



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:49 PM UTC

PDB ID : 7PA9 / pdb_00007pa9
Title : JC polyomavirus VP1 in complex with Fab 98D3
Authors : Stroeh, L.J.; Harprecht, C.; Freytag, J.; Stehle, T.
Deposited on : 2021-07-29
Resolution : 2.75 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

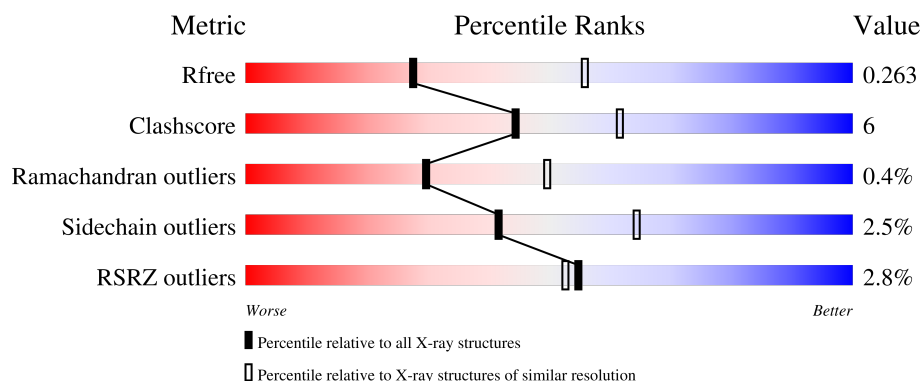
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



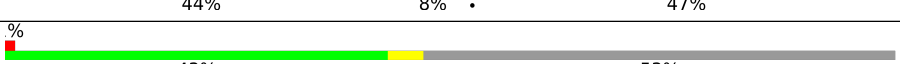
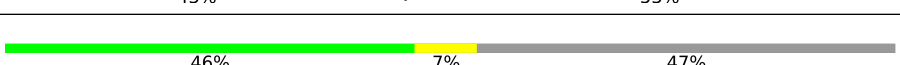
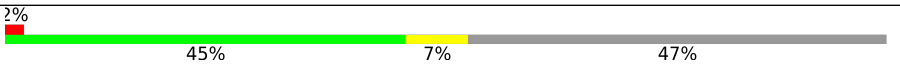
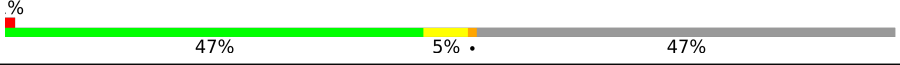
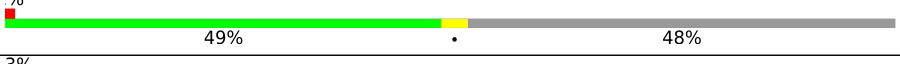
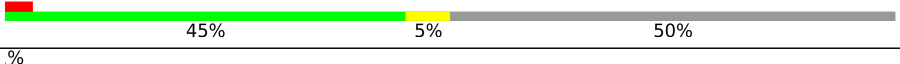
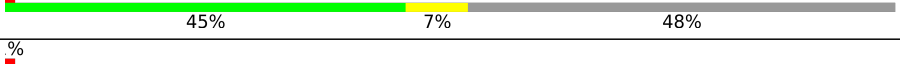
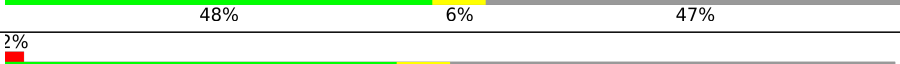
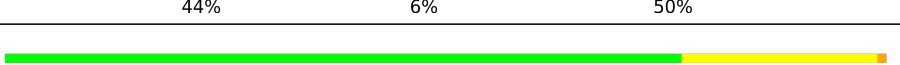
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	AAA	272	2% 81% 13% • 5%
1	BBB	272	% 78% 16% • 5%
1	CCC	272	82% 12% • 5%
1	DDD	272	2% 81% 14% 5%
1	EEE	272	% 81% 13% • 5%

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Mol	Chain	Length	Quality of chain
1	FFF	272	
1	GGG	272	
1	HHH	272	
1	III	272	
1	JJJ	272	
2	KKK	404	
2	MMM	404	
2	OOO	404	
2	QQQ	404	
2	TTT	404	
2	VVV	404	
2	XXX	404	
2	YYY	404	
2	bbb	404	
2	ccc	404	
3	LLL	212	
3	NNN	212	
3	PPP	212	
3	RRR	212	
3	SSS	212	
3	UUU	212	
3	WWW	212	
3	ZZZ	212	
3	aaa	212	
3	ddd	212	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51021 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	259	Total	C	N	O	S	0	0	0
			2014	1270	347	386	11			
1	BBB	258	Total	C	N	O	S	0	0	0
			2010	1269	344	386	11			
1	CCC	258	Total	C	N	O	S	0	0	0
			2009	1267	346	385	11			
1	DDD	259	Total	C	N	O	S	0	0	0
			2020	1274	347	388	11			
1	EEE	259	Total	C	N	O	S	0	0	0
			2023	1275	348	389	11			
1	FFF	259	Total	C	N	O	S	0	0	0
			2016	1272	347	386	11			
1	GGG	258	Total	C	N	O	S	0	0	0
			2015	1271	346	387	11			
1	HHH	258	Total	C	N	O	S	0	0	0
			2007	1264	345	387	11			
1	III	259	Total	C	N	O	S	0	0	0
			2016	1271	346	388	11			
1	JJJ	259	Total	C	N	O	S	0	0	0
			2018	1272	347	388	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	GLY	-	expression tag	UNP P03089
AAA	19	SER	-	expression tag	UNP P03089
AAA	20	HIS	-	expression tag	UNP P03089
AAA	21	MET	-	expression tag	UNP P03089
BBB	18	GLY	-	expression tag	UNP P03089
BBB	19	SER	-	expression tag	UNP P03089
BBB	20	HIS	-	expression tag	UNP P03089
BBB	21	MET	-	expression tag	UNP P03089
CCC	18	GLY	-	expression tag	UNP P03089

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	19	SER	-	expression tag	UNP P03089
CCC	20	HIS	-	expression tag	UNP P03089
CCC	21	MET	-	expression tag	UNP P03089
DDD	18	GLY	-	expression tag	UNP P03089
DDD	19	SER	-	expression tag	UNP P03089
DDD	20	HIS	-	expression tag	UNP P03089
DDD	21	MET	-	expression tag	UNP P03089
EEE	18	GLY	-	expression tag	UNP P03089
EEE	19	SER	-	expression tag	UNP P03089
EEE	20	HIS	-	expression tag	UNP P03089
EEE	21	MET	-	expression tag	UNP P03089
FFF	18	GLY	-	expression tag	UNP P03089
FFF	19	SER	-	expression tag	UNP P03089
FFF	20	HIS	-	expression tag	UNP P03089
FFF	21	MET	-	expression tag	UNP P03089
GGG	18	GLY	-	expression tag	UNP P03089
GGG	19	SER	-	expression tag	UNP P03089
GGG	20	HIS	-	expression tag	UNP P03089
GGG	21	MET	-	expression tag	UNP P03089
HHH	18	GLY	-	expression tag	UNP P03089
HHH	19	SER	-	expression tag	UNP P03089
HHH	20	HIS	-	expression tag	UNP P03089
HHH	21	MET	-	expression tag	UNP P03089
III	18	GLY	-	expression tag	UNP P03089
III	19	SER	-	expression tag	UNP P03089
III	20	HIS	-	expression tag	UNP P03089
III	21	MET	-	expression tag	UNP P03089
JJJ	18	GLY	-	expression tag	UNP P03089
JJJ	19	SER	-	expression tag	UNP P03089
JJJ	20	HIS	-	expression tag	UNP P03089
JJJ	21	MET	-	expression tag	UNP P03089

- Molecule 2 is a protein called Fab 98D3 VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	KKK	214	Total	C	N	O	S	0	0	0
			1599	1013	268	313	5			
2	MMM	191	Total	C	N	O	S	0	0	0
			1401	886	236	274	5			
2	OOO	215	Total	C	N	O	S	0	0	0
			1593	1011	267	310	5			
2	QQQ	213	Total	C	N	O	S	0	0	0
			1561	987	259	310	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	TTT	214	Total	C	N	O	S	0	0	0
			1575	996	264	310	5			
2	VVV	212	Total	C	N	O	S	0	0	0
			1579	1004	264	306	5			
2	XXX	203	Total	C	N	O	S	0	0	0
			1500	955	249	291	5			
2	YYY	212	Total	C	N	O	S	0	0	0
			1584	1004	267	308	5			
2	bbb	215	Total	C	N	O	S	0	0	0
			1588	1008	264	311	5			
2	ccc	202	Total	C	N	O	S	0	0	0
			1503	958	250	290	5			

- Molecule 3 is a protein called Fab 98D3 VL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	LLL	211	Total	C	N	O	S	0	0	0
			1592	993	266	328	5			
3	NNN	157	Total	C	N	O	S	0	0	0
			1160	728	183	245	4			
3	PPP	211	Total	C	N	O	S	0	0	0
			1570	977	263	325	5			
3	RRR	202	Total	C	N	O	S	0	0	0
			1515	947	249	314	5			
3	SSS	199	Total	C	N	O	S	0	0	0
			1493	930	248	310	5			
3	UUU	175	Total	C	N	O	S	0	0	0
			1328	831	221	272	4			
3	WWW	212	Total	C	N	O	S	0	0	0
			1605	1000	270	330	5			
3	ZZZ	211	Total	C	N	O	S	0	0	0
			1614	1010	270	329	5			
3	aaa	211	Total	C	N	O	S	0	0	0
			1595	994	267	329	5			
3	ddd	206	Total	C	N	O	S	0	0	0
			1572	983	263	321	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	31	Total 31	O 31	0	0
4	CCC	27	Total 27	O 27	0	0
4	DDD	23	Total 23	O 23	0	0
4	EEE	29	Total 29	O 29	0	0
4	FFF	22	Total 22	O 22	0	0
4	GGG	35	Total 35	O 35	0	0
4	HHH	34	Total 34	O 34	0	0
4	III	31	Total 31	O 31	0	0
4	JJJ	31	Total 31	O 31	0	0
4	KKK	9	Total 9	O 9	0	0
4	LLL	9	Total 9	O 9	0	0
4	MMM	4	Total 4	O 4	0	0
4	NNN	2	Total 2	O 2	0	0
4	OOO	3	Total 3	O 3	0	0
4	PPP	3	Total 3	O 3	0	0
4	QQQ	6	Total 6	O 6	0	0
4	RRR	4	Total 4	O 4	0	0
4	SSS	3	Total 3	O 3	0	0
4	TTT	2	Total 2	O 2	0	0
4	UUU	2	Total 2	O 2	0	0
4	VVV	3	Total 3	O 3	0	0

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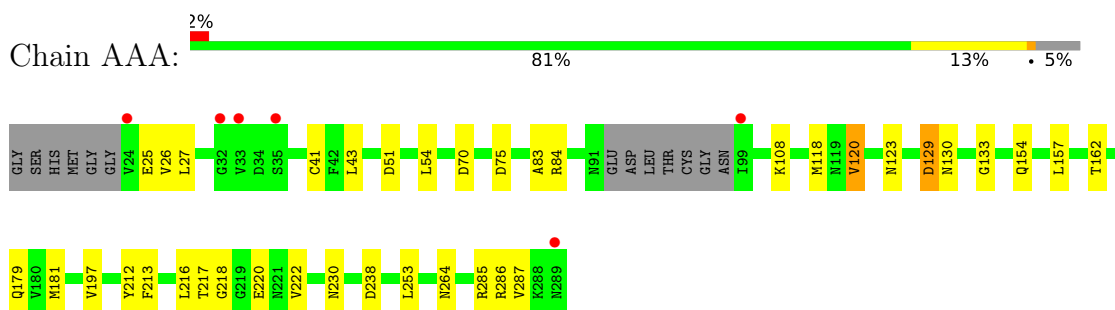
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	WWW	1	Total	O	0	0
			1	1		
4	XXX	1	Total	O	0	0
			1	1		
4	YYY	1	Total	O	0	0
			1	1		
4	ZZZ	1	Total	O	0	0
			1	1		
4	bbb	1	Total	O	0	0
			1	1		
4	ccc	4	Total	O	0	0
			4	4		
4	ddd	2	Total	O	0	0
			2	2		

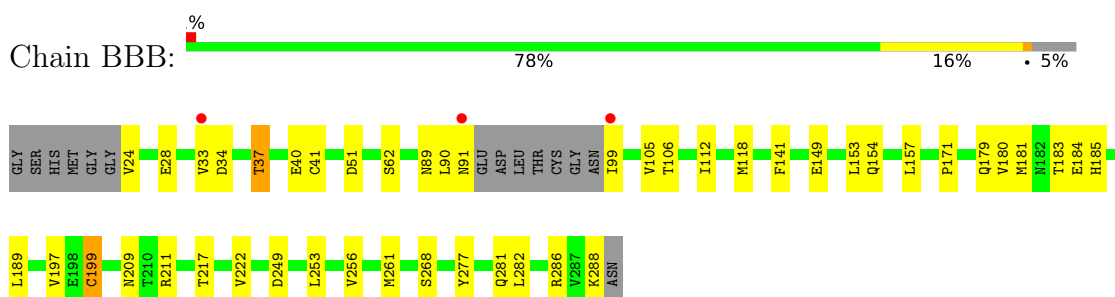
3 Residue-property plots [i](#)

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.

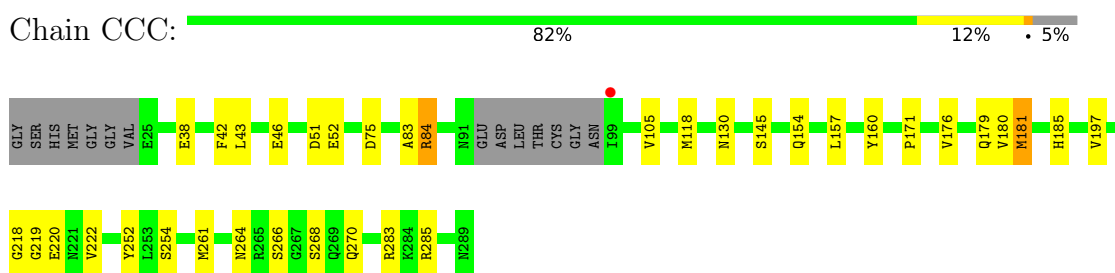
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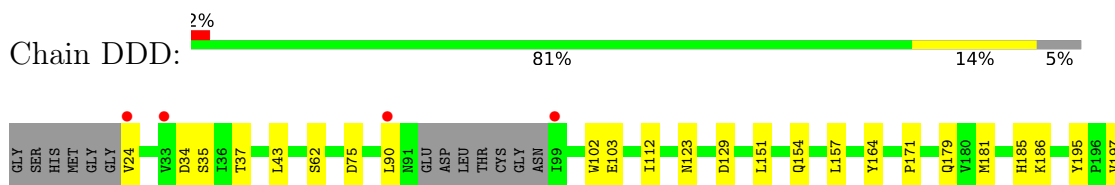
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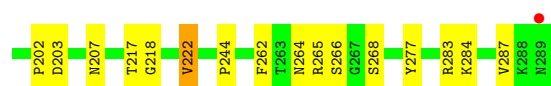


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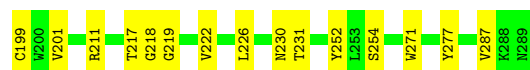
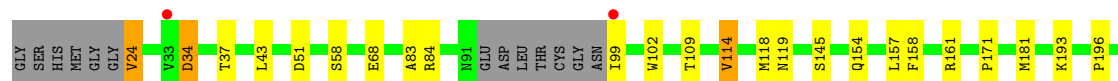
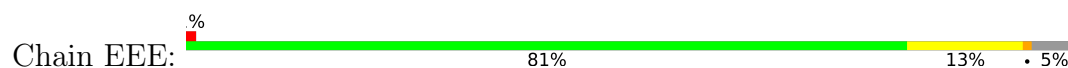


- Molecule 1: Major capsid protein VP1

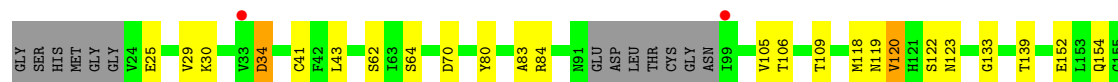
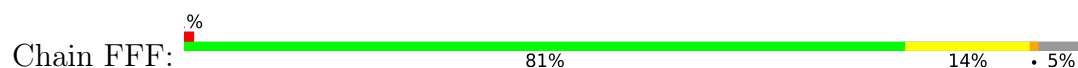




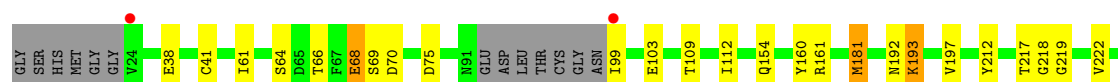
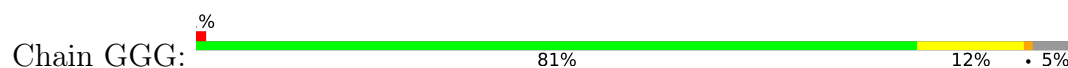
- Molecule 1: Major capsid protein VP1



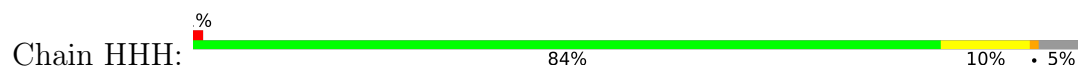
- Molecule 1: Major capsid protein VP1



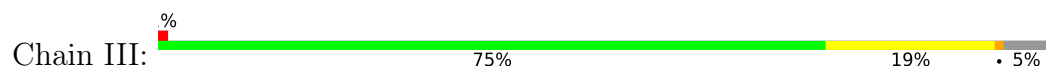
- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



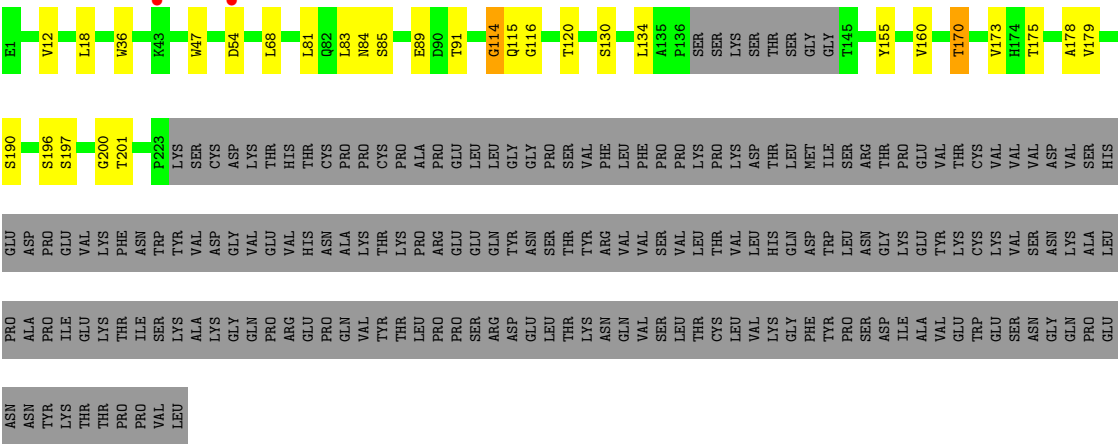
- Molecule 1: Major capsid protein VP1



GLY
GLN
PRO
GLU
ASN
TYR
THR
PRO
PRO
VAL
LEU

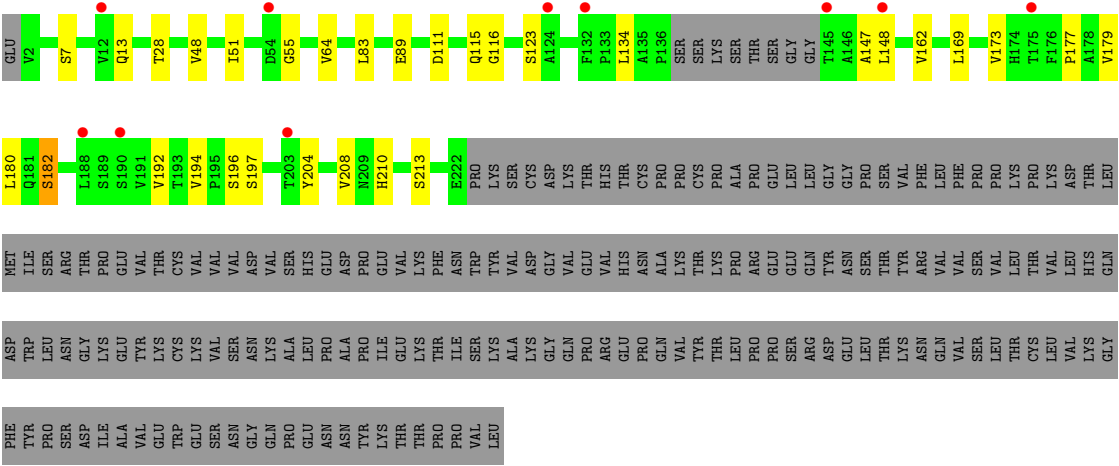
● Molecule 2: Fab 98D3 VH

Chain OOO: 46% 7% 47%



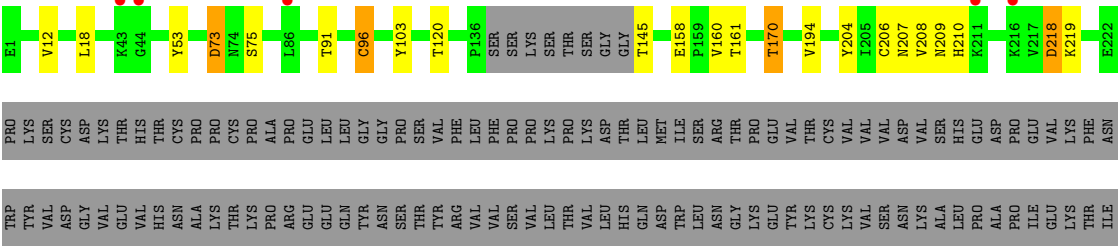
● Molecule 2: Fab 98D3 VH

Chain QQQ: 2% 45% 7% 47%



● Molecule 2: Fab 98D3 VH

Chain TTT: 47% 5% 47%



- Molecule 2: Fab 98D3 VH

[illegible]

- Molecule 2: Fab 98D3 VH

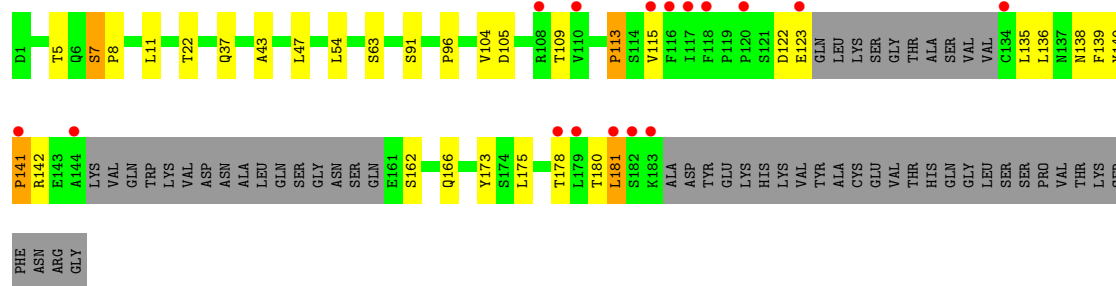
Chain XXX:

3% 45% 5% 50%

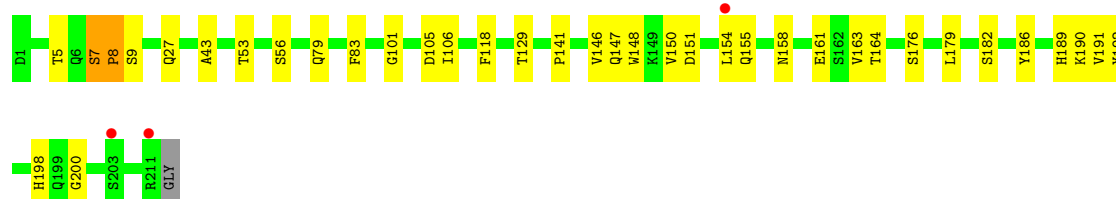
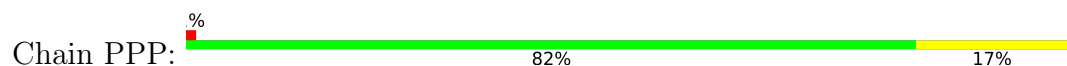
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- Molecule 2: Fab 98D3 VH

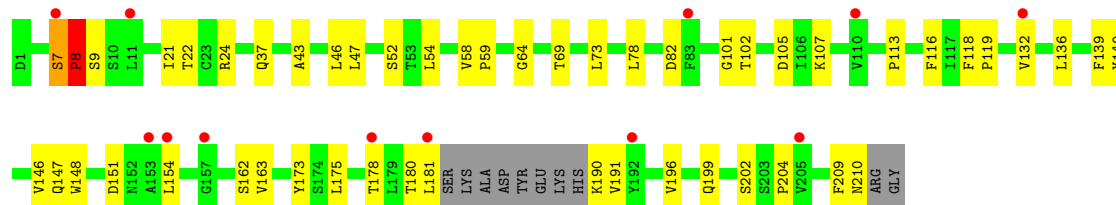
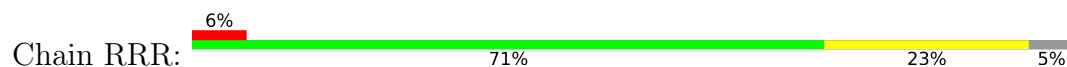
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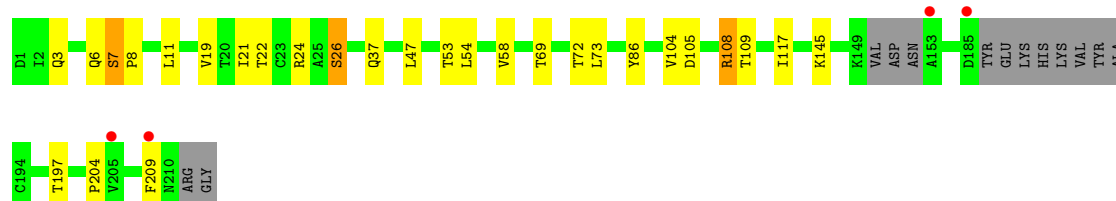
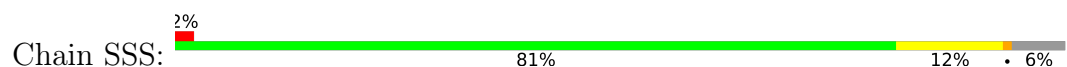
• Molecule 3: Fab 98D3 VL



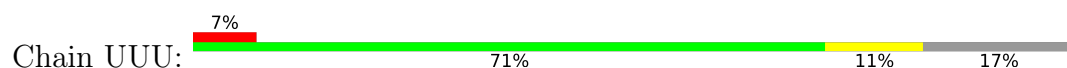
• Molecule 3: Fab 98D3 VL

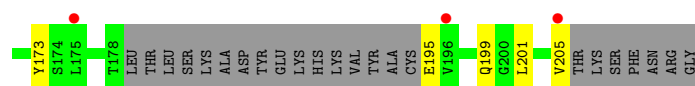


• Molecule 3: Fab 98D3 VL

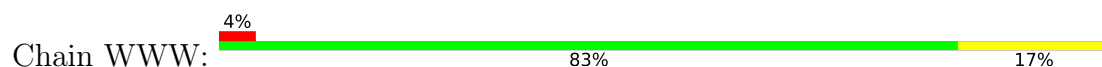


• Molecule 3: Fab 98D3 VL

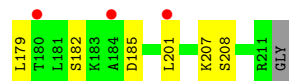
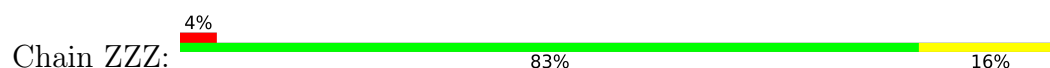




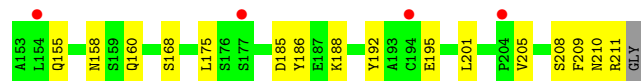
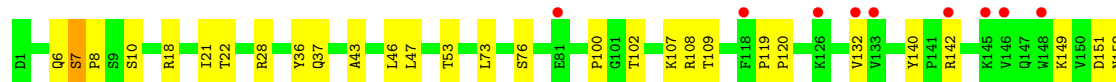
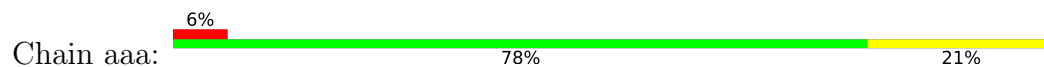
• Molecule 3: Fab 98D3 VL



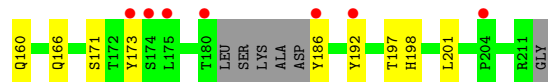
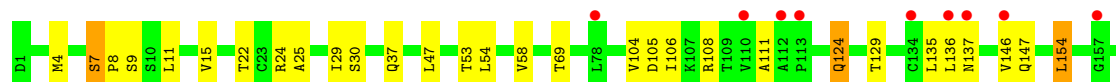
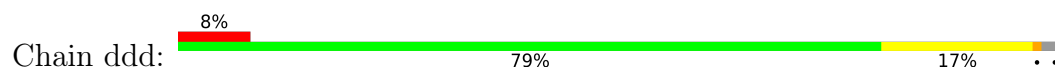
• Molecule 3: Fab 98D3 VL



• Molecule 3: Fab 98D3 VL



• Molecule 3: Fab 98D3 VL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.97Å 202.31Å 251.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.75 49.15 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.75) 100.0 (49.15-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.207 , 0.263 0.210 , 0.263	Depositor DCC
R_{free} test set	11285 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	51021	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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	AAA	1.01	0/2059	1.37	4/2797 (0.1%)
1	BBB	1.00	0/2055	1.37	2/2792 (0.1%)
1	CCC	0.99	0/2054	1.36	4/2790 (0.1%)
1	DDD	0.98	0/2065	1.37	8/2805 (0.3%)
1	EEE	1.00	0/2068	1.33	3/2809 (0.1%)
1	FFF	0.99	0/2061	1.36	4/2800 (0.1%)
1	GGG	0.97	0/2060	1.36	5/2798 (0.2%)
1	HHH	0.98	0/2052	1.36	3/2788 (0.1%)
1	III	0.99	0/2061	1.35	2/2801 (0.1%)
1	JJJ	1.01	0/2063	1.38	8/2802 (0.3%)
2	KKK	1.02	0/1636	1.38	4/2227 (0.2%)
2	MMM	1.07	0/1434	1.37	1/1956 (0.1%)
2	OOO	1.03	0/1632	1.34	6/2227 (0.3%)
2	QQQ	1.04	0/1599	1.33	5/2190 (0.2%)
2	TTT	1.06	0/1612	1.43	5/2200 (0.2%)
2	VVV	1.03	0/1618	1.35	0/2207
2	XXX	1.04	0/1536	1.36	2/2096 (0.1%)
2	YYY	1.03	0/1622	1.37	3/2211 (0.1%)
2	bbb	1.03	0/1627	1.36	4/2222 (0.2%)
2	ccc	1.06	0/1539	1.41	5/2097 (0.2%)
3	LLL	1.03	0/1628	1.38	6/2221 (0.3%)
3	NNN	1.09	0/1186	1.44	2/1622 (0.1%)
3	PPP	1.06	1/1606 (0.1%)	1.38	3/2197 (0.1%)
3	RRR	1.08	1/1548 (0.1%)	1.40	7/2113 (0.3%)
3	SSS	1.07	0/1524	1.38	3/2076 (0.1%)
3	UUU	1.03	0/1353	1.36	3/1837 (0.2%)
3	WWW	1.07	0/1641	1.40	2/2234 (0.1%)
3	ZZZ	1.05	0/1650	1.34	0/2243
3	aaa	1.05	0/1629	1.40	2/2216 (0.1%)
3	ddd	1.10	0/1607	1.43	3/2185 (0.1%)
All	All	1.03	2/51825 (0.0%)	1.37	109/70559 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	RRR	8	PRO	C-O	-5.52	1.16	1.24
3	PPP	79	GLN	N-CA	5.46	1.49	1.46

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	RRR	8	PRO	CA-N-CD	-7.73	101.18	112.00
1	HHH	32	GLY	CA-C-O	-7.48	117.07	122.23
1	CCC	219	GLY	CA-C-O	-7.25	117.51	122.22
3	LLL	53	THR	CA-CB-OG1	-7.21	98.78	109.60
2	ccc	53	TYR	CA-C-N	6.93	131.22	120.82

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2014	0	1965	42	0
1	BBB	2010	0	1963	32	0
1	CCC	2009	0	1963	22	0
1	DDD	2020	0	1976	23	0
1	EEE	2023	0	1980	30	0
1	FFF	2016	0	1972	31	0
1	GGG	2015	0	1974	26	0
1	HHH	2007	0	1949	19	0
1	III	2016	0	1965	36	0
1	JJJ	2018	0	1969	27	0
2	KKK	1599	0	1542	19	0
2	MMM	1401	0	1295	11	0
2	OOO	1593	0	1529	12	0
2	QQQ	1561	0	1458	16	0
2	TTT	1575	0	1501	9	0
2	VVV	1579	0	1521	6	0
2	XXX	1500	0	1418	13	0
2	YYY	1584	0	1528	21	0
2	bbb	1588	0	1515	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	ccc	1503	0	1438	14	0
3	LLL	1592	0	1506	34	0
3	NNN	1160	0	1073	26	0
3	PPP	1570	0	1453	21	0
3	RRR	1515	0	1436	31	0
3	SSS	1493	0	1418	22	0
3	UUU	1328	0	1288	16	0
3	WWW	1605	0	1526	24	0
3	ZZZ	1614	0	1567	16	0
3	aaa	1595	0	1530	28	0
3	ddd	1572	0	1510	29	0
4	AAA	22	0	0	0	0
4	BBB	31	0	0	0	0
4	CCC	27	0	0	0	0
4	DDD	23	0	0	0	0
4	EEE	29	0	0	1	0
4	FFF	22	0	0	0	0
4	GGG	35	0	0	1	0
4	HHH	34	0	0	0	0
4	III	31	0	0	0	0
4	JJJ	31	0	0	0	0
4	KKK	9	0	0	0	0
4	LLL	9	0	0	1	0
4	MMM	4	0	0	0	0
4	NNN	2	0	0	0	0
4	OOO	3	0	0	0	0
4	PPP	3	0	0	0	0
4	QQQ	6	0	0	0	0
4	RRR	4	0	0	0	0
4	SSS	3	0	0	0	0
4	TTT	2	0	0	0	0
4	UUU	2	0	0	0	0
4	VVV	3	0	0	0	0
4	WWW	1	0	0	0	0
4	XXX	1	0	0	0	0
4	YYY	1	0	0	0	0
4	ZZZ	1	0	0	0	0
4	bbb	1	0	0	0	0
4	ccc	4	0	0	0	0
4	ddd	2	0	0	0	0
All	All	51021	0	48728	594	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 594 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)
1:AAA:26:VAL:CG1	1:AAA:285:ARG:HH11	1.29	1.45
1:AAA:26:VAL:CG1	1:AAA:285:ARG:NH1	1.92	1.28
3:PPP:147:GLN:NE2	3:PPP:154:LEU:HD23	1.60	1.17
1:AAA:26:VAL:HG12	1:AAA:285:ARG:HH11	0.94	1.08
1:AAA:26:VAL:HG11	1:AAA:285:ARG:NH1	1.75	1.01

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	AAA	255/272 (94%)	240 (94%)	15 (6%)	0	100	100
1	BBB	254/272 (93%)	242 (95%)	12 (5%)	0	100	100
1	CCC	254/272 (93%)	238 (94%)	14 (6%)	2 (1%)	16	30
1	DDD	255/272 (94%)	245 (96%)	10 (4%)	0	100	100
1	EEE	255/272 (94%)	242 (95%)	13 (5%)	0	100	100
1	FFF	255/272 (94%)	244 (96%)	11 (4%)	0	100	100
1	GGG	254/272 (93%)	243 (96%)	10 (4%)	1 (0%)	30	50
1	HHH	254/272 (93%)	242 (95%)	12 (5%)	0	100	100
1	III	255/272 (94%)	241 (94%)	14 (6%)	0	100	100
1	JJJ	255/272 (94%)	244 (96%)	11 (4%)	0	100	100
2	KKK	208/404 (52%)	195 (94%)	11 (5%)	2 (1%)	12	24
2	MMM	185/404 (46%)	176 (95%)	9 (5%)	0	100	100
2	OOO	211/404 (52%)	202 (96%)	8 (4%)	1 (0%)	24	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QQQ	209/404 (52%)	200 (96%)	8 (4%)	1 (0%)	24	43
2	TTT	210/404 (52%)	201 (96%)	9 (4%)	0	100	100
2	VVV	208/404 (52%)	197 (95%)	9 (4%)	2 (1%)	12	24
2	XXX	197/404 (49%)	190 (96%)	7 (4%)	0	100	100
2	YYY	208/404 (52%)	200 (96%)	8 (4%)	0	100	100
2	bbb	211/404 (52%)	201 (95%)	9 (4%)	1 (0%)	24	43
2	ccc	196/404 (48%)	185 (94%)	11 (6%)	0	100	100
3	LLL	209/212 (99%)	195 (93%)	13 (6%)	1 (0%)	24	43
3	NNN	151/212 (71%)	134 (89%)	13 (9%)	4 (3%)	4	7
3	PPP	209/212 (99%)	192 (92%)	14 (7%)	3 (1%)	9	17
3	RRR	198/212 (93%)	186 (94%)	11 (6%)	1 (0%)	24	43
3	SSS	193/212 (91%)	177 (92%)	14 (7%)	2 (1%)	12	24
3	UUU	163/212 (77%)	148 (91%)	15 (9%)	0	100	100
3	WWW	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	24	43
3	ZZZ	209/212 (99%)	196 (94%)	13 (6%)	0	100	100
3	aaa	209/212 (99%)	196 (94%)	12 (6%)	1 (0%)	24	43
3	ddd	202/212 (95%)	191 (95%)	9 (4%)	2 (1%)	12	24
All	All	6542/8880 (74%)	6183 (94%)	334 (5%)	25 (0%)	30	50

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	LLL	7	SER
3	NNN	7	SER
3	RRR	8	PRO
3	SSS	7	SER
3	WWW	7	SER

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	AAA	225/237 (95%)	221 (98%)	4 (2%)	51	71
1	BBB	225/237 (95%)	219 (97%)	6 (3%)	39	62
1	CCC	225/237 (95%)	221 (98%)	4 (2%)	51	71
1	DDD	227/237 (96%)	225 (99%)	2 (1%)	70	82
1	EEE	228/237 (96%)	224 (98%)	4 (2%)	51	71
1	FFF	226/237 (95%)	220 (97%)	6 (3%)	39	62
1	GGG	227/237 (96%)	225 (99%)	2 (1%)	70	82
1	HHH	224/237 (94%)	216 (96%)	8 (4%)	31	55
1	III	226/237 (95%)	222 (98%)	4 (2%)	51	71
1	JJJ	226/237 (95%)	222 (98%)	4 (2%)	51	71
2	KKK	176/353 (50%)	172 (98%)	4 (2%)	44	66
2	MMM	147/353 (42%)	144 (98%)	3 (2%)	48	69
2	OOO	173/353 (49%)	165 (95%)	8 (5%)	24	45
2	QQQ	168/353 (48%)	160 (95%)	8 (5%)	23	44
2	TTT	170/353 (48%)	163 (96%)	7 (4%)	27	49
2	VVV	173/353 (49%)	171 (99%)	2 (1%)	63	78
2	XXX	160/353 (45%)	158 (99%)	2 (1%)	61	76
2	YYY	174/353 (49%)	170 (98%)	4 (2%)	44	66
2	bbb	172/353 (49%)	166 (96%)	6 (4%)	32	56
2	ccc	162/353 (46%)	159 (98%)	3 (2%)	50	70
3	LLL	180/187 (96%)	175 (97%)	5 (3%)	38	61
3	NNN	131/187 (70%)	126 (96%)	5 (4%)	29	52
3	PPP	174/187 (93%)	169 (97%)	5 (3%)	37	61
3	RRR	173/187 (92%)	165 (95%)	8 (5%)	24	45
3	SSS	171/187 (91%)	169 (99%)	2 (1%)	63	78
3	UUU	155/187 (83%)	152 (98%)	3 (2%)	50	70
3	WWW	182/187 (97%)	177 (97%)	5 (3%)	39	62
3	ZZZ	186/187 (100%)	178 (96%)	8 (4%)	26	47
3	aaa	182/187 (97%)	177 (97%)	5 (3%)	39	62
3	ddd	180/187 (96%)	175 (97%)	5 (3%)	38	61
All	All	5648/7770 (73%)	5506 (98%)	142 (2%)	42	64

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	ZZZ	20	THR
3	ZZZ	156	SER
2	bbb	197	SER
3	LLL	9	SER
2	KKK	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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	AAA	259/272 (95%)	-0.28	6 (2%) 61 59	26, 37, 57, 83	0
1	BBB	258/272 (94%)	-0.36	3 (1%) 76 76	24, 36, 55, 92	0
1	CCC	258/272 (94%)	-0.41	1 (0%) 88 89	23, 32, 53, 72	0
1	DDD	259/272 (95%)	-0.45	5 (1%) 66 64	23, 31, 50, 73	0
1	EEE	259/272 (95%)	-0.41	2 (0%) 82 82	24, 34, 54, 81	0
1	FFF	259/272 (95%)	-0.39	3 (1%) 76 76	23, 34, 53, 88	0
1	GGG	258/272 (94%)	-0.46	3 (1%) 76 76	23, 31, 51, 81	0
1	HHH	258/272 (94%)	-0.41	4 (1%) 70 69	22, 33, 53, 80	0
1	III	259/272 (95%)	-0.37	3 (1%) 76 76	25, 35, 55, 84	0
1	JJJ	259/272 (95%)	-0.40	1 (0%) 88 89	23, 35, 56, 82	0
2	KKK	214/404 (52%)	0.02	5 (2%) 61 59	23, 48, 79, 96	0
2	MMM	191/404 (47%)	0.25	5 (2%) 57 55	34, 57, 82, 91	0
2	OOO	215/404 (53%)	0.15	2 (0%) 81 81	25, 54, 77, 90	0
2	QQQ	213/404 (52%)	0.44	10 (4%) 36 36	30, 64, 95, 103	0
2	TTT	214/404 (52%)	0.38	5 (2%) 61 59	34, 61, 82, 99	0
2	VVV	212/404 (52%)	0.03	3 (1%) 73 73	32, 52, 83, 101	0
2	XXX	203/404 (50%)	0.18	12 (5%) 28 28	23, 50, 107, 129	0
2	YYY	212/404 (52%)	0.14	3 (1%) 73 73	25, 54, 81, 96	0
2	bbb	215/404 (53%)	0.03	5 (2%) 61 59	27, 51, 74, 84	0
2	ccc	202/404 (50%)	0.24	9 (4%) 38 37	26, 58, 83, 96	0
3	LLL	211/212 (99%)	0.19	1 (0%) 87 87	27, 59, 85, 112	0
3	NNN	157/212 (74%)	0.59	16 (10%) 12 11	33, 64, 100, 119	0
3	PPP	211/212 (99%)	0.33	3 (1%) 73 73	29, 57, 98, 108	0
3	RRR	202/212 (95%)	0.70	12 (5%) 28 28	29, 75, 100, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	SSS	199/212 (93%)	0.35	4 (2%) 65 63	31, 60, 94, 108	0
3	UUU	175/212 (82%)	0.36	15 (8%) 16 16	28, 53, 105, 128	0
3	WWW	212/212 (100%)	0.36	8 (3%) 44 41	32, 60, 92, 107	0
3	ZZZ	211/212 (99%)	0.36	8 (3%) 44 41	29, 58, 96, 113	0
3	aaa	211/212 (99%)	0.50	13 (6%) 26 26	28, 64, 100, 113	0
3	ddd	206/212 (97%)	0.61	16 (7%) 19 19	26, 67, 98, 119	0
All	All	6672/8880 (75%)	0.03	186 (2%) 55 53	22, 46, 89, 129	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	KKK	140	SER	5.6
3	NNN	183	LYS	4.8
3	NNN	179	LEU	4.2
2	TTT	211	LYS	4.1
3	ddd	134	CYS	3.9

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.