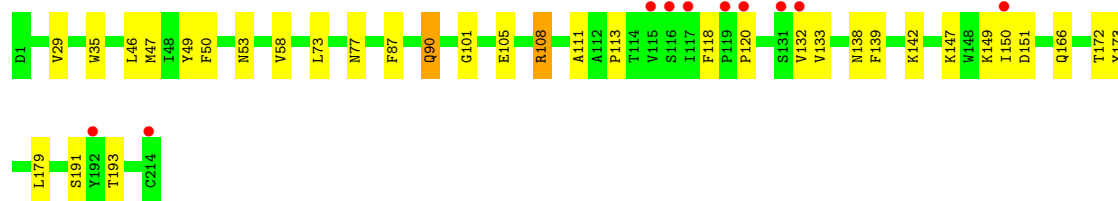
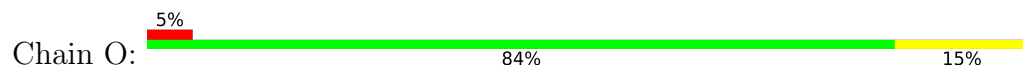
- Molecule 3: Light chain of 13H5



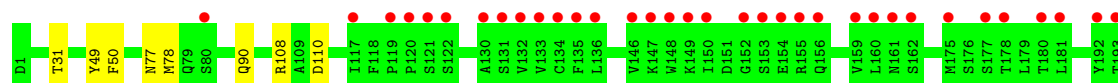
- Molecule 3: Light chain of 13H5

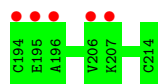


- Molecule 3: Light chain of 13H5

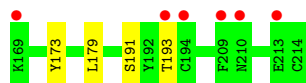
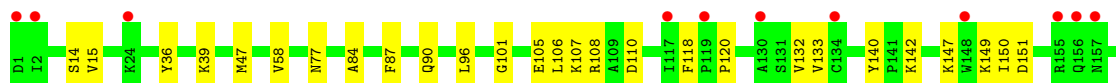
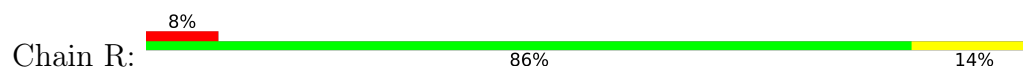


- Molecule 3: Light chain of 13H5

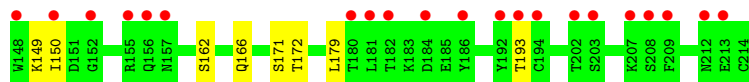
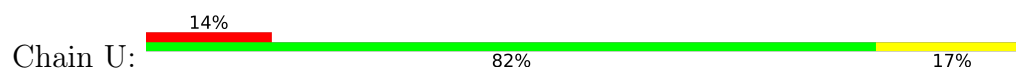




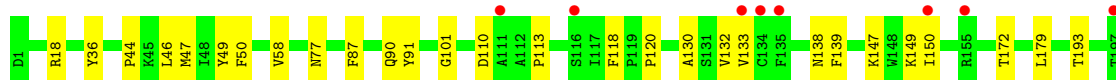
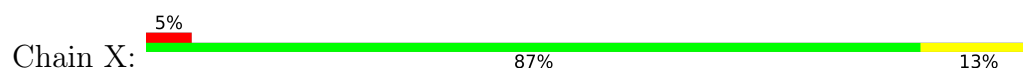
- Molecule 3: Light chain of 13H5



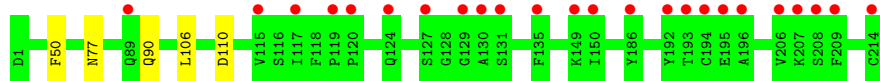
- Molecule 3: Light chain of 13H5



- Molecule 3: Light chain of 13H5



- Molecule 3: Light chain of 13H5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.09Å 208.31Å 205.95Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	49.02 – 3.61 49.71 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.02-3.61) 99.5 (49.71-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.31	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.252 , 0.293 0.251 , 0.291	Depositor DCC
R_{free} test set	6719 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	65550	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/3342	0.46	0/4544
1	D	0.25	0/3342	0.46	0/4544
1	G	0.26	0/3342	0.46	0/4544
1	J	0.26	0/3342	0.46	0/4544
1	M	0.26	0/3342	0.46	0/4544
1	P	0.26	0/3342	0.46	0/4544
1	S	0.26	0/3342	0.47	0/4544
1	V	0.25	0/3342	0.46	0/4544
1	Y	0.25	0/3342	0.46	0/4544
1	b	0.25	0/3342	0.46	0/4544
2	B	0.26	0/1686	0.58	2/2309 (0.1%)
2	E	0.27	0/1686	0.59	3/2309 (0.1%)
2	H	0.27	0/1686	0.56	1/2309 (0.0%)
2	K	0.26	0/1686	0.57	1/2309 (0.0%)
2	N	0.27	0/1686	0.58	3/2309 (0.1%)
2	Q	0.27	0/1686	0.57	1/2309 (0.0%)
2	T	0.27	0/1686	0.56	2/2309 (0.1%)
2	W	0.26	0/1686	0.57	2/2309 (0.1%)
2	Z	0.26	0/1686	0.55	1/2309 (0.0%)
2	g	0.28	0/1686	0.59	2/2309 (0.1%)
3	C	0.26	0/1688	0.47	0/2286
3	F	0.26	0/1688	0.52	2/2286 (0.1%)
3	I	0.25	0/1688	0.46	0/2286
3	L	0.25	0/1688	0.46	0/2286
3	O	0.25	0/1688	0.46	0/2286
3	R	0.26	0/1688	0.47	0/2286
3	U	0.26	0/1688	0.48	0/2286
3	X	0.25	0/1688	0.45	0/2286
3	a	0.26	0/1688	0.46	0/2286
3	j	0.26	0/1688	0.48	0/2286
All	All	0.26	0/67160	0.50	20/91390 (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
2	B	0	3
2	E	0	2
2	H	0	2
2	N	0	2
2	T	0	2
2	W	0	1
2	Z	0	2
2	g	0	2
3	F	0	1
All	All	0	17

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	58	VAL	N-CA-C	-7.51	90.72	111.00
2	K	76	SER	C-N-CA	7.11	139.48	121.70
2	E	107	PHE	C-N-CD	-6.65	105.98	120.60
2	Q	76	SER	C-N-CA	6.05	136.82	121.70
2	T	30	LYS	C-N-CA	5.99	136.67	121.70

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	30	LYS	Peptide
2	B	76	SER	Peptide
2	B	78	THR	Peptide
2	E	76	SER	Peptide
2	E	78	THR	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	A	3258	0	3150	52	0
1	D	3258	0	3150	52	0
1	G	3258	0	3150	53	0
1	J	3258	0	3150	54	0
1	M	3258	0	3150	61	0
1	P	3258	0	3150	52	0
1	S	3258	0	3150	53	1
1	V	3258	0	3150	58	0
1	Y	3258	0	3150	44	0
1	b	3258	0	3150	0	0
2	B	1643	0	1590	53	0
2	E	1643	0	1590	48	0
2	H	1643	0	1590	46	0
2	K	1643	0	1590	43	0
2	N	1643	0	1590	59	0
2	Q	1643	0	1590	48	1
2	T	1643	0	1590	54	0
2	W	1643	0	1590	52	0
2	Z	1643	0	1590	43	0
2	g	1643	0	1590	0	0
3	C	1654	0	1582	14	0
3	F	1654	0	1582	21	1
3	I	1654	0	1582	29	1
3	L	1654	0	1582	17	0
3	O	1654	0	1582	24	0
3	R	1654	0	1582	19	0
3	U	1654	0	1582	26	0
3	X	1654	0	1582	20	0
3	a	1654	0	1582	0	0
3	j	1654	0	1582	0	0
All	All	65550	0	63220	941	2

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 8.

The worst 5 of 941 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:H:30:LYS:HA	2:H:31:ASP:HB2	1.52	0.90
3:U:83:LEU:HD21	3:U:106:LEU:HG	1.53	0.89
2:E:30:LYS:HA	2:E:31:ASP:HB2	1.55	0.86
2:W:30:LYS:HA	2:W:31:ASP:HB2	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:106:LEU:HB2	3:U:166:GLN:HE22	1.37	0.85

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:77:ASP:OD2	3:F:189:HIS:NE2[2_545]	2.05	0.15
3:I:127:SER:OG	2:Q:5:GLN:OE1[1_565]	2.11	0.09

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	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15 55
1	D	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15 55
1	G	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15 55
1	J	412/496 (83%)	383 (93%)	24 (6%)	5 (1%)	13 51
1	M	412/496 (83%)	384 (93%)	24 (6%)	4 (1%)	15 55
1	P	412/496 (83%)	386 (94%)	22 (5%)	4 (1%)	15 55
1	S	412/496 (83%)	382 (93%)	28 (7%)	2 (0%)	29 68
1	V	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15 55
1	Y	412/496 (83%)	381 (92%)	26 (6%)	5 (1%)	13 51
1	b	412/496 (83%)	382 (93%)	27 (7%)	3 (1%)	22 61
2	B	216/221 (98%)	189 (88%)	20 (9%)	7 (3%)	4 31
2	E	216/221 (98%)	187 (87%)	20 (9%)	9 (4%)	3 25
2	H	216/221 (98%)	187 (87%)	22 (10%)	7 (3%)	4 31
2	K	216/221 (98%)	190 (88%)	18 (8%)	8 (4%)	3 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	216/221 (98%)	186 (86%)	21 (10%)	9 (4%)	3	25
2	Q	216/221 (98%)	191 (88%)	21 (10%)	4 (2%)	8	42
2	T	216/221 (98%)	191 (88%)	20 (9%)	5 (2%)	6	38
2	W	216/221 (98%)	186 (86%)	21 (10%)	9 (4%)	3	25
2	Z	216/221 (98%)	186 (86%)	23 (11%)	7 (3%)	4	31
2	g	216/221 (98%)	188 (87%)	18 (8%)	10 (5%)	2	23
3	C	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	F	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	I	212/214 (99%)	202 (95%)	8 (4%)	2 (1%)	17	57
3	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	O	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	R	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	29	68
3	U	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	17	57
3	X	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	a	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	j	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	29	68
All	All	8400/9310 (90%)	7731 (92%)	543 (6%)	126 (2%)	10	47

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	273	THR
1	Y	263	THR
1	Y	273	THR
2	B	31	ASP
2	B	77	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	A	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	D	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	G	363/432 (84%)	360 (99%)	3 (1%)	81	91
1	J	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	M	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	P	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	S	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	V	363/432 (84%)	360 (99%)	3 (1%)	81	91
1	Y	363/432 (84%)	356 (98%)	7 (2%)	57	80
1	b	363/432 (84%)	359 (99%)	4 (1%)	73	88
2	B	184/187 (98%)	171 (93%)	13 (7%)	14	48
2	E	184/187 (98%)	175 (95%)	9 (5%)	25	59
2	H	184/187 (98%)	174 (95%)	10 (5%)	22	57
2	K	184/187 (98%)	174 (95%)	10 (5%)	22	57
2	N	184/187 (98%)	172 (94%)	12 (6%)	17	51
2	Q	184/187 (98%)	171 (93%)	13 (7%)	14	48
2	T	184/187 (98%)	174 (95%)	10 (5%)	22	57
2	W	184/187 (98%)	179 (97%)	5 (3%)	44	73
2	Z	184/187 (98%)	176 (96%)	8 (4%)	29	63
2	g	184/187 (98%)	171 (93%)	13 (7%)	14	48
3	C	189/189 (100%)	187 (99%)	2 (1%)	73	88
3	F	189/189 (100%)	182 (96%)	7 (4%)	34	66
3	I	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	L	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	O	189/189 (100%)	186 (98%)	3 (2%)	62	83
3	R	189/189 (100%)	186 (98%)	3 (2%)	62	83
3	U	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	X	189/189 (100%)	186 (98%)	3 (2%)	62	83
3	a	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	j	189/189 (100%)	182 (96%)	7 (4%)	34	66
All	All	7360/8080 (91%)	7169 (97%)	191 (3%)	46	74

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	123	THR
2	Q	70	MET
3	O	90	GLN
2	g	124	THR
2	Q	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	38	GLN
3	O	77	ASN
3	a	166	GLN
3	U	77	ASN
3	U	166	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](#)

There are no ligands in this entry.

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, 95th 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	A	416/496 (83%)	-0.08	6 (1%) 75 61	27, 62, 124, 168	0
1	D	416/496 (83%)	-0.11	7 (1%) 70 55	37, 70, 124, 189	0
1	G	416/496 (83%)	-0.05	5 (1%) 79 66	41, 70, 132, 183	0
1	J	416/496 (83%)	-0.17	1 (0%) 95 91	31, 64, 122, 185	0
1	M	416/496 (83%)	-0.21	1 (0%) 95 91	28, 59, 118, 184	0
1	P	416/496 (83%)	-0.01	9 (2%) 62 45	34, 64, 123, 186	0
1	S	416/496 (83%)	-0.13	2 (0%) 91 83	31, 60, 119, 174	0
1	V	416/496 (83%)	-0.06	7 (1%) 70 55	30, 64, 118, 183	0
1	Y	416/496 (83%)	-0.11	5 (1%) 79 66	40, 71, 132, 169	0
1	b	416/496 (83%)	-0.08	1 (0%) 95 91	43, 69, 124, 163	0
2	B	218/221 (98%)	0.05	4 (1%) 68 53	34, 63, 123, 163	0
2	E	218/221 (98%)	0.47	16 (7%) 15 9	52, 109, 174, 217	0
2	H	218/221 (98%)	0.46	15 (6%) 16 10	52, 91, 133, 172	0
2	K	218/221 (98%)	1.38	56 (25%) 0 0	40, 108, 220, 258	0
2	N	218/221 (98%)	0.28	12 (5%) 25 15	38, 73, 144, 204	0
2	Q	218/221 (98%)	0.45	16 (7%) 15 9	53, 98, 148, 174	0
2	T	218/221 (98%)	0.52	16 (7%) 15 9	47, 109, 171, 191	0
2	W	218/221 (98%)	0.29	9 (4%) 37 24	35, 70, 161, 191	0
2	Z	218/221 (98%)	0.52	15 (6%) 16 10	49, 99, 157, 210	0
2	g	218/221 (98%)	0.76	37 (16%) 1 1	58, 105, 196, 218	0
3	C	214/214 (100%)	-0.03	0 100 100	27, 59, 102, 125	12 (5%)
3	F	214/214 (100%)	0.48	17 (7%) 12 7	35, 98, 175, 211	12 (5%)
3	I	214/214 (100%)	0.35	10 (4%) 31 19	47, 104, 154, 191	12 (5%)
3	L	214/214 (100%)	1.20	56 (26%) 0 0	44, 118, 223, 275	12 (5%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	O	214/214 (100%)	0.51	10 (4%) 31 19	30, 78, 140, 193	12 (5%)
3	R	214/214 (100%)	0.48	17 (7%) 12 7	51, 97, 150, 195	12 (5%)
3	U	214/214 (100%)	0.75	30 (14%) 2 2	46, 113, 202, 229	12 (5%)
3	X	214/214 (100%)	0.19	10 (4%) 31 19	29, 80, 141, 189	12 (5%)
3	a	214/214 (100%)	0.52	24 (11%) 5 3	35, 77, 142, 194	12 (5%)
3	j	214/214 (100%)	0.78	39 (18%) 1 0	53, 114, 183, 218	12 (5%)
All	All	8480/9310 (91%)	0.22	453 (5%) 26 16	27, 75, 167, 275	120 (1%)

The worst 5 of 453 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	132	ALA	12.1
2	K	147	CYS	9.9
2	K	186	SER	9.3
2	K	158	THR	9.2
2	K	187	SER	9.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.