



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:04 AM UTC

PDB ID : 7PAA / pdb_00007paa
Title : JC polyomavirus VP1 in complex with scFv 29B1
Authors : Harprecht, C.; Stroeh, L.J.; Freytag, J.; Stehle, T.
Deposited on : 2021-07-29
Resolution : 3.10 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

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:

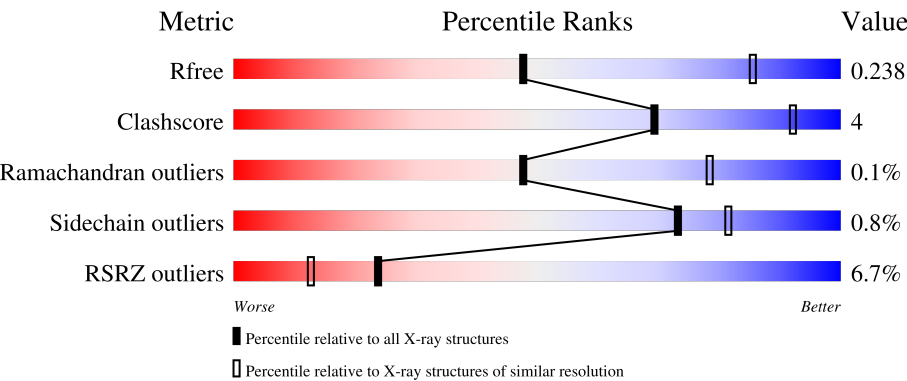
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	KKK	252	8% 81%10%8%
1	WWW	252	4% 84%9%6%
1	XXX	252	45% 84%7%9%
1	YYY	252	7% 83%10%7%
1	ZZZ	252	6% 81%10%8%

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Mol	Chain	Length	Quality of chain
1	aaa	252	
1	bbb	252	
1	ccc	252	
1	ddd	252	
1	eee	252	
2	AAA	272	
2	BBB	272	
2	CCC	272	
2	DDD	272	
2	EEE	272	
2	FFF	272	
2	GGG	272	
2	HHH	272	
2	III	272	
2	JJJ	272	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37872 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 scFv 29B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	ZZZ	232	Total	C	N	O	S	0	0	0
			1735	1084	299	344	8			
1	KKK	232	Total	C	N	O	S	0	0	0
			1750	1093	305	344	8			
1	aaa	236	Total	C	N	O	S	0	0	0
			1765	1102	305	350	8			
1	bbb	232	Total	C	N	O	S	0	0	0
			1746	1090	304	344	8			
1	ccc	234	Total	C	N	O	S	0	0	0
			1750	1095	301	346	8			
1	ddd	233	Total	C	N	O	S	0	0	0
			1743	1092	300	343	8			
1	eee	235	Total	C	N	O	S	0	0	0
			1750	1095	299	348	8			
1	WWW	236	Total	C	N	O	S	0	0	0
			1773	1108	307	350	8			
1	XXX	229	Total	C	N	O	S	0	0	0
			1713	1071	296	338	8			
1	YYY	234	Total	C	N	O	S	0	0	0
			1756	1098	304	346	8			

- Molecule 2 is a protein called Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AAA	264	Total	C	N	O	S	0	3	0
			2062	1299	352	399	12			
2	BBB	259	Total	C	N	O	S	0	5	0
			2037	1288	347	391	11			
2	CCC	259	Total	C	N	O	S	0	7	0
			2045	1293	351	390	11			
2	DDD	259	Total	C	N	O	S	0	5	0
			2031	1282	347	391	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	EEE	259	Total 2026	C 1278	N 349	O 388	S 11	0	2	0
2	FFF	259	Total 2028	C 1280	N 347	O 390	S 11	0	4	0
2	GGG	258	Total 2032	C 1285	N 346	O 390	S 11	0	5	0
2	HHH	258	Total 2047	C 1295	N 352	O 389	S 11	0	8	0
2	III	259	Total 2031	C 1282	N 347	O 391	S 11	0	5	0
2	JJJ	259	Total 2029	C 1279	N 350	O 389	S 11	0	2	0

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

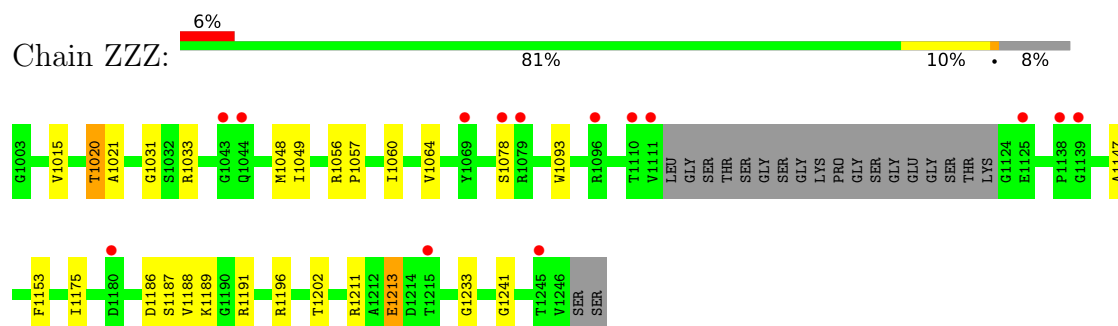
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	ZZZ	1	Total O 1 1	0	0
3	AAA	2	Total O 2 2	0	0
3	BBB	3	Total O 3 3	0	0
3	CCC	1	Total O 1 1	0	0
3	DDD	1	Total O 1 1	0	0
3	EEE	5	Total O 5 5	0	0
3	FFF	1	Total O 1 1	0	0
3	GGG	2	Total O 2 2	0	0
3	HHH	2	Total O 2 2	0	0
3	ccc	1	Total O 1 1	0	0
3	WWW	2	Total O 2 2	0	0
3	XXX	1	Total O 1 1	0	0
3	YYY	1	Total O 1 1	0	0

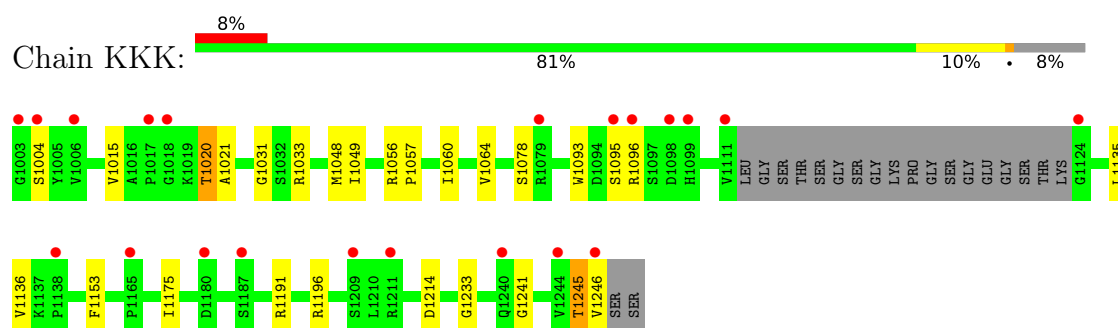
3 Residue-property plots

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.

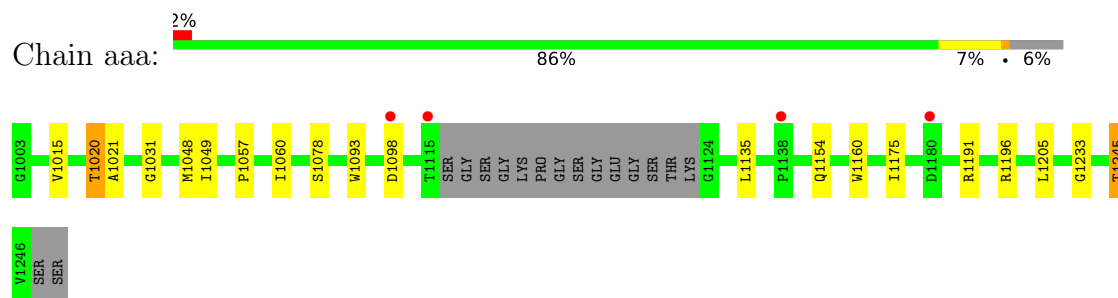
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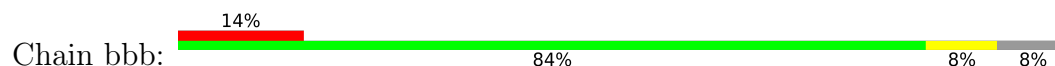
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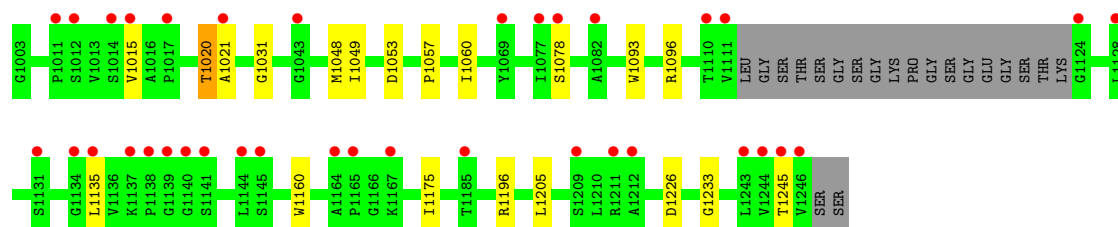


- Molecule 1: scFv 29B1

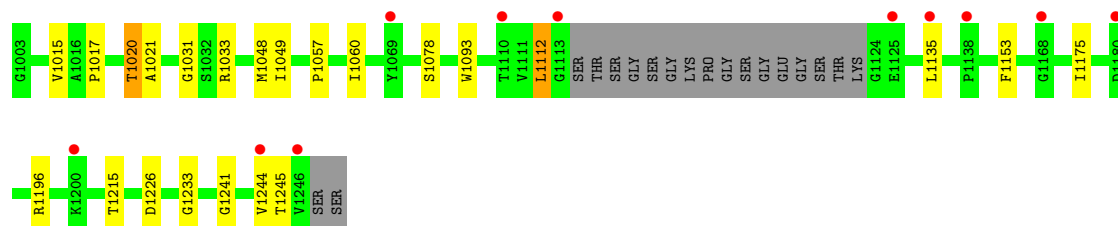
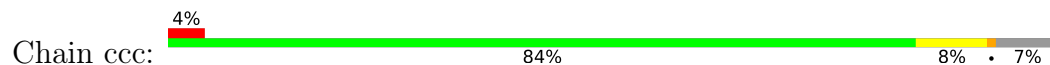


- Molecule 1: scFv 29B1

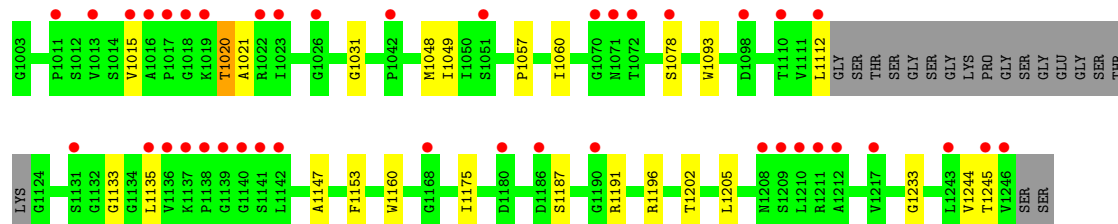
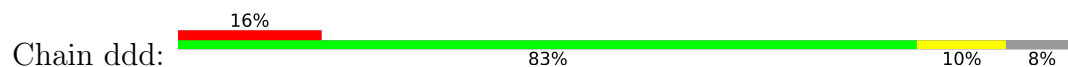




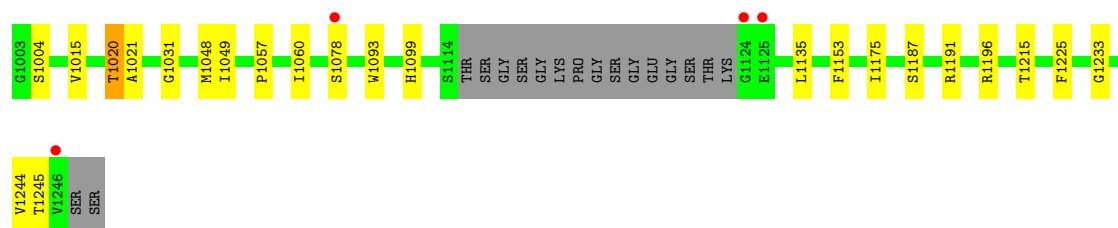
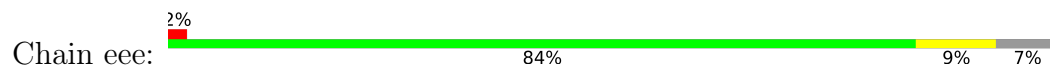
• Molecule 1: scFv 29B1



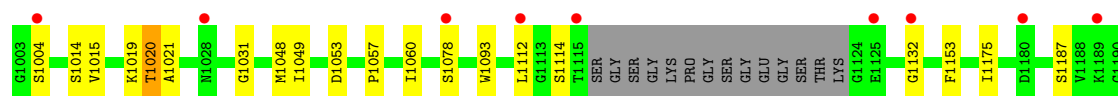
• Molecule 1: scFv 29B1



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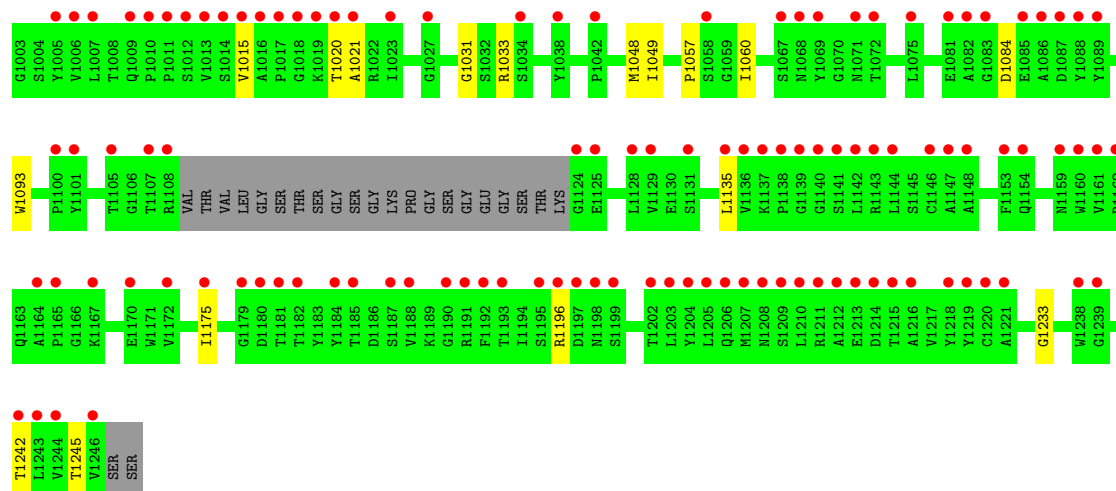
• Molecule 1: scFv 29B1





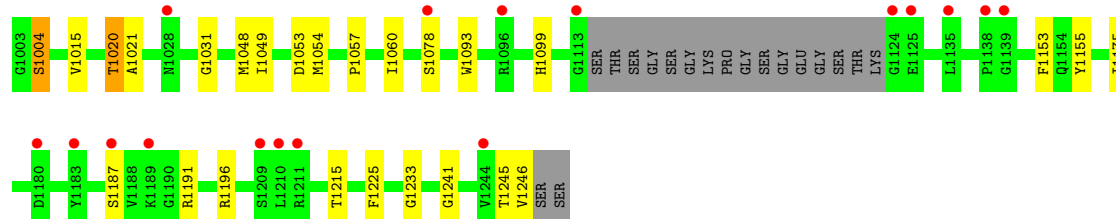
• Molecule 1: scFv 29B1

Chain XXX: 45% 84% 7% 9%



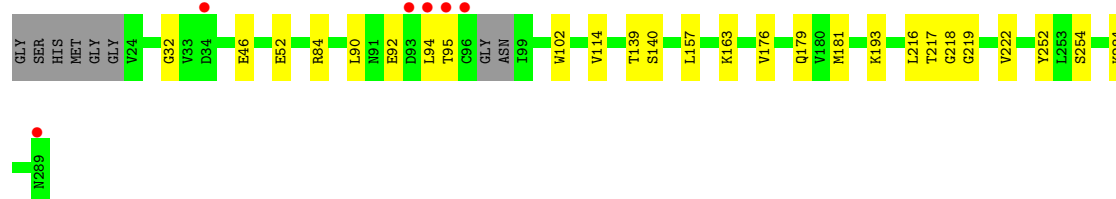
• Molecule 1: scFv 29B1

Chain YYY: 7% 83% 10% 7%



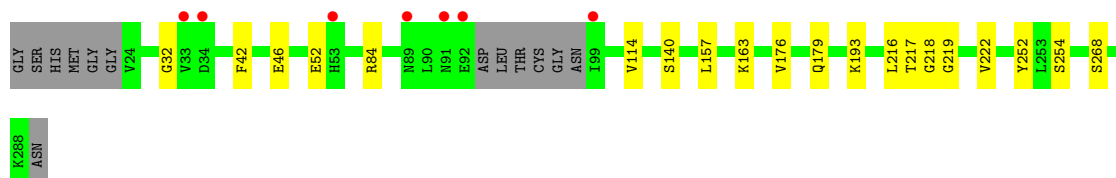
• Molecule 2: Major capsid protein VP1

Chain AAA: 2% 88% 10%

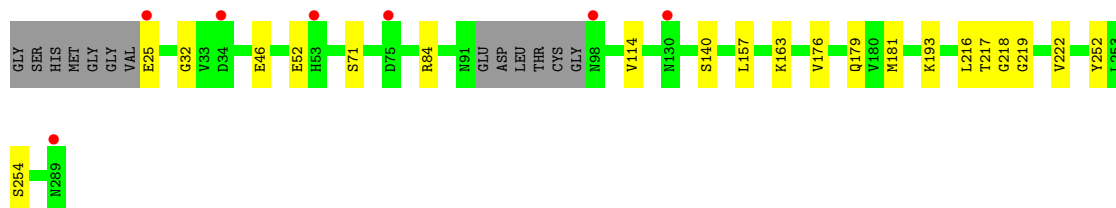
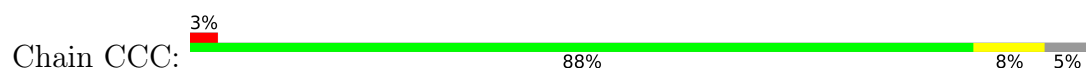


• Molecule 2: Major capsid protein VP1

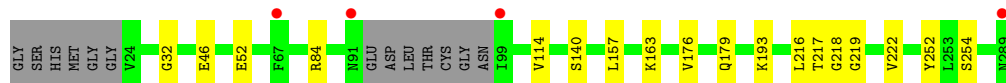
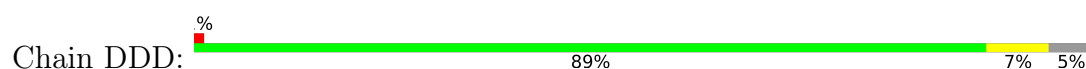
Chain BBB: 3% 88% 7% 5%



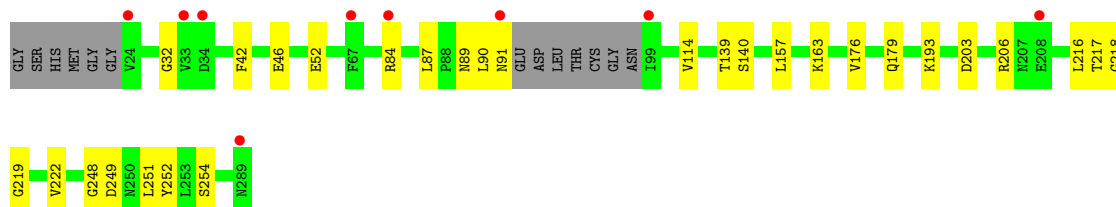
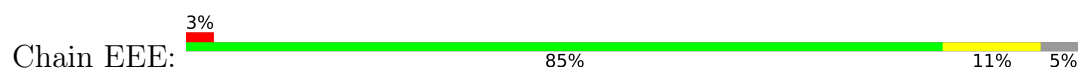
- Molecule 2: Major capsid protein VP1



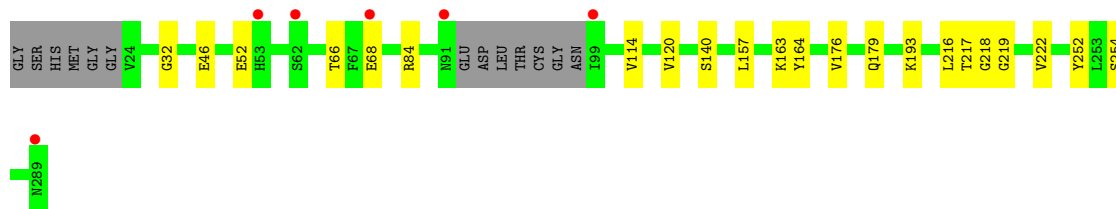
- Molecule 2: Major capsid protein VP1



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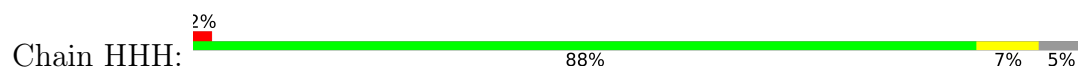


- Molecule 2: Major capsid protein VP1

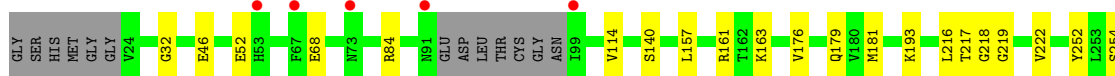
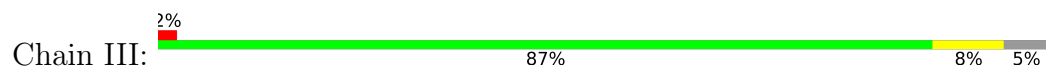




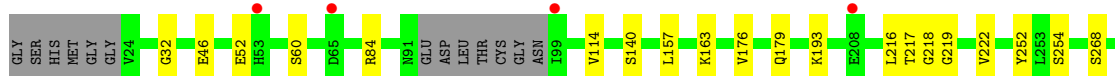
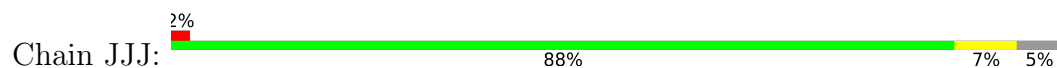
- Molecule 2: Major capsid protein VP1



- Molecule 2: Major capsid protein VP1



- Molecule 2: Major capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.13Å 172.53Å 159.71Å 90.00° 104.53° 90.00°	Depositor
Resolution (Å)	48.51 – 3.10 48.51 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.51-3.10) 99.9 (48.51-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.225 , 0.240 0.223 , 0.238	Depositor DCC
R_{free} test set	5881 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	37872	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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	KKK	1.02	0/1793	1.29	1/2442 (0.0%)
1	WWW	1.01	0/1816	1.27	0/2473
1	XXX	1.03	0/1756	1.28	1/2393 (0.0%)
1	YYY	1.01	0/1799	1.27	1/2451 (0.0%)
1	ZZZ	1.02	0/1778	1.28	1/2424 (0.0%)
1	aaa	1.01	0/1808	1.30	0/2465
1	bbb	1.03	0/1789	1.29	0/2438
1	ccc	1.02	0/1793	1.29	1/2444 (0.0%)
1	ddd	1.03	0/1786	1.28	0/2435
1	eee	1.02	0/1793	1.29	0/2445
2	AAA	0.98	0/2116	1.27	3/2875 (0.1%)
2	BBB	0.98	0/2098	1.25	2/2850 (0.1%)
2	CCC	0.97	0/2112	1.24	2/2868 (0.1%)
2	DDD	0.99	0/2091	1.25	2/2841 (0.1%)
2	EEE	0.97	0/2077	1.27	3/2821 (0.1%)
2	FFF	0.97	0/2085	1.25	3/2833 (0.1%)
2	GGG	0.97	0/2093	1.25	2/2843 (0.1%)
2	HHH	0.98	0/2118	1.26	2/2876 (0.1%)
2	III	0.99	0/2091	1.25	2/2841 (0.1%)
2	JJJ	0.97	0/2080	1.25	2/2825 (0.1%)
All	All	1.00	0/38872	1.27	28/52883 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	92	GLU	N-CA-C	-8.52	103.01	112.72
2	FFF	219	GLY	CA-C-O	-7.34	117.45	122.22
2	EEE	219	GLY	CA-C-O	-7.11	117.60	122.22
2	DDD	219	GLY	CA-C-O	-6.97	117.69	122.22
2	HHH	219	GLY	CA-C-O	-6.73	117.85	122.22
2	AAA	219	GLY	CA-C-O	-6.63	117.91	122.22
1	KKK	1241	GLY	CA-C-O	-6.51	117.74	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	219	GLY	CA-C-O	-6.37	118.08	122.22
2	GGG	32	GLY	CA-C-O	-6.36	117.72	122.37
2	GGG	219	GLY	CA-C-O	-6.36	118.09	122.22
2	EEE	249	ASP	CB-CA-C	6.30	120.31	111.86
2	BBB	219	GLY	CA-C-O	-6.28	118.14	122.22
2	DDD	32	GLY	CA-C-O	-6.22	117.83	122.37
2	BBB	32	GLY	CA-C-O	-6.08	117.94	122.37
1	YYY	1241	GLY	CA-C-O	-5.99	117.79	122.52
2	CCC	32	GLY	CA-C-O	-5.95	118.03	122.37
2	III	219	GLY	CA-C-O	-5.94	118.36	122.22
2	AAA	32	GLY	CA-C-O	-5.70	118.21	122.37
2	EEE	32	GLY	CA-C-O	-5.64	118.25	122.37
2	FFF	32	GLY	CA-C-O	-5.55	118.32	122.37
1	XXX	1084	ASP	N-CA-C	-5.54	106.19	113.17
2	JJJ	219	GLY	CA-C-O	-5.44	118.68	122.22
2	HHH	32	GLY	CA-C-O	-5.43	118.41	122.37
2	III	32	GLY	CA-C-O	-5.41	118.42	122.37
1	ZZZ	1241	GLY	CA-C-O	-5.39	118.26	122.52
1	ccc	1241	GLY	CA-C-O	-5.33	117.60	122.24
2	FFF	164	TYR	CB-CA-C	5.12	117.45	109.42
2	JJJ	32	GLY	CA-C-O	-5.11	118.64	122.37

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	KKK	1750	0	1637	14	0
1	WWW	1773	0	1663	12	1
1	XXX	1713	0	1586	8	0
1	YYY	1756	0	1640	17	0
1	ZZZ	1735	0	1606	15	0
1	aaa	1765	0	1641	9	0
1	bbb	1746	0	1626	14	0
1	ccc	1750	0	1629	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ddd	1743	0	1624	15	0
1	eee	1750	0	1623	13	0
2	AAA	2062	0	2009	28	0
2	BBB	2037	0	1995	18	0
2	CCC	2045	0	2005	23	0
2	DDD	2031	0	1988	16	0
2	EEE	2026	0	1983	21	1
2	FFF	2028	0	1983	15	0
2	GGG	2032	0	1993	17	0
2	HHH	2047	0	2010	19	0
2	III	2031	0	1988	16	0
2	JJJ	2029	0	1987	14	0
3	AAA	2	0	0	0	0
3	BBB	3	0	0	0	0
3	CCC	1	0	0	1	0
3	DDD	1	0	0	0	0
3	EEE	5	0	0	0	0
3	FFF	1	0	0	0	0
3	GGG	2	0	0	0	0
3	HHH	2	0	0	0	0
3	WWW	2	0	0	0	0
3	XXX	1	0	0	0	0
3	YYY	1	0	0	0	0
3	ZZZ	1	0	0	0	0
3	ccc	1	0	0	0	0
All	All	37872	0	36216	261	1

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 (261) 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:ZZZ:1211:ARG:CB	1:ZZZ:1213:GLU:OE2	1.97	1.13
2:AAA:94:LEU:HD12	2:AAA:95:THR:N	1.86	0.90
1:bbb:1135:LEU:HD23	1:bbb:1245:THR:HG23	1.55	0.89
1:ddd:1135:LEU:HD23	1:ddd:1245:THR:HG23	1.57	0.85
2:AAA:94:LEU:HD12	2:AAA:95:THR:O	1.79	0.82
1:bbb:1135:LEU:HD23	1:bbb:1245:THR:CG2	2.14	0.78
1:ddd:1135:LEU:HD23	1:ddd:1245:THR:CG2	2.14	0.77
2:AAA:139:THR:HG23	2:AAA:218:GLY:HA2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GGG:52:GLU:O	2:HHH:176:VAL:HG23	1.90	0.72
2:FFF:176:VAL:HG23	2:JJJ:52:GLU:O	1.89	0.72
2:AAA:94:LEU:CD1	2:AAA:95:THR:N	2.55	0.70
2:BBB:163:LYS:HE3	1:WWW:1031:GLY:O	1.95	0.66
2:AAA:90:LEU:HD22	2:AAA:284:LYS:HE2	1.78	0.66
1:XXX:1135:LEU:HD23	1:XXX:1245:THR:OG1	1.97	0.64
2:AAA:90:LEU:HD21	2:AAA:102:TRP:CZ2	2.33	0.63
2:AAA:94:LEU:CD1	2:AAA:95:THR:O	2.46	0.62
2:AAA:140:SER:O	2:AAA:216:LEU:HD12	2.00	0.62
1:ccc:1215:THR:HA	1:ccc:1244:VAL:O	1.98	0.62
2:AAA:52:GLU:O	2:BBB:176:VAL:HG23	2.01	0.61
2:JJJ:163:LYS:HE3	1:eee:1031:GLY:O	2.00	0.61
2:GGG:163:LYS:HE3	1:bbb:1031:GLY:O	2.01	0.60
2:JJJ:140:SER:O	2:JJJ:216:LEU:HD12	2.02	0.59
2:CCC:25:GLU:N	3:CCC:301:HOH:O	2.34	0.59
1:ZZZ:1187:SER:O	1:ZZZ:1191:ARG:NH1	2.34	0.59
2:CCC:52:GLU:O	2:DDD:176:VAL:HG23	2.02	0.59
2:III:140:SER:O	2:III:216:LEU:HD12	2.03	0.59
2:BBB:52:GLU:O	2:CCC:176:VAL:HG23	2.03	0.59
1:YYY:1187:SER:O	1:YYY:1191:ARG:NH1	2.35	0.59
1:KKK:1136:VAL:O	1:KKK:1246:VAL:HA	2.03	0.58
2:HHH:140:SER:O	2:HHH:216:LEU:HD12	2.04	0.58
2:AAA:114:VAL:O	2:BBB:216:LEU:HD22	2.04	0.58
2:AAA:176:VAL:HG23	2:EEE:52:GLU:O	2.04	0.58
2:BBB:218:GLY:O	2:BBB:222:VAL:HG21	2.05	0.57
2:CCC:163:LYS:HE3	1:YYY:1031:GLY:O	2.03	0.57
1:ccc:1135:LEU:HD23	1:ccc:1245:THR:OG1	2.03	0.57
1:aaa:1048:MET:HE3	1:aaa:1057:PRO:HG3	1.85	0.57
2:JJJ:218:GLY:O	2:JJJ:222:VAL:HG21	2.05	0.57
1:KKK:1135:LEU:HD23	1:KKK:1245:THR:OG1	2.04	0.57
2:DDD:140:SER:O	2:DDD:216:LEU:HD12	2.05	0.57
2:III:52:GLU:O	2:JJJ:176:VAL:HG23	2.05	0.57
2:AAA:90:LEU:HD21	2:AAA:102:TRP:CE2	2.39	0.57
2:CCC:140:SER:O	2:CCC:216:LEU:HD12	2.04	0.56
2:EEE:140:SER:O	2:EEE:216:LEU:HD12	2.05	0.56
1:YYY:1048:MET:HE3	1:YYY:1057:PRO:HG3	1.87	0.56
2:FFF:163:LYS:HE3	1:aaa:1031:GLY:O	2.05	0.56
2:FFF:176:VAL:CG2	2:JJJ:52:GLU:O	2.54	0.56
2:AAA:94:LEU:HD12	2:AAA:94:LEU:C	2.30	0.55
2:FFF:140:SER:O	2:FFF:216:LEU:HD12	2.05	0.55
1:eee:1048:MET:HE3	1:eee:1057:PRO:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:140:SER:O	2:BBB:216:LEU:HD12	2.06	0.55
1:ddd:1048:MET:HE3	1:ddd:1057:PRO:HG3	1.89	0.55
2:DDD:52:GLU:O	2:EEE:176:VAL:HG23	2.06	0.55
2:HHH:114:VAL:O	2:III:216:LEU:HD22	2.06	0.55
1:ddd:1133:GLY:HA2	1:ddd:1244:VAL:HG12	1.87	0.55
2:AAA:218:GLY:O	2:AAA:222:VAL:HG21	2.06	0.55
2:FFF:217:THR:HG22	2:FFF:222:VAL:HG11	1.89	0.55
2:GGG:140:SER:O	2:GGG:216:LEU:HD12	2.07	0.55
1:aaa:1135:LEU:HD23	1:aaa:1245:THR:OG1	2.07	0.55
1:ZZZ:1093:TRP:CG	1:ZZZ:1233:GLY:HA3	2.42	0.55
2:DDD:218:GLY:O	2:DDD:222:VAL:HG21	2.07	0.55
1:bbb:1048:MET:HE3	1:bbb:1057:PRO:HG3	1.90	0.54
1:bbb:1135:LEU:CD2	1:bbb:1245:THR:HG23	2.32	0.54
2:HHH:163:LYS:NZ	1:ccc:1033:ARG:O	2.40	0.54
1:YYY:1049:ILE:HA	1:YYY:1060:ILE:HG12	1.90	0.54
1:YYY:1175:ILE:HD13	1:YYY:1196:ARG:HG3	1.90	0.54
2:HHH:218:GLY:O	2:HHH:222:VAL:HG21	2.07	0.54
1:YYY:1215:THR:HG22	1:YYY:1246:VAL:N	2.23	0.54
2:EEE:84:ARG:HD2	2:EEE:252:TYR:OH	2.07	0.54
1:WWW:1093:TRP:CG	1:WWW:1233:GLY:HA3	2.43	0.54
2:GGG:52:GLU:O	2:HHH:176:VAL:CG2	2.56	0.54
1:ZZZ:1048:MET:HE3	1:ZZZ:1057:PRO:HG3	1.90	0.54
1:bbb:1096:ARG:O	1:bbb:1096:ARG:HG3	2.07	0.54
1:ccc:1093:TRP:CG	1:ccc:1233:GLY:HA3	2.43	0.54
2:DDD:114:VAL:O	2:EEE:216:LEU:HD22	2.08	0.54
2:HHH:217:THR:HG22	2:HHH:222:VAL:HG11	1.91	0.54
2:BBB:84:ARG:HD2	2:BBB:252:TYR:OH	2.09	0.53
2:DDD:217:THR:HG22	2:DDD:222:VAL:HG11	1.91	0.53
1:ccc:1175:ILE:HD13	1:ccc:1196:ARG:HG3	1.90	0.53
2:GGG:217:THR:HG22	2:GGG:222:VAL:HG11	1.91	0.53
1:ZZZ:1049:ILE:HA	1:ZZZ:1060:ILE:HG12	1.90	0.53
1:KKK:1191:ARG:NH2	1:KKK:1214:ASP:OD2	2.41	0.53
2:GGG:218:GLY:O	2:GGG:222:VAL:HG21	2.09	0.53
1:bbb:1049:ILE:HA	1:bbb:1060:ILE:HG12	1.90	0.53
1:WWW:1175:ILE:HD13	1:WWW:1196:ARG:HG3	1.91	0.53
1:KKK:1048:MET:HE3	1:KKK:1057:PRO:HG3	1.89	0.53
2:HHH:52:GLU:O	2:III:176:VAL:HG23	2.08	0.53
2:JJJ:217:THR:HG22	2:JJJ:222:VAL:HG11	1.91	0.53
1:XXX:1093:TRP:CG	1:XXX:1233:GLY:HA3	2.44	0.53
1:ZZZ:1175:ILE:HD13	1:ZZZ:1196:ARG:HG3	1.91	0.53
2:AAA:163:LYS:HE3	1:KKK:1031:GLY:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:217:THR:HG22	2:CCC:222:VAL:HG11	1.91	0.53
1:bbb:1093:TRP:CG	1:bbb:1233:GLY:HA3	2.44	0.53
1:bbb:1175:ILE:HD13	1:bbb:1196:ARG:HG3	1.91	0.53
2:III:217:THR:HG22	2:III:222:VAL:HG11	1.91	0.52
1:ddd:1175:ILE:HD13	1:ddd:1196:ARG:HG3	1.90	0.52
2:AAA:217:THR:HG22	2:AAA:222:VAL:HG11	1.92	0.52
1:ccc:1048:MET:HE3	1:ccc:1057:PRO:HG3	1.90	0.52
2:CCC:46:GLU:HG2	2:CCC:193:LYS:CG	2.40	0.52
2:EEE:217:THR:HG22	2:EEE:222:VAL:HG11	1.92	0.52
1:ddd:1093:TRP:CG	1:ddd:1233:GLY:HA3	2.44	0.52
1:eee:1049:ILE:HA	1:eee:1060:ILE:HG12	1.91	0.52
2:BBB:217:THR:HG22	2:BBB:222:VAL:HG11	1.92	0.52
2:III:163:LYS:HE3	1:ddd:1031:GLY:O	2.09	0.52
1:XXX:1175:ILE:HD13	1:XXX:1196:ARG:HG3	1.91	0.52
1:aaa:1175:ILE:HD13	1:aaa:1196:ARG:HG3	1.91	0.52
1:ddd:1049:ILE:HA	1:ddd:1060:ILE:HG12	1.91	0.52
1:ddd:1187:SER:O	1:ddd:1191:ARG:NH1	2.43	0.52
1:XXX:1049:ILE:HA	1:XXX:1060:ILE:HG12	1.92	0.52
2:EEE:218:GLY:O	2:EEE:222:VAL:HG21	2.09	0.52
2:AAA:46:GLU:HG2	2:AAA:193:LYS:CG	2.40	0.52
2:III:84:ARG:HD2	2:III:252:TYR:OH	2.10	0.52
2:AAA:216:LEU:HD22	2:EEE:114:VAL:O	2.09	0.51
1:KKK:1049:ILE:HA	1:KKK:1060:ILE:HG12	1.92	0.51
1:ccc:1049:ILE:HA	1:ccc:1060:ILE:HG12	1.92	0.51
1:eee:1093:TRP:CG	1:eee:1233:GLY:HA3	2.45	0.51
1:ddd:1135:LEU:CD2	1:ddd:1245:THR:HG23	2.36	0.51
2:FFF:218:GLY:O	2:FFF:222:VAL:HG21	2.10	0.51
2:FFF:216:LEU:HD22	2:JJJ:114:VAL:O	2.10	0.51
1:WWW:1049:ILE:HA	1:WWW:1060:ILE:HG12	1.91	0.51
1:XXX:1048:MET:HE3	1:XXX:1057:PRO:HG3	1.92	0.51
2:JJJ:46:GLU:HG2	2:JJJ:193:LYS:CG	2.41	0.51
2:DDD:163:LYS:HE3	1:XXX:1031:GLY:O	2.10	0.51
2:HHH:46:GLU:HG2	2:HHH:193:LYS:CG	2.41	0.51
1:YYY:1093:TRP:CG	1:YYY:1233:GLY:HA3	2.46	0.51
1:aaa:1093:TRP:CG	1:aaa:1233:GLY:HA3	2.45	0.50
2:GGG:46:GLU:HG2	2:GGG:193:LYS:CG	2.41	0.50
1:aaa:1049:ILE:HA	1:aaa:1060:ILE:HG12	1.91	0.50
2:DDD:46:GLU:HG2	2:DDD:193:LYS:CG	2.41	0.50
2:III:46:GLU:HG2	2:III:193:LYS:CG	2.42	0.50
1:KKK:1093:TRP:CG	1:KKK:1233:GLY:HA3	2.47	0.50
1:KKK:1175:ILE:HD13	1:KKK:1196:ARG:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:46:GLU:HG2	2:BBB:193:LYS:CG	2.42	0.50
2:III:218:GLY:O	2:III:222:VAL:HG21	2.12	0.50
2:CCC:218:GLY:O	2:CCC:222:VAL:HG21	2.12	0.49
1:YYY:1215:THR:HG22	1:YYY:1246:VAL:H	1.77	0.49
2:FFF:114:VAL:O	2:GGG:216:LEU:HD22	2.13	0.49
1:eee:1175:ILE:HD13	1:eee:1196:ARG:HG3	1.93	0.49
2:BBB:42[A]:PHE:CD2	2:CCC:181:MET:HG2	2.47	0.49
2:HHH:84:ARG:HD2	2:HHH:252:TYR:OH	2.12	0.49
1:ZZZ:1031:GLY:O	2:EEE:163:LYS:HE3	2.13	0.49
1:ccc:1020:THR:HB	1:ccc:1078:SER:HA	1.95	0.48
2:FFF:66:THR:OG1	2:FFF:68[B]:GLU:HG2	2.13	0.48
2:HHH:163:LYS:HE3	1:ccc:1031:GLY:O	2.14	0.48
1:WWW:1048:MET:HE3	1:WWW:1057:PRO:HG3	1.95	0.48
2:AAA:90:LEU:CD2	2:AAA:284:LYS:HE2	2.43	0.48
2:EEE:84:ARG:HD2	2:EEE:252:TYR:CZ	2.48	0.48
2:FFF:120:VAL:HG11	2:GGG:261:MET:HE1	1.96	0.48
2:DDD:84:ARG:HD2	2:DDD:252:TYR:OH	2.14	0.48
1:aaa:1020:THR:HB	1:aaa:1078:SER:HA	1.96	0.48
2:FFF:46:GLU:HG2	2:FFF:193:LYS:CG	2.44	0.48
2:GGG:114:VAL:O	2:HHH:216:LEU:HD22	2.13	0.48
1:eee:1020:THR:HB	1:eee:1078:SER:HA	1.95	0.47
2:AAA:157:LEU:O	2:AAA:179:GLN:HA	2.15	0.47
2:CCC:114:VAL:O	2:DDD:216:LEU:HD22	2.14	0.47
1:ZZZ:1020:THR:HB	1:ZZZ:1078:SER:HA	1.96	0.47
1:KKK:1095:SER:O	1:KKK:1096:ARG:HG2	2.15	0.47
2:CCC:84:ARG:HD2	2:CCC:252:TYR:OH	2.14	0.47
2:EEE:46:GLU:HG2	2:EEE:193:LYS:CG	2.45	0.47
1:WWW:1020:THR:HB	1:WWW:1078:SER:HA	1.97	0.47
2:AAA:163:LYS:NZ	1:KKK:1033:ARG:O	2.46	0.46
2:CCC:52:GLU:HB3	1:YYY:1225:PHE:CD1	2.51	0.46
2:EEE:87:LEU:HD21	2:EEE:251:LEU:HB2	1.97	0.46
2:BBB:163:LYS:NZ	1:WWW:1053:ASP:OD2	2.49	0.46
2:GGG:139:THR:HG23	2:GGG:218:GLY:HA2	1.98	0.46
1:ZZZ:1033:ARG:O	2:EEE:163:LYS:NZ	2.48	0.46
1:WWW:1014:SER:HB3	1:WWW:1112:LEU:HD23	1.97	0.46
1:ZZZ:1188:VAL:HA	1:ZZZ:1191:ARG:NH1	2.31	0.46
2:FFF:84:ARG:HD2	2:FFF:252:TYR:OH	2.15	0.46
2:CCC:163:LYS:NZ	1:YYY:1053:ASP:OD2	2.43	0.46
2:EEE:203:ASP:OD2	2:EEE:206[A]:ARG:HD2	2.16	0.45
2:JJJ:84:ARG:HD2	2:JJJ:252:TYR:OH	2.16	0.45
1:KKK:1020:THR:HB	1:KKK:1078:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WWW:1191:ARG:NH2	1:WWW:1214:ASP:OD2	2.50	0.45
2:AAA:46:GLU:HG2	2:AAA:193:LYS:HG2	1.98	0.45
2:DDD:163:LYS:NZ	1:XXX:1033:ARG:O	2.49	0.45
2:HHH:42[B]:PHE:CE1	2:III:181:MET:HE2	2.52	0.45
1:YYY:1004:SER:HB3	1:YYY:1099:HIS:CE1	2.51	0.45
2:AAA:94:LEU:CD1	2:AAA:95:THR:H	2.28	0.45
2:BBB:157:LEU:O	2:BBB:179:GLN:HA	2.17	0.45
1:ccc:1017:PRO:HD3	1:ccc:1112:LEU:HB2	1.98	0.45
2:AAA:84:ARG:HD2	2:AAA:252:TYR:OH	2.16	0.45
2:CCC:157:LEU:O	2:CCC:179:GLN:HA	2.16	0.45
2:GGG:84:ARG:HD2	2:GGG:252:TYR:OH	2.17	0.45
2:CCC:46:GLU:HG2	2:CCC:193:LYS:HG2	1.99	0.45
2:CCC:71[A]:SER:HB3	1:YYY:1054:MET:HG2	1.99	0.45
1:XXX:1015:VAL:HG21	1:XXX:1021:ALA:HB2	1.97	0.45
2:CCC:71[B]:SER:HB3	1:YYY:1054:MET:HG2	1.99	0.44
1:aaa:1015:VAL:HG21	1:aaa:1021:ALA:HB2	2.00	0.44
2:GGG:157:LEU:O	2:GGG:179:GLN:HA	2.17	0.44
1:ddd:1015:VAL:HG21	1:ddd:1021:ALA:HB2	1.99	0.44
1:KKK:1015:VAL:HG21	1:KKK:1021:ALA:HB2	2.00	0.44
1:YYY:1015:VAL:HG21	1:YYY:1021:ALA:HB2	1.98	0.44
1:bbb:1020:THR:HB	1:bbb:1078:SER:HA	2.00	0.44
2:BBB:42[B]:PHE:CE1	2:CCC:181:MET:HE2	2.53	0.44
2:JJJ:46:GLU:HG2	2:JJJ:193:LYS:HG2	1.99	0.44
1:ZZZ:1153:PHE:O	1:ZZZ:1196:ARG:NH2	2.51	0.44
2:DDD:46:GLU:HG2	2:DDD:193:LYS:HG2	2.00	0.44
1:eee:1015:VAL:HG21	1:eee:1021:ALA:HB2	1.99	0.44
1:WWW:1015:VAL:HG21	1:WWW:1021:ALA:HB2	1.99	0.44
2:EEE:90:LEU:O	2:EEE:91:ASN:C	2.61	0.44
2:HHH:193:LYS:NZ	1:ccc:1226:ASP:OD1	2.51	0.44
1:bbb:1015:VAL:HG21	1:bbb:1021:ALA:HB2	1.99	0.44
1:ccc:1015:VAL:HG21	1:ccc:1021:ALA:HB2	1.99	0.44
2:BBB:52:GLU:O	2:CCC:176:VAL:CG2	2.65	0.43
2:BBB:84:ARG:HD2	2:BBB:252:TYR:CZ	2.53	0.43
1:ZZZ:1015:VAL:HG21	1:ZZZ:1021:ALA:HB2	2.00	0.43
2:EEE:89:ASN:OD1	2:EEE:89:ASN:O	2.35	0.43
1:ddd:1020:THR:HB	1:ddd:1078:SER:HA	2.00	0.43
2:III:157:LEU:O	2:III:179:GLN:HA	2.19	0.43
2:FFF:157:LEU:O	2:FFF:179:GLN:HA	2.18	0.43
2:GGG:163:LYS:NZ	1:bbb:1053:ASP:OD2	2.51	0.43
2:III:46:GLU:HG2	2:III:193:LYS:HG2	2.00	0.43
2:BBB:114:VAL:O	2:CCC:216:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YYY:1020:THR:HB	1:YYY:1078:SER:HA	2.01	0.43
2:EEE:157:LEU:O	2:EEE:179:GLN:HA	2.19	0.43
2:HHH:46:GLU:HG2	2:HHH:193:LYS:HG2	2.01	0.43
2:GGG:46:GLU:HG2	2:GGG:193:LYS:HG2	2.01	0.43
2:BBB:46:GLU:HG2	2:BBB:193:LYS:HG2	2.01	0.42
2:GGG:193:LYS:NZ	1:bbb:1226:ASP:OD1	2.53	0.42
2:HHH:84:ARG:HD2	2:HHH:252:TYR:CZ	2.54	0.42
2:CCC:52:GLU:O	2:DDD:176:VAL:CG2	2.67	0.42
2:FFF:52:GLU:O	2:GGG:176:VAL:HG23	2.19	0.42
2:JJJ:52:GLU:HB3	1:eee:1225:PHE:CD1	2.54	0.42
2:EEE:139:THR:HG23	2:EEE:218:GLY:HA2	2.01	0.42
1:aaa:1160:TRP:NE1	1:aaa:1205:LEU:HB2	2.35	0.42
2:III:114:VAL:O	2:JJJ:216:LEU:HD22	2.18	0.42
2:AAA:52:GLU:O	2:BBB:176:VAL:CG2	2.66	0.42
2:III:84:ARG:HD2	2:III:252:TYR:CZ	2.54	0.42
1:eee:1215:THR:HA	1:eee:1244:VAL:O	2.19	0.42
1:KKK:1056:ARG:HD3	1:KKK:1064:VAL:O	2.20	0.42
2:CCC:46:GLU:HG2	2:CCC:193:LYS:HG3	2.02	0.42
2:DDD:84:ARG:HD2	2:DDD:252:TYR:CZ	2.55	0.42
2:HHH:120:VAL:HG11	2:III:261:MET:HE1	2.00	0.42
1:eee:1187:SER:O	1:eee:1191:ARG:NH1	2.53	0.42
2:DDD:157:LEU:O	2:DDD:179:GLN:HA	2.20	0.41
1:ddd:1160:TRP:NE1	1:ddd:1205:LEU:HB2	2.35	0.41
1:eee:1153:PHE:O	1:eee:1196:ARG:NH2	2.53	0.41
2:CCC:84:ARG:HD2	2:CCC:252:TYR:CZ	2.55	0.41
2:HHH:157:LEU:O	2:HHH:179:GLN:HA	2.20	0.41
2:JJJ:157:LEU:O	2:JJJ:179:GLN:HA	2.21	0.41
1:KKK:1153:PHE:O	1:KKK:1196:ARG:NH2	2.54	0.41
1:eee:1004:SER:HB2	1:eee:1099:HIS:CE1	2.55	0.41
2:EEE:46:GLU:HG2	2:EEE:193:LYS:HG2	2.03	0.41
2:III:68[A]:GLU:CG	2:III:161:ARG:NH1	2.84	0.41
1:YYY:1153:PHE:O	1:YYY:1196:ARG:NH2	2.54	0.41
2:AAA:176:VAL:CG2	2:EEE:52:GLU:O	2.68	0.41
1:ddd:1147:ALA:HA	1:ddd:1202:THR:HG22	2.03	0.41
2:FFF:84:ARG:HD2	2:FFF:252:TYR:CZ	2.56	0.41
1:ZZZ:1056:ARG:HD3	1:ZZZ:1064:VAL:O	2.21	0.41
1:ccc:1153:PHE:O	1:ccc:1196:ARG:NH2	2.54	0.41
1:eee:1135:LEU:HD23	1:eee:1245:THR:HB	2.02	0.41
1:WWW:1187:SER:O	1:WWW:1191:ARG:NH1	2.53	0.41
1:ZZZ:1186:ASP:HA	1:ZZZ:1189:LYS:HE3	2.03	0.41
2:AAA:181:MET:HG2	2:EEE:42:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ddd:1153:PHE:O	1:ddd:1196:ARG:NH2	2.54	0.41
2:DDD:176:VAL:HG11	1:YYY:1155:TYR:CE2	2.56	0.40
2:HHH:46:GLU:HG2	2:HHH:193:LYS:HG3	2.02	0.40
2:AAA:94:LEU:HD12	2:AAA:95:THR:C	2.45	0.40
1:WWW:1153:PHE:O	1:WWW:1196:ARG:NH2	2.55	0.40
1:bbb:1160:TRP:NE1	1:bbb:1205:LEU:HB2	2.36	0.40
1:ZZZ:1147:ALA:HA	1:ZZZ:1202:THR:HG22	2.04	0.40

All (1) 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)
2:EEE:248:GLY:O	1:WWW:1132:GLY:O[2_654]	1.83	0.37

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	KKK	228/252 (90%)	211 (92%)	17 (8%)	0	100	100
1	WWW	232/252 (92%)	215 (93%)	16 (7%)	1 (0%)	30	61
1	XXX	225/252 (89%)	208 (92%)	16 (7%)	1 (0%)	30	61
1	YYY	230/252 (91%)	212 (92%)	17 (7%)	1 (0%)	30	61
1	ZZZ	228/252 (90%)	210 (92%)	18 (8%)	0	100	100
1	aaa	232/252 (92%)	216 (93%)	16 (7%)	0	100	100
1	bbb	228/252 (90%)	210 (92%)	18 (8%)	0	100	100
1	ccc	230/252 (91%)	214 (93%)	15 (6%)	1 (0%)	30	61
1	ddd	229/252 (91%)	213 (93%)	16 (7%)	0	100	100
1	eee	231/252 (92%)	213 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AAA	263/272 (97%)	250 (95%)	13 (5%)	0	100	100
2	BBB	260/272 (96%)	248 (95%)	12 (5%)	0	100	100
2	CCC	262/272 (96%)	250 (95%)	12 (5%)	0	100	100
2	DDD	260/272 (96%)	249 (96%)	11 (4%)	0	100	100
2	EEE	257/272 (94%)	244 (95%)	13 (5%)	0	100	100
2	FFF	259/272 (95%)	247 (95%)	12 (5%)	0	100	100
2	GGG	259/272 (95%)	247 (95%)	12 (5%)	0	100	100
2	HHH	262/272 (96%)	250 (95%)	12 (5%)	0	100	100
2	III	260/272 (96%)	248 (95%)	12 (5%)	0	100	100
2	JJJ	257/272 (94%)	244 (95%)	13 (5%)	0	100	100
All	All	4892/5240 (93%)	4599 (94%)	289 (6%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	WWW	1114	SER
1	YYY	1004	SER
1	ccc	1112	LEU
1	XXX	1242	THR

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	KKK	184/204 (90%)	181 (98%)	3 (2%)	55	75
1	WWW	187/204 (92%)	184 (98%)	3 (2%)	55	75
1	XXX	178/204 (87%)	177 (99%)	1 (1%)	78	83
1	YYY	184/204 (90%)	182 (99%)	2 (1%)	65	78
1	ZZZ	181/204 (89%)	179 (99%)	2 (1%)	65	78
1	aaa	185/204 (91%)	180 (97%)	5 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	bbb	183/204 (90%)	182 (100%)	1 (0%)	81	85
1	ccc	183/204 (90%)	182 (100%)	1 (0%)	81	85
1	ddd	182/204 (89%)	180 (99%)	2 (1%)	65	78
1	eee	183/204 (90%)	182 (100%)	1 (0%)	81	85
2	AAA	232/237 (98%)	231 (100%)	1 (0%)	84	86
2	BBB	230/237 (97%)	227 (99%)	3 (1%)	61	77
2	CCC	230/237 (97%)	229 (100%)	1 (0%)	84	86
2	DDD	229/237 (97%)	228 (100%)	1 (0%)	84	86
2	EEE	227/237 (96%)	226 (100%)	1 (0%)	84	86
2	FFF	228/237 (96%)	227 (100%)	1 (0%)	84	86
2	GGG	230/237 (97%)	229 (100%)	1 (0%)	84	86
2	HHH	231/237 (98%)	230 (100%)	1 (0%)	84	86
2	III	229/237 (97%)	228 (100%)	1 (0%)	84	86
2	JJJ	228/237 (96%)	225 (99%)	3 (1%)	61	77
All	All	4124/4410 (94%)	4089 (99%)	35 (1%)	73	81

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ZZZ	1020	THR
1	ZZZ	1213	GLU
2	AAA	254	SER
2	BBB	254	SER
2	BBB	268[A]	SER
2	BBB	268[B]	SER
2	CCC	254	SER
2	DDD	254	SER
2	EEE	254	SER
2	FFF	254	SER
2	GGG	254	SER
2	HHH	254	SER
2	III	254	SER
2	JJJ	60	SER
2	JJJ	254	SER
2	JJJ	268	SER
1	KKK	1004	SER
1	KKK	1020	THR

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Mol	Chain	Res	Type
1	KKK	1245	THR
1	aaa	1020	THR
1	aaa	1098	ASP
1	aaa	1154	GLN
1	aaa	1191	ARG
1	aaa	1245	THR
1	bbb	1020	THR
1	ccc	1020	THR
1	ddd	1020	THR
1	ddd	1112	LEU
1	eee	1020	THR
1	WWW	1004	SER
1	WWW	1019	LYS
1	WWW	1020	THR
1	XXX	1020	THR
1	YYY	1020	THR
1	YYY	1245	THR

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 ⓘ

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	KKK	232/252 (92%)	0.78	21 (9%) 15 8	33, 57, 96, 117	0
1	WWW	236/252 (93%)	0.26	9 (3%) 44 25	20, 39, 62, 88	0
1	XXX	229/252 (90%)	2.10	113 (49%) 0 0	30, 93, 137, 162	0
1	YYY	234/252 (92%)	0.68	17 (7%) 21 11	20, 53, 93, 124	0
1	ZZZ	232/252 (92%)	0.57	14 (6%) 27 15	32, 51, 78, 99	0
1	aaa	236/252 (93%)	0.35	4 (1%) 69 48	26, 48, 67, 81	0
1	bbb	232/252 (92%)	1.13	36 (15%) 5 2	34, 79, 123, 161	0
1	ccc	234/252 (92%)	0.57	11 (4%) 36 19	32, 55, 85, 105	0
1	ddd	233/252 (92%)	1.28	41 (17%) 4 2	33, 79, 119, 144	0
1	eee	235/252 (93%)	0.33	4 (1%) 69 48	34, 48, 68, 81	0
2	AAA	264/272 (97%)	0.04	6 (2%) 61 39	21, 33, 53, 81	3 (1%)
2	BBB	259/272 (95%)	-0.04	7 (2%) 56 35	18, 32, 52, 68	5 (1%)
2	CCC	259/272 (95%)	0.11	7 (2%) 56 35	17, 33, 53, 69	7 (2%)
2	DDD	259/272 (95%)	0.11	4 (1%) 72 52	22, 38, 56, 71	5 (1%)
2	EEE	259/272 (95%)	0.11	9 (3%) 47 27	19, 35, 53, 66	2 (0%)
2	FFF	259/272 (95%)	0.14	6 (2%) 61 39	22, 37, 57, 72	4 (1%)
2	GGG	258/272 (94%)	0.15	5 (1%) 66 45	24, 40, 58, 75	5 (1%)
2	HHH	258/272 (94%)	0.15	6 (2%) 61 39	21, 40, 56, 69	8 (3%)
2	III	259/272 (95%)	0.14	6 (2%) 61 39	23, 39, 55, 68	5 (1%)
2	JJJ	259/272 (95%)	0.05	5 (1%) 66 45	19, 37, 54, 71	2 (0%)
All	All	4926/5240 (94%)	0.43	331 (6%) 24 13	17, 44, 95, 162	46 (0%)

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	XXX	1209	SER	5.7
1	ddd	1112	LEU	5.3
1	XXX	1211	ARG	5.3
2	FFF	91	ASN	5.3
1	XXX	1207	MET	4.9
1	XXX	1138	PRO	4.9
2	CCC	98	ASN	4.7
1	ccc	1113	GLY	4.7
1	ZZZ	1180	ASP	4.5
2	BBB	92	GLU	4.5
1	ddd	1138	PRO	4.5
1	KKK	1180	ASP	4.4
1	XXX	1212	ALA	4.3
1	XXX	1221	ALA	4.3
1	bbb	1138	PRO	4.3
2	III	99	ILE	4.2
1	ddd	1180	ASP	4.2
1	XXX	1220	CYS	4.2
1	KKK	1099	HIS	4.1
1	WWW	1132	GLY	4.1
1	aaa	1180	ASP	4.0
1	XXX	1017	PRO	3.9
1	XXX	1205	LEU	3.9
1	XXX	1142	LEU	3.9
1	bbb	1012	SER	3.8
1	ddd	1212	ALA	3.8
1	ddd	1137	LYS	3.8
2	HHH	91	ASN	3.7
2	III	289	ASN	3.7
1	YYY	1078	SER	3.7
1	XXX	1210	LEU	3.7
1	KKK	1138	PRO	3.7
1	YYY	1138	PRO	3.6
1	ZZZ	1069	TYR	3.6
1	KKK	1003	GLY	3.5
1	KKK	1096	ARG	3.5
1	XXX	1006	VAL	3.5
1	XXX	1180	ASP	3.5
1	ddd	1135	LEU	3.5
1	XXX	1011	PRO	3.5
1	XXX	1144	LEU	3.5
1	XXX	1179	GLY	3.5
1	XXX	1243	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	XXX	1137	LYS	3.4
1	XXX	1191	ARG	3.4
1	XXX	1206	GLN	3.4
2	FFF	289	ASN	3.4
2	III	91	ASN	3.4
1	XXX	1016	ALA	3.4
2	AAA	95	THR	3.4
1	XXX	1244	VAL	3.4
1	XXX	1021	ALA	3.4
2	DDD	91	ASN	3.3
1	KKK	1098	ASP	3.3
1	YYY	1180	ASP	3.3
2	CCC	289	ASN	3.3
1	bbb	1243	LEU	3.3
1	XXX	1187	SER	3.3
1	XXX	1038	TYR	3.3
1	bbb	1110	THR	3.3
2	GGG	91	ASN	3.3
1	XXX	1082	ALA	3.3
1	bbb	1165	PRO	3.3
1	XXX	1135	LEU	3.3
2	HHH	289	ASN	3.3
1	ddd	1141	SER	3.2
1	KKK	1017	PRO	3.2
1	XXX	1042	PRO	3.2
1	XXX	1105	THR	3.2
1	ccc	1125	GLU	3.2
2	EEE	67	PHE	3.2
1	ddd	1211	ARG	3.2
1	ddd	1246	VAL	3.2
1	XXX	1136	VAL	3.2
2	CCC	53	HIS	3.2
1	XXX	1213	GLU	3.1
2	CCC	25	GLU	3.1
1	XXX	1246	VAL	3.1
2	BBB	91	ASN	3.1
1	XXX	1128	LEU	3.1
1	XXX	1160	TRP	3.1
2	BBB	33	VAL	3.1
1	XXX	1216	ALA	3.1
1	ddd	1139	GLY	3.1
1	XXX	1069	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	XXX	1204	TYR	3.1
1	XXX	1170	GLU	3.0
1	XXX	1088	TYR	3.0
1	bbb	1246	VAL	3.0
1	bbb	1078	SER	3.0
1	XXX	1175	ILE	3.0
1	aaa	1138	PRO	3.0
1	XXX	1203	LEU	3.0
1	XXX	1196	ARG	3.0
2	AAA	96	CYS	3.0
2	EEE	91	ASN	3.0
1	WWW	1078	SER	3.0
1	bbb	1043	GLY	3.0
1	XXX	1146	CYS	3.0
1	bbb	1164	ALA	2.9
1	XXX	1058	SER	2.9
1	XXX	1139	GLY	2.9
2	JJJ	289	ASN	2.9
1	XXX	1125	GLU	2.9
1	ccc	1069	TYR	2.9
1	XXX	1108	ARG	2.9
1	ccc	1180	ASP	2.9
2	AAA	93	ASP	2.9
1	ZZZ	1138	PRO	2.9
1	bbb	1134	GLY	2.9
1	bbb	1139	GLY	2.9
1	XXX	1089	TYR	2.9
1	XXX	1219	TYR	2.9
2	HHH	53	HIS	2.8
1	XXX	1242	THR	2.8
1	KKK	1006	VAL	2.8
1	YYY	1113	GLY	2.8
2	BBB	99	ILE	2.8
1	XXX	1131	SER	2.8
1	XXX	1124	GLY	2.8
2	AAA	94	LEU	2.8
1	XXX	1147	ALA	2.8
1	ddd	1072	THR	2.8
1	ddd	1110	THR	2.8
1	bbb	1185	THR	2.8
2	JJJ	208	GLU	2.8
1	XXX	1153	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	XXX	1239	GLY	2.7
1	XXX	1208	ASN	2.7
1	YYY	1028	ASN	2.7
1	ddd	1019	LYS	2.7
1	XXX	1081	GLU	2.7
1	ddd	1016	ALA	2.7
1	XXX	1188	VAL	2.7
1	YYY	1125	GLU	2.7
1	YYY	1139	GLY	2.7
1	ccc	1200	LYS	2.7
1	XXX	1184	TYR	2.7
1	XXX	1161	VAL	2.7
2	HHH	25	GLU	2.7
1	XXX	1167	LYS	2.7
1	XXX	1215	THR	2.7
1	KKK	1246	VAL	2.7
1	XXX	1192	PHE	2.7
1	XXX	1181	THR	2.7
1	ddd	1243	LEU	2.7
2	DDD	289	ASN	2.7
1	XXX	1140	GLY	2.6
1	XXX	1107	THR	2.6
1	bbb	1131	SER	2.6
2	EEE	99	ILE	2.6
2	CCC	130	ASN	2.6
1	eee	1125	GLU	2.6
1	XXX	1202	THR	2.6
1	XXX	1141	SER	2.6
1	XXX	1165	PRO	2.6
2	GGG	67	PHE	2.6
1	WWW	1180	ASP	2.6
1	ZZZ	1125	GLU	2.6
1	ddd	1131	SER	2.6
1	XXX	1067	SER	2.6
1	ccc	1138	PRO	2.6
2	HHH	208	GLU	2.6
1	bbb	1140	GLY	2.6
1	YYY	1124	GLY	2.6
1	XXX	1198	ASN	2.6
2	CCC	34	ASP	2.6
1	bbb	1135	LEU	2.6
1	ddd	1142	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	III	67	PHE	2.5
1	YYY	1211	ARG	2.5
1	bbb	1082	ALA	2.5
1	XXX	1199	SER	2.5
1	WWW	1189	LYS	2.5
2	FFF	99	ILE	2.5
1	XXX	1193	THR	2.5
1	XXX	1218	TYR	2.5
1	KKK	1079	ARG	2.5
1	XXX	1007	LEU	2.5
1	XXX	1172	VAL	2.5
1	bbb	1077	ILE	2.5
2	AAA	289	ASN	2.5
2	JJJ	65	ASP	2.5
1	ddd	1017	PRO	2.5
1	XXX	1010	PRO	2.5
1	bbb	1211	ARG	2.5
1	XXX	1101	TYR	2.5
1	XXX	1143	ARG	2.5
1	YYY	1183	TYR	2.5
1	XXX	1197	ASP	2.5
2	EEE	34	ASP	2.5
1	XXX	1072	THR	2.5
1	bbb	1137	LYS	2.5
1	XXX	1027	GLY	2.5
1	bbb	1015	VAL	2.5
1	bbb	1111	VAL	2.5
1	XXX	1154	GLN	2.5
1	ddd	1011	PRO	2.4
1	YYY	1096	ARG	2.4
1	WWW	1115	THR	2.4
1	KKK	1124	GLY	2.4
1	eee	1124	GLY	2.4
1	XXX	1015	VAL	2.4
1	XXX	1012	SER	2.4
1	KKK	1244	VAL	2.4
1	ccc	1246	VAL	2.4
1	ddd	1015	VAL	2.4
1	ddd	1098	ASP	2.4
1	ddd	1026	GLY	2.4
1	bbb	1021	ALA	2.4
1	XXX	1086	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	DDD	99	ILE	2.4
1	bbb	1144	LEU	2.4
1	bbb	1145	SER	2.4
2	BBB	89	ASN	2.4
1	KKK	1165	PRO	2.4
1	ddd	1018	GLY	2.3
2	FFF	68[A]	GLU	2.3
1	XXX	1013	VAL	2.3
1	KKK	1004	SER	2.3
1	XXX	1195	SER	2.3
1	ccc	1168	GLY	2.3
1	ddd	1140	GLY	2.3
1	ddd	1210	LEU	2.3
2	EEE	33	VAL	2.3
1	XXX	1100	PRO	2.3
1	ZZZ	1043	GLY	2.3
1	eee	1078	SER	2.3
2	GGG	99	ILE	2.3
1	XXX	1020	THR	2.3
1	XXX	1068	ASN	2.3
2	EEE	289	ASN	2.3
1	KKK	1111	VAL	2.3
1	KKK	1187	SER	2.3
1	bbb	1014	SER	2.3
1	XXX	1034	SER	2.3
1	XXX	1087	ASP	2.3
1	XXX	1190	GLY	2.3
1	ZZZ	1110	THR	2.3
1	aaa	1115	THR	2.3
1	ccc	1110	THR	2.3
1	ddd	1208	ASN	2.3
1	KKK	1240	GLN	2.3
1	ccc	1244	VAL	2.3
1	KKK	1018	GLY	2.2
1	XXX	1148	ALA	2.2
1	ZZZ	1245	THR	2.2
1	ddd	1209	SER	2.2
2	EEE	84	ARG	2.2
1	aaa	1098	ASP	2.2
1	ZZZ	1139	GLY	2.2
1	ddd	1042	PRO	2.2
1	ddd	1190	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	WWW	1112	LEU	2.2
1	XXX	1018	GLY	2.2
1	XXX	1185	THR	2.2
2	JJJ	53	HIS	2.2
1	ddd	1022	ARG	2.2
1	XXX	1162	ARG	2.2
1	YYY	1209	SER	2.2
1	XXX	1009	GLN	2.2
1	WWW	1028	ASN	2.2
1	XXX	1023	ILE	2.2
1	bbb	1124	GLY	2.2
1	ccc	1135	LEU	2.2
1	XXX	1214	ASP	2.2
1	KKK	1211	ARG	2.2
1	XXX	1238	TRP	2.2
1	ZZZ	1215	THR	2.2
1	bbb	1069	TYR	2.2
1	ddd	1136	VAL	2.2
1	ZZZ	1078	SER	2.2
1	bbb	1209	SER	2.2
2	FFF	62	SER	2.2
2	HHH	122	SER	2.2
2	III	73	ASN	2.2
1	XXX	1075	LEU	2.2
1	ddd	1070	GLY	2.2
1	XXX	1083	GLY	2.2
2	BBB	34	ASP	2.2
2	CCC	75	ASP	2.2
2	EEE	24	VAL	2.2
1	ZZZ	1044	GLN	2.2
1	YYY	1187	SER	2.2
1	bbb	1128	LEU	2.2
1	YYY	1210	LEU	2.2
2	BBB	53	HIS	2.2
1	YYY	1244	VAL	2.1
1	XXX	1014	SER	2.1
2	GGG	208	GLU	2.1
2	AAA	34	ASP	2.1
1	bbb	1244	VAL	2.1
2	FFF	53	HIS	2.1
1	ddd	1245	THR	2.1
1	XXX	1005	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	KKK	1209	SER	2.1
1	bbb	1017	PRO	2.1
1	ddd	1071	ASN	2.1
1	XXX	1159	ASN	2.1
1	ddd	1186	ASP	2.1
1	eee	1246	VAL	2.1
1	ddd	1023	ILE	2.1
2	JJJ	99	ILE	2.1
1	XXX	1085	GLU	2.1
2	EEE	208	GLU	2.1
1	ddd	1051	SER	2.1
1	ddd	1078	SER	2.1
1	XXX	1129	VAL	2.1
1	YYY	1189	LYS	2.1
1	ZZZ	1096	ARG	2.1
1	WWW	1125	GLU	2.1
1	ddd	1013	VAL	2.1
1	bbb	1167	LYS	2.1
1	ZZZ	1079	ARG	2.1
1	ddd	1168	GLY	2.1
1	bbb	1011	PRO	2.1
1	ZZZ	1111	VAL	2.0
1	ddd	1217	VAL	2.0
1	KKK	1095	SER	2.0
1	WWW	1004	SER	2.0
1	YYY	1135	LEU	2.0
1	bbb	1141	SER	2.0
1	XXX	1071	ASN	2.0
2	III	53	HIS	2.0
1	bbb	1212	ALA	2.0
1	bbb	1245	THR	2.0
1	XXX	1164	ALA	2.0
1	XXX	1182	THR	2.0
2	DDD	67	PHE	2.0
2	GGG	218	GLY	2.0
1	XXX	1019	LYS	2.0

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 oligosaccharides 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.