



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 7PA6 / pdb_00007pa6
Title : JC polyomavirus VP1 in complex with scFv 27C11
Authors : Harprecht, C.; Stroeh, L.J.; Nagel, F.; Freytag, J.; Stehle, T.
Deposited on : 2021-07-29
Resolution : 1.90 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

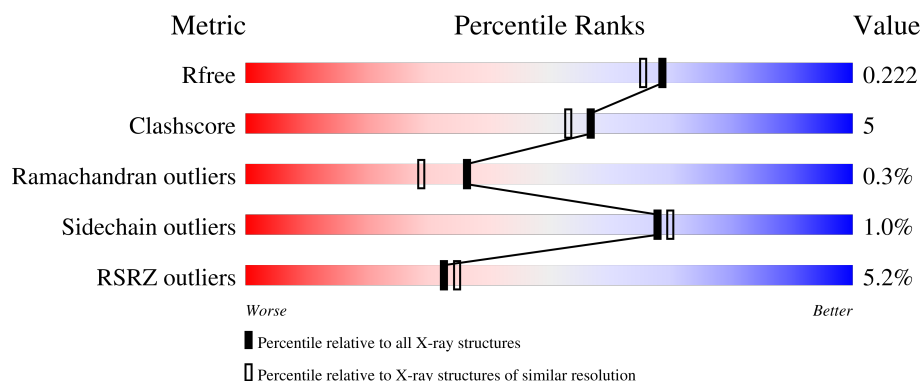
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	253	3% 82% 12% 6%
1	LLL	253	4% 83% 11% 6%
1	MMM	253	15% 73% 18% 9%
1	NNN	253	5% 81% 11% 9%
1	OOO	253	10% 81% 12% 7%

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Mol	Chain	Length	Quality of chain
1	PPP	253	
1	QQQ	253	
1	RRR	253	
1	SSS	253	
1	TTT	253	
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 40319 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 27C11 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	KKK	238	Total	C	N	O	S	0	0	0
			1805	1142	302	354	7			
1	LLL	238	Total	C	N	O	S	0	0	0
			1795	1136	300	352	7			
1	MMM	230	Total	C	N	O	S	0	0	0
			1690	1064	285	334	7			
1	NNN	231	Total	C	N	O	S	0	1	0
			1753	1105	297	344	7			
1	OOO	235	Total	C	N	O	S	0	1	0
			1772	1124	298	343	7			
1	PPP	231	Total	C	N	O	S	0	1	0
			1710	1074	287	343	6			
1	QQQ	232	Total	C	N	O	S	0	1	0
			1758	1109	297	346	6			
1	RRR	236	Total	C	N	O	S	0	0	0
			1774	1119	299	349	7			
1	SSS	237	Total	C	N	O	S	0	0	0
			1786	1129	296	354	7			
1	TTT	238	Total	C	N	O	S	0	0	0
			1775	1121	299	348	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AAA	268	Total	C	N	O	S	0	2	0
			2071	1302	356	401	12			
2	BBB	261	Total	C	N	O	S	0	1	0
			2030	1279	350	390	11			
2	CCC	264	Total	C	N	O	S	0	4	0
			2067	1304	357	394	12			
2	DDD	262	Total	C	N	O	S	0	2	0
			2032	1282	350	389	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	EEE	261	Total	C	N	O	S	0	3	0
			2049	1290	354	394	11			
2	FFF	260	Total	C	N	O	S	0	4	0
			2026	1277	347	391	11			
2	GGG	261	Total	C	N	O	S	0	3	0
			2046	1291	352	392	11			
2	HHH	262	Total	C	N	O	S	0	5	0
			2058	1301	354	392	11			
2	III	263	Total	C	N	O	S	0	1	0
			2027	1275	350	391	11			
2	JJJ	264	Total	C	N	O	S	0	2	0
			2046	1288	355	391	12			

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	KKK	112	Total O 112 112	0	0
3	LLL	90	Total O 90 90	0	0
3	MMM	33	Total O 33 33	0	0
3	NNN	85	Total O 85 85	0	0
3	OOO	83	Total O 83 83	0	0
3	PPP	37	Total O 37 37	0	0
3	QQQ	66	Total O 66 66	0	0
3	RRR	106	Total O 106 106	0	0
3	SSS	121	Total O 121 121	0	0
3	TTT	105	Total O 105 105	0	0
3	AAA	144	Total O 144 144	0	0
3	BBB	134	Total O 134 134	0	0
3	CCC	136	Total O 136 136	0	0

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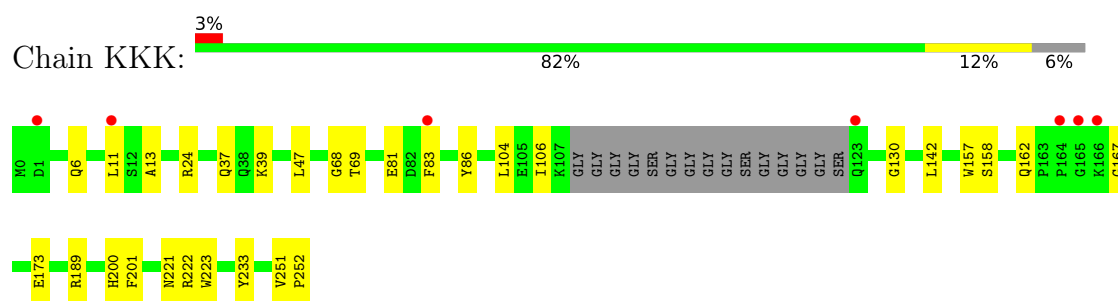
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DDD	142	Total 142	O 142	0	0
3	EEE	145	Total 145	O 145	0	0
3	FFF	138	Total 138	O 138	0	0
3	GGG	140	Total 140	O 140	0	0
3	HHH	143	Total 143	O 143	0	0
3	III	150	Total 150	O 150	0	0
3	JJJ	139	Total 139	O 139	0	0

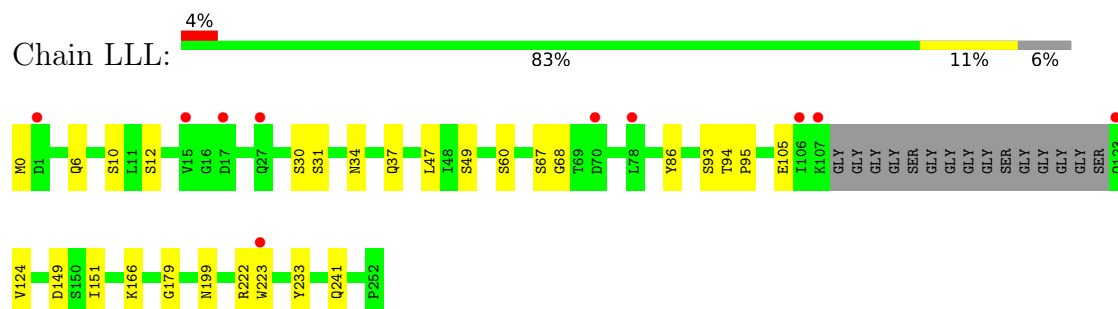
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

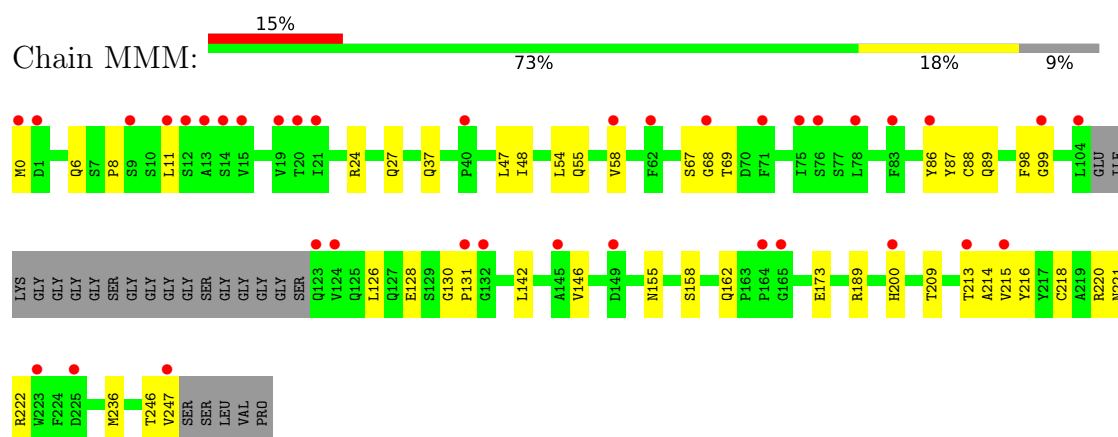
- Molecule 1: scFv 27C11 antibody heavy chain



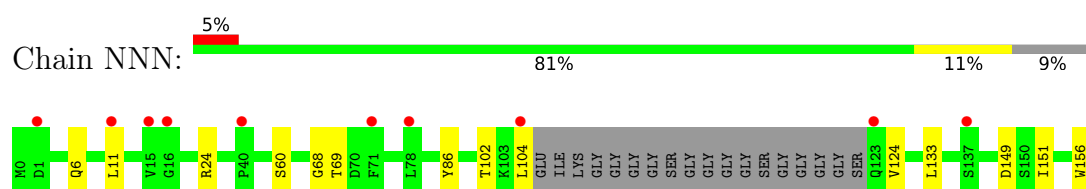
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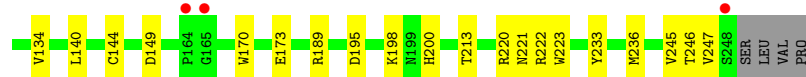
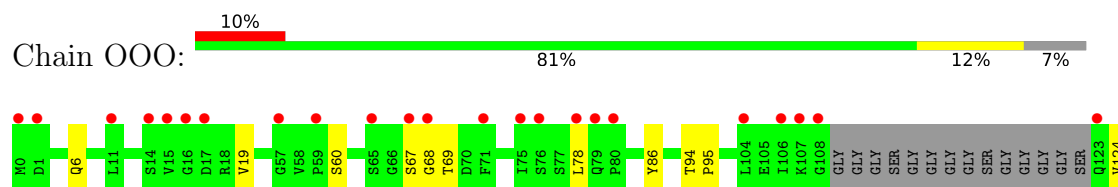
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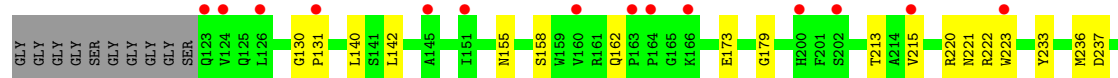
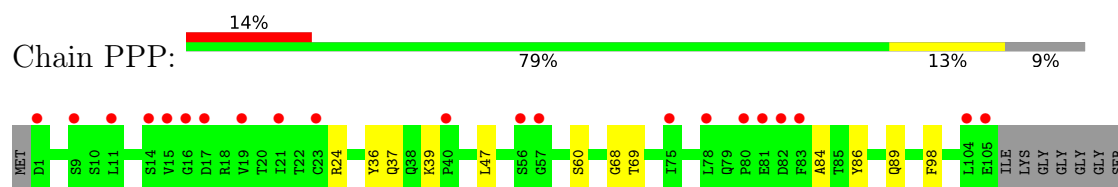
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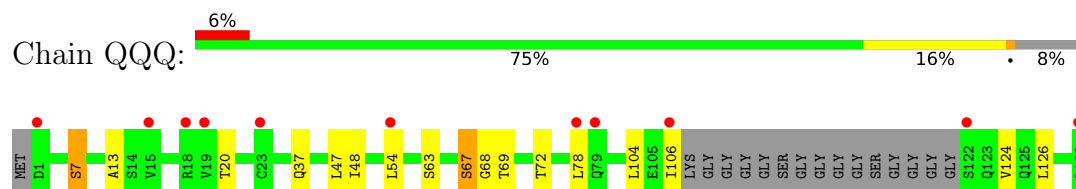
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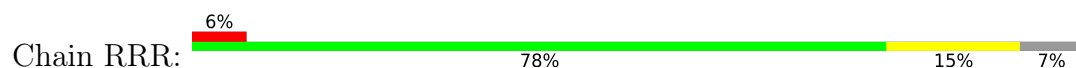
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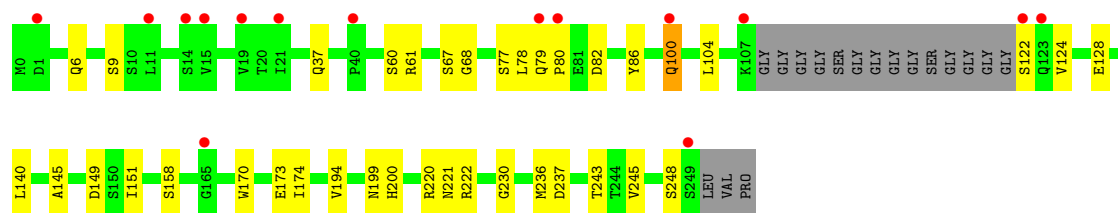


- Molecule 1: scFv 27C11 antibody heavy chain

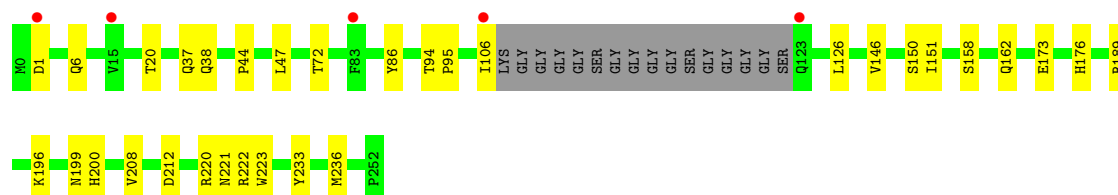
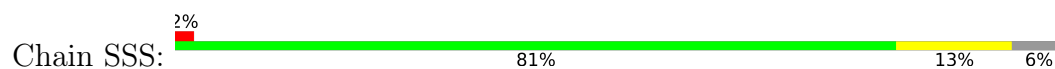


- Molecule 1: scFv 27C11 antibody heavy chain

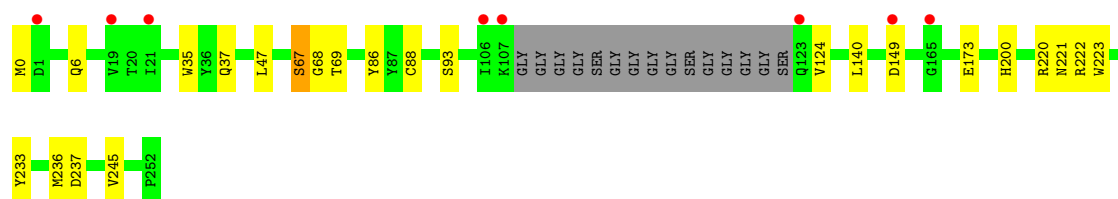
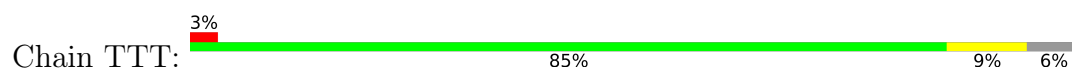




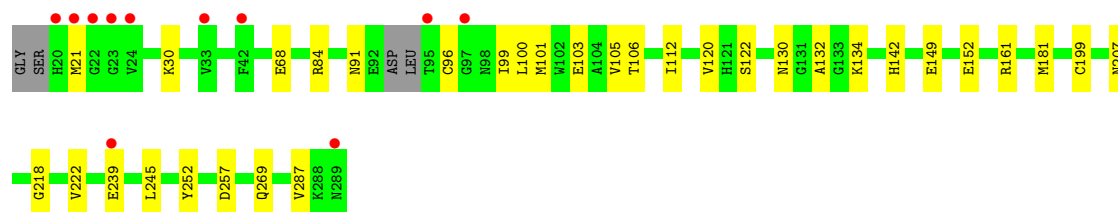
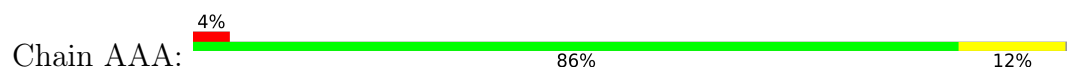
• Molecule 1: scFv 27C11 antibody heavy chain



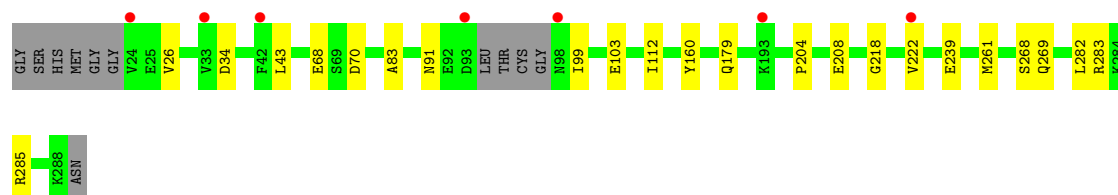
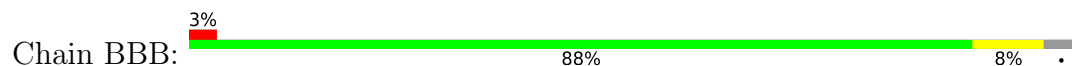
• Molecule 1: scFv 27C11 antibody heavy chain



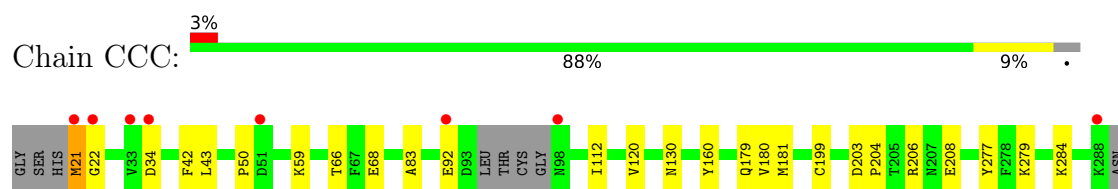
• Molecule 2: Major capsid protein VP1



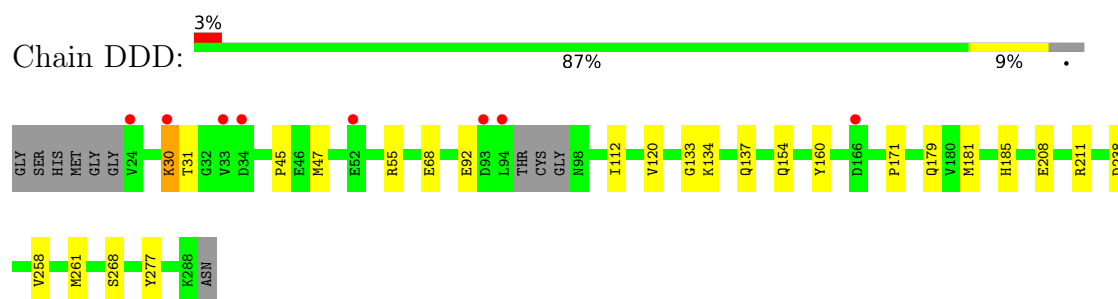
• Molecule 2: Major capsid protein VP1



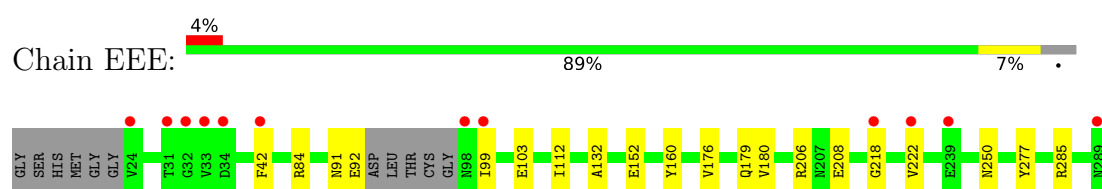
- Molecule 2: Major capsid protein VP1



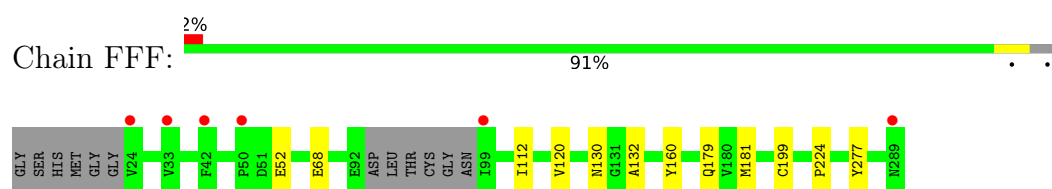
- Molecule 2: Major capsid protein VP1



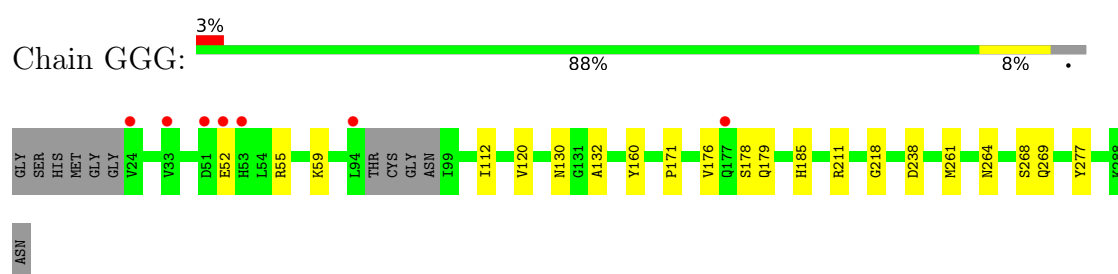
- Molecule 2: Major capsid protein VP1



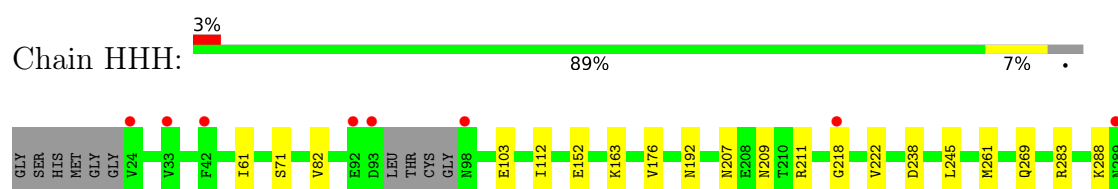
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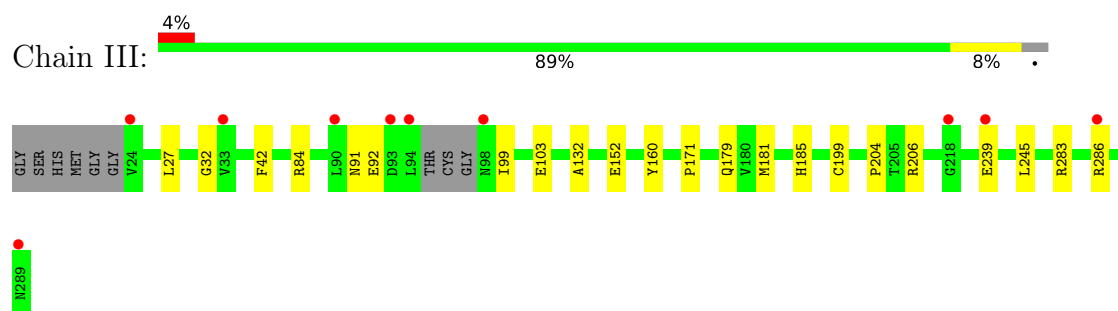
- Molecule 2: Major capsid protein VP1



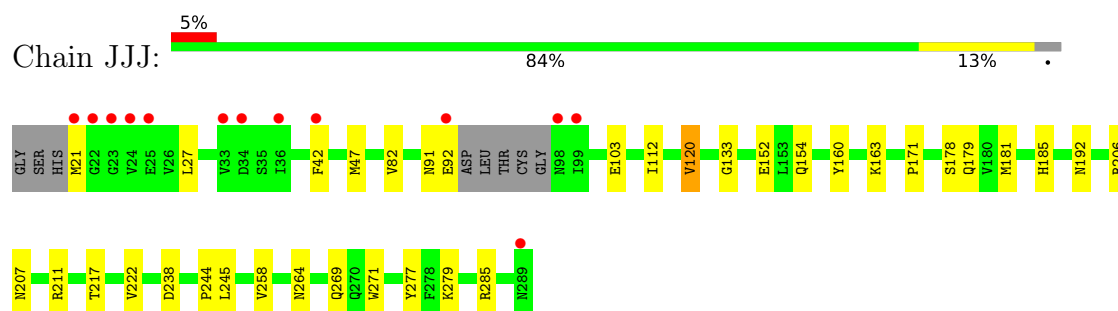
- Molecule 2: Major capsid protein VP1



- Molecule 2: Major capsid protein VP1



- Molecule 2: Major capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.09Å 96.11Å 190.41Å 100.91° 93.01° 113.83°	Depositor
Resolution (Å)	47.81 – 1.90 47.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.81-1.90) 97.6 (47.81-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.216 (Not available) , 0.222	Depositor DCC
R_{free} test set	23290 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.5	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	0.96	EDS
Total number of atoms	40319	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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	0.81	0/1851	0.72	0/2518
1	LLL	0.80	0/1840	0.71	0/2504
1	MMM	0.80	0/1733	0.67	0/2368
1	NNN	0.78	0/1801	0.71	0/2454
1	OOO	0.77	0/1821	0.69	0/2479
1	PPP	0.80	0/1753	0.69	0/2395
1	QQQ	0.79	0/1806	0.73	1/2461 (0.0%)
1	RRR	0.80	0/1819	0.75	0/2478
1	SSS	0.81	0/1832	0.73	0/2496
1	TTT	0.80	0/1820	0.70	0/2481
2	AAA	0.82	0/2122	0.83	1/2881 (0.0%)
2	BBB	0.83	0/2078	0.80	1/2824 (0.0%)
2	CCC	0.81	0/2126	0.78	1/2886 (0.0%)
2	DDD	0.84	0/2083	0.85	1/2832 (0.0%)
2	EEE	0.83	0/2104	0.84	0/2859
2	FFF	0.82	0/2084	0.79	0/2835
2	GGG	0.82	0/2101	0.81	0/2855
2	HHH	0.84	0/2120	0.84	0/2881
2	III	0.81	0/2075	0.86	1/2821 (0.0%)
2	JJJ	0.82	0/2098	0.84	1/2849 (0.0%)
All	All	0.81	0/39067	0.77	7/53157 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	III	32	GLY	CA-C-O	-6.01	117.98	122.37
2	JJJ	120	VAL	N-CA-CB	-5.64	104.83	112.22
2	CCC	199	CYS	CB-CA-C	-5.28	100.46	109.65
2	BBB	239	GLU	CB-CA-C	-5.27	102.38	110.81
1	QQQ	7	SER	CA-C-O	-5.25	113.87	119.22
2	AAA	96	CYS	CA-C-O	-5.14	115.26	121.32
2	DDD	30	LYS	N-CA-CB	-5.04	102.46	110.06

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	1805	0	1720	15	0
1	LLL	1795	0	1704	14	0
1	MMM	1690	0	1530	28	0
1	NNN	1753	0	1648	15	0
1	OOO	1772	0	1672	17	0
1	PPP	1710	0	1545	20	0
1	QQQ	1758	0	1654	29	0
1	RRR	1774	0	1661	22	0
1	SSS	1786	0	1677	21	0
1	TTT	1775	0	1653	11	0
2	AAA	2071	0	1999	24	0
2	BBB	2030	0	1978	18	0
2	CCC	2067	0	2007	18	0
2	DDD	2032	0	1973	19	0
2	EEE	2049	0	1995	16	0
2	FFF	2026	0	1949	12	0
2	GGG	2046	0	2000	20	0
2	HHH	2058	0	2006	14	0
2	III	2027	0	1948	16	0
2	JJJ	2046	0	1978	32	0
3	AAA	144	0	0	2	0
3	BBB	134	0	0	0	0
3	CCC	136	0	0	0	0
3	DDD	142	0	0	0	0
3	EEE	145	0	0	0	0
3	FFF	138	0	0	0	0
3	GGG	140	0	0	1	0
3	HHH	143	0	0	1	0
3	III	150	0	0	0	0
3	JJJ	139	0	0	2	0
3	KKK	112	0	0	0	0
3	LLL	90	0	0	0	0
3	MMM	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	NNN	85	0	0	0	0
3	OOO	83	0	0	0	0
3	PPP	37	0	0	0	0
3	QQQ	66	0	0	0	0
3	RRR	106	0	0	0	0
3	SSS	121	0	0	0	0
3	TTT	105	0	0	0	0
All	All	40319	0	36297	341	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 5.

All (341) 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:CCC:160:TYR:H	2:CCC:179:GLN:HE21	1.11	0.98
2:DDD:160:TYR:H	2:DDD:179:GLN:HE21	1.10	0.97
2:BBB:160:TYR:H	2:BBB:179:GLN:HE21	1.13	0.96
2:III:160:TYR:H	2:III:179:GLN:HE21	1.14	0.95
2:GGG:160:TYR:H	2:GGG:179:GLN:HE21	1.17	0.92
2:FFF:160:TYR:H	2:FFF:179:GLN:HE21	1.15	0.92
2:EEE:160:TYR:H	2:EEE:179:GLN:HE21	1.19	0.91
2:AAA:132:ALA:H	2:BBB:269:GLN:HE21	1.20	0.88
2:GGG:132:ALA:H	2:HHH:269:GLN:HE21	1.20	0.87
2:III:132:ALA:H	2:JJJ:269:GLN:HE21	1.21	0.86
2:HHH:209:ASN:HD21	2:HHH:245:LEU:H	1.21	0.86
1:QQQ:213:THR:HG22	1:QQQ:247:VAL:H	1.41	0.86
2:FFF:132:ALA:H	2:GGG:269:GLN:HE21	1.24	0.86
1:PPP:213:THR:HG22	1:PPP:247:VAL:H	1.44	0.82
2:HHH:152:GLU:H	2:HHH:207:ASN:HD21	1.27	0.82
2:HHH:112:ILE:HG21	2:III:181:MET:HE1	1.62	0.81
2:AAA:269:GLN:HE21	2:EEE:132:ALA:H	1.26	0.81
2:JJJ:152:GLU:H	2:JJJ:207:ASN:HD21	1.29	0.80
2:AAA:152:GLU:H	2:AAA:207:ASN:HD21	1.28	0.78
1:OOO:213:THR:HG22	1:OOO:247:VAL:H	1.48	0.78
1:MMM:213:THR:HG23	1:MMM:247:VAL:HG12	1.63	0.78
1:RRR:151:ILE:H	1:RRR:199:ASN:HD21	1.32	0.77
1:SSS:38:GLN:HE22	1:SSS:162:GLN:HE22	1.33	0.76
1:MMM:128:GLU:HG2	1:MMM:218:CYS:SG	2.27	0.75
1:LLL:60:SER:OG	1:MMM:189:ARG:HD3	1.86	0.74
1:RRR:60:SER:HB2	1:SSS:189:ARG:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JJJ:112:ILE:HD11	2:JJJ:277:TYR:HB2	1.70	0.74
1:KKK:39:LYS:NZ	1:KKK:81:GLU:O	2.20	0.72
2:JJJ:47:MET:CE	2:JJJ:271:TRP:HB3	2.19	0.72
1:MMM:6:GLN:HE22	1:MMM:87:TYR:HA	1.54	0.71
1:TTT:173:GLU:OE2	1:TTT:221:ASN:ND2	2.20	0.71
1:OOO:67:SER:O	1:OOO:69:THR:N	2.23	0.70
2:III:103:GLU:OE2	2:III:283:ARG:NE	2.23	0.69
1:KKK:173:GLU:OE2	1:KKK:221:ASN:ND2	2.24	0.69
2:JJJ:47:MET:HE1	2:JJJ:258:VAL:HG22	1.73	0.69
2:CCC:34:ASP:O	2:CCC:284:LYS:NZ	2.26	0.68
1:NNN:60:SER:HB2	1:OOO:189:ARG:HD3	1.75	0.68
1:QQQ:151:ILE:H	1:QQQ:199:ASN:HD21	1.40	0.67
2:AAA:134:LYS:NZ	3:AAA:301:HOH:O	2.24	0.67
1:RRR:140:LEU:HD13	1:RRR:245:VAL:HG11	1.76	0.66
1:LLL:151:ILE:H	1:LLL:199:ASN:HD21	1.44	0.66
1:PPP:39:LYS:HD3	1:PPP:84:ALA:HB2	1.79	0.65
1:PPP:24:ARG:HH21	1:PPP:24:ARG:HB3	1.63	0.64
2:EEE:91:ASN:O	2:EEE:92:GLU:HG3	1.97	0.64
1:QQQ:78:LEU:HD11	1:QQQ:104:LEU:HD21	1.80	0.63
2:AAA:101:MET:HE2	2:AAA:287:VAL:HG21	1.80	0.63
1:LLL:179:GLY:HA3	2:BBB:68:GLU:OE2	1.99	0.63
2:JJJ:178:SER:OG	2:JJJ:185:HIS:HE1	1.82	0.62
2:CCC:112:ILE:HD11	2:CCC:277:TYR:HB2	1.80	0.62
2:III:27:LEU:HG	2:III:286:ARG:NH2	2.14	0.62
2:GGG:178:SER:OG	2:GGG:185:HIS:HE1	1.83	0.62
1:MMM:213:THR:HG22	1:MMM:246:THR:HA	1.82	0.61
1:OOO:213:THR:CG2	1:OOO:247:VAL:H	2.13	0.61
2:EEE:208:GLU:H	2:EEE:208:GLU:CD	2.07	0.61
1:PPP:140:LEU:HD13	1:PPP:245:VAL:HG11	1.81	0.61
1:KKK:11:LEU:HD23	1:KKK:104:LEU:HD13	1.83	0.60
2:JJJ:47:MET:HE2	2:JJJ:271:TRP:HB3	1.83	0.60
1:NNN:163:PRO:HG2	1:NNN:166:LYS:HB2	1.83	0.60
1:KKK:6:GLN:NE2	1:KKK:86:TYR:O	2.32	0.59
1:SSS:6:GLN:NE2	1:SSS:86:TYR:O	2.35	0.59
1:RRR:222:ARG:HD3	1:RRR:237:ASP:OD2	2.02	0.59
1:SSS:151:ILE:H	1:SSS:199:ASN:HD21	1.50	0.59
1:LLL:124:VAL:HG22	1:LLL:149:ASP:HB2	1.84	0.59
1:NNN:151:ILE:H	1:NNN:199:ASN:HD21	1.50	0.59
1:SSS:173:GLU:OE2	1:SSS:221:ASN:ND2	2.32	0.59
2:AAA:142:HIS:HD2	2:AAA:257:ASP:OD1	1.86	0.58
2:CCC:208:GLU:CD	2:CCC:208:GLU:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AAA:181:MET:HE1	2:EEE:112:ILE:HG21	1.86	0.58
2:JJJ:277:TYR:OH	2:JJJ:279:LYS:HE3	2.03	0.58
1:RRR:6:GLN:NE2	1:RRR:86:TYR:O	2.35	0.58
1:OOO:170:TRP:HZ2	1:OOO:173:GLU:HG3	1.69	0.58
1:QQQ:67:SER:O	1:QQQ:69:THR:N	2.36	0.58
2:III:27:LEU:HG	2:III:286:ARG:HH21	1.67	0.58
1:QQQ:173:GLU:OE2	1:QQQ:221:ASN:ND2	2.26	0.58
2:JJJ:154:GLN:CD	2:JJJ:181:MET:HE1	2.28	0.58
1:MMM:213:THR:HG22	1:MMM:247:VAL:H	1.69	0.58
1:RRR:79:GLN:HG2	1:RRR:80:PRO:HD2	1.86	0.57
1:QQQ:151:ILE:H	1:QQQ:199:ASN:ND2	2.01	0.57
1:TTT:37:GLN:HB3	1:TTT:47:LEU:HD11	1.86	0.57
1:QQQ:213:THR:CG2	1:QQQ:247:VAL:H	2.13	0.57
1:RRR:173:GLU:OE2	1:RRR:221:ASN:ND2	2.24	0.57
1:PPP:179:GLY:HA3	2:FFF:68[A]:GLU:OE1	2.05	0.56
1:RRR:151:ILE:H	1:RRR:199:ASN:ND2	2.00	0.56
1:TTT:222:ARG:HD3	1:TTT:237:ASP:OD2	2.05	0.56
1:LLL:37:GLN:HB2	1:LLL:47:LEU:HD11	1.88	0.56
1:SSS:37:GLN:HB2	1:SSS:47:LEU:HD11	1.88	0.56
2:DDD:208:GLU:CD	2:DDD:208:GLU:H	2.13	0.56
2:HHH:61:ILE:HG13	2:HHH:261:MET:HE2	1.87	0.56
2:CCC:160:TYR:N	2:CCC:179:GLN:HE21	1.93	0.56
1:QQQ:37:GLN:HB3	1:QQQ:47:LEU:HD11	1.87	0.55
2:FFF:181:MET:HE1	2:JJJ:112:ILE:HG21	1.89	0.55
1:MMM:209:THR:O	1:MMM:247:VAL:HG11	2.06	0.55
1:SSS:151:ILE:H	1:SSS:199:ASN:ND2	2.05	0.55
2:CCC:277:TYR:OH	2:CCC:279:LYS:HE3	2.07	0.55
2:III:239:GLU:H	2:III:239:GLU:CD	2.15	0.55
2:EEE:84:ARG:NH1	2:EEE:250:ASN:OD1	2.41	0.54
1:SSS:38:GLN:HB2	1:SSS:44:PRO:HA	1.90	0.54
1:QQQ:140:LEU:HD13	1:QQQ:245:VAL:HG11	1.88	0.54
2:AAA:101:MET:HE2	2:AAA:287:VAL:HG11	1.89	0.54
2:CCC:42[B]:PHE:HD2	2:CCC:112:ILE:HD13	1.73	0.54
2:AAA:122:SER:HB3	2:BBB:70:ASP:OD2	2.08	0.54
2:FFF:120:VAL:HG21	2:GGG:261:MET:HE1	1.88	0.54
1:RRR:61:ARG:NH1	1:RRR:82:ASP:OD2	2.40	0.54
2:DDD:134:LYS:HE2	2:DDD:137:GLN:HE21	1.73	0.54
2:HHH:209:ASN:ND2	2:HHH:245:LEU:H	1.99	0.53
2:GGG:112:ILE:HD11	2:GGG:277:TYR:HB2	1.89	0.53
2:JJJ:160:TYR:HD1	2:JJJ:179:GLN:OE1	1.91	0.53
2:CCC:43:LEU:HD21	2:CCC:83:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AAA:239:GLU:CD	2:AAA:239:GLU:H	2.17	0.53
2:HHH:103:GLU:OE2	2:HHH:283:ARG:NE	2.38	0.53
1:OOO:6:GLN:NE2	1:OOO:86:TYR:O	2.42	0.52
2:JJJ:120:VAL:HG22	2:JJJ:133:GLY:O	2.09	0.52
1:NNN:6:GLN:NE2	1:NNN:86:TYR:O	2.34	0.52
1:QQQ:48:ILE:HG12	1:QQQ:54:LEU:HD23	1.91	0.52
2:AAA:218:GLY:O	2:AAA:222:VAL:HG11	2.10	0.52
1:MMM:6:GLN:NE2	1:MMM:88:CYS:H	2.08	0.52
2:AAA:91:ASN:ND2	2:AAA:99:ILE:HG12	2.24	0.52
2:EEE:160:TYR:N	2:EEE:179:GLN:HE21	1.99	0.51
1:MMM:220:ARG:O	1:MMM:236:MET:HA	2.11	0.51
2:BBB:208:GLU:H	2:BBB:208:GLU:CD	2.16	0.51
2:HHH:82:VAL:O	2:HHH:192[B]:ASN:ND2	2.41	0.51
2:AAA:132:ALA:N	2:BBB:269:GLN:HE21	2.00	0.51
2:DDD:55:ARG:HB3	2:EEE:176:VAL:HG22	1.91	0.51
2:III:132:ALA:N	2:JJJ:269:GLN:HE21	1.98	0.51
1:OOO:140:LEU:HD13	1:OOO:245:VAL:HG11	1.93	0.51
1:NNN:179:GLY:HA3	2:DDD:68:GLU:OE1	2.11	0.51
1:QQQ:227:ASN:OD1	2:GGG:59:LYS:NZ	2.44	0.50
2:III:160:TYR:N	2:III:179:GLN:HE21	1.96	0.50
1:PPP:37:GLN:HG3	1:PPP:86:TYR:CE2	2.46	0.50
2:JJJ:154:GLN:OE1	2:JJJ:181:MET:HE1	2.11	0.50
2:JJJ:82:VAL:O	2:JJJ:192:ASN:ND2	2.45	0.50
2:CCC:42[B]:PHE:HD2	2:CCC:112:ILE:CD1	2.24	0.50
1:NNN:124:VAL:HG22	1:NNN:149:ASP:HB2	1.93	0.50
1:MMM:213:THR:CG2	1:MMM:247:VAL:HG12	2.37	0.50
1:LLL:34:ASN:HD22	1:LLL:49:SER:HA	1.77	0.49
1:NNN:151:ILE:H	1:NNN:199:ASN:ND2	2.09	0.49
2:CCC:120:VAL:HG21	2:DDD:261:MET:HE1	1.92	0.49
1:LLL:30:SER:OG	1:LLL:31:SER:N	2.45	0.49
2:DDD:120:VAL:HG23	2:DDD:133:GLY:O	2.13	0.49
2:AAA:68[A]:GLU:HG3	2:AAA:161:ARG:HD2	1.93	0.49
2:AAA:103:GLU:HB3	2:AAA:245:LEU:HD23	1.93	0.49
1:LLL:12:SER:HA	1:LLL:105:GLU:O	2.13	0.49
2:EEE:103:GLU:OE1	2:EEE:285:ARG:HD3	2.13	0.49
1:KKK:37:GLN:HB2	1:KKK:47:LEU:HD11	1.95	0.49
2:GGG:160:TYR:N	2:GGG:179:GLN:HE21	1.98	0.49
2:DDD:112:ILE:HD11	2:DDD:277:TYR:HB2	1.95	0.49
1:MMM:8:PRO:HG3	1:MMM:11:LEU:HD13	1.95	0.48
1:LLL:151:ILE:H	1:LLL:199:ASN:ND2	2.09	0.48
1:PPP:222:ARG:HD3	1:PPP:237:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RRR:220:ARG:O	1:RRR:236:MET:HA	2.14	0.48
1:QQQ:213:THR:HG22	1:QQQ:247:VAL:N	2.18	0.48
2:DDD:120:VAL:CG2	2:DDD:133:GLY:O	2.62	0.48
2:JJJ:211:ARG:NH2	2:JJJ:238:ASP:HB3	2.28	0.48
2:JJJ:264:ASN:HB2	3:JJJ:337:HOH:O	2.13	0.48
1:RRR:124:VAL:HG22	1:RRR:149:ASP:HB2	1.95	0.48
2:HHH:163:LYS:NZ	3:HHH:302:HOH:O	2.45	0.48
1:MMM:130:GLY:HA3	1:MMM:142:LEU:HD23	1.96	0.48
1:PPP:89:GLN:HB2	1:PPP:98:PHE:CD2	2.49	0.48
2:BBB:34:ASP:OD1	2:BBB:34:ASP:N	2.37	0.48
2:CCC:50:PRO:HB3	2:CCC:59:LYS:HB2	1.95	0.48
1:SSS:38:GLN:NE2	1:SSS:162:GLN:HE22	2.08	0.47
1:SSS:20:THR:HG23	1:SSS:72:THR:HG23	1.95	0.47
2:DDD:160:TYR:N	2:DDD:179:GLN:HE21	1.94	0.47
1:RRR:174:ILE:HD13	1:RRR:194:VAL:HG13	1.97	0.47
2:FFF:132:ALA:H	2:GGG:269:GLN:NE2	2.04	0.47
1:MMM:6:GLN:HE21	1:MMM:99:GLY:HA3	1.79	0.47
1:SSS:150:SER:HA	1:SSS:199:ASN:HD21	1.79	0.47
1:OOO:19:VAL:HG21	1:OOO:78:LEU:HD22	1.97	0.47
2:III:91:ASN:ND2	2:III:99:ILE:HB	2.30	0.47
1:PPP:24:ARG:HB3	1:PPP:24:ARG:NH2	2.27	0.47
2:EEE:218:GLY:O	2:EEE:222:VAL:HG11	2.15	0.47
2:JJJ:171:PRO:HB3	2:JJJ:185:HIS:CG	2.50	0.47
1:PPP:24:ARG:HA	1:PPP:69:THR:O	2.15	0.47
1:RRR:61:ARG:HH12	1:RRR:82:ASP:CG	2.22	0.47
1:RRR:78:LEU:HD11	1:RRR:104:LEU:HD21	1.96	0.47
1:SSS:158:SER:OG	1:SSS:173:GLU:HG2	2.15	0.47
2:JJJ:152:GLU:H	2:JJJ:207:ASN:ND2	2.06	0.47
2:CCC:21:MET:HG3	2:CCC:22:GLY:N	2.29	0.47
1:MMM:158:SER:OG	1:MMM:173:GLU:HG2	2.14	0.46
1:QQQ:185:SER:OG	1:QQQ:186:LEU:HG	2.16	0.46
1:QQQ:186:LEU:O	1:QQQ:190:VAL:HG23	2.15	0.46
2:GGG:211:ARG:NH2	2:GGG:238:ASP:HB3	2.29	0.46
1:OOO:213:THR:HG22	1:OOO:246:THR:HA	1.96	0.46
1:QQQ:222:ARG:HD3	1:QQQ:237:ASP:OD2	2.16	0.46
1:NNN:220:ARG:O	1:NNN:236:MET:HA	2.15	0.46
2:HHH:211:ARG:NH2	2:HHH:238:ASP:HB3	2.31	0.46
2:III:103:GLU:HB3	2:III:245:LEU:HD23	1.96	0.46
2:JJJ:217:THR:CG2	2:JJJ:222:VAL:HG21	2.45	0.46
1:OOO:94:THR:HA	1:OOO:95:PRO:C	2.41	0.46
1:PPP:155:ASN:ND2	1:PPP:220:ARG:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FFF:112:ILE:HD11	2:FFF:277:TYR:HB2	1.96	0.46
1:KKK:158:SER:OG	1:KKK:173:GLU:HG2	2.16	0.46
1:MMM:37:GLN:HG3	1:MMM:86:TYR:CZ	2.51	0.46
2:EEE:42:PHE:CD1	2:EEE:112:ILE:HD13	2.50	0.46
2:GGG:55:ARG:HB3	2:HHH:176:VAL:HG22	1.98	0.46
1:QQQ:20:THR:HG23	1:QQQ:72:THR:HG23	1.97	0.46
1:QQQ:126:LEU:HD22	1:QQQ:146:VAL:HG22	1.96	0.46
1:TTT:124:VAL:HG22	1:TTT:149:ASP:HB2	1.98	0.46
2:FFF:224:PRO:HD2	2:GGG:218:GLY:HA3	1.97	0.46
2:JJJ:163:LYS:NZ	3:JJJ:303:HOH:O	2.48	0.46
1:PPP:173:GLU:OE2	1:PPP:221:ASN:ND2	2.37	0.46
2:III:84:ARG:HH11	2:III:84:ARG:HG2	1.81	0.45
1:LLL:0:MET:HE3	1:LLL:93:SER:HB2	1.97	0.45
1:QQQ:158:SER:OG	1:QQQ:173:GLU:HG2	2.15	0.45
2:DDD:211:ARG:NH2	2:DDD:238:ASP:HB3	2.31	0.45
2:JJJ:91:ASN:O	2:JJJ:92:GLU:C	2.59	0.45
2:JJJ:120:VAL:CG2	2:JJJ:133:GLY:O	2.64	0.45
1:QQQ:190:VAL:HG22	1:QQQ:205:LEU:HD23	1.98	0.45
1:QQQ:220:ARG:O	1:QQQ:236:MET:HA	2.15	0.45
1:PPP:158:SER:OG	1:PPP:173:GLU:HG2	2.16	0.45
2:JJJ:103:GLU:OE2	2:JJJ:285:ARG:HD3	2.16	0.45
1:NNN:186:LEU:O	1:NNN:190:VAL:HG12	2.17	0.45
1:OOO:170:TRP:CZ2	1:OOO:173:GLU:HG3	2.49	0.45
2:BBB:26:VAL:HG13	2:BBB:285:ARG:HD3	1.99	0.45
1:PPP:223:TRP:HA	1:PPP:233:TYR:O	2.17	0.45
1:TTT:6:GLN:NE2	1:TTT:86:TYR:O	2.40	0.45
2:JJJ:42:PHE:HD1	2:JJJ:112:ILE:CD1	2.30	0.45
2:GGG:264:ASN:HB2	3:GGG:353:HOH:O	2.16	0.45
2:III:42:PHE:CE2	2:JJJ:181:MET:HE2	2.52	0.45
1:PPP:162:GLN:HB3	1:PPP:215:VAL:HG13	1.99	0.44
1:RRR:60:SER:CB	1:SSS:189:ARG:HG2	2.44	0.44
1:OOO:134:VAL:O	1:OOO:247:VAL:HA	2.17	0.44
1:RRR:158:SER:OG	1:RRR:221:ASN:HB2	2.17	0.44
1:NNN:133:LEU:HD23	1:NNN:246:THR:O	2.17	0.44
1:OOO:223:TRP:HA	1:OOO:233:TYR:O	2.17	0.44
2:BBB:43:LEU:HD21	2:BBB:83:ALA:HB2	1.99	0.44
1:MMM:126:LEU:HD22	1:MMM:146:VAL:HG22	2.00	0.44
2:JJJ:103:GLU:CB	2:JJJ:245:LEU:HD23	2.48	0.44
1:OOO:220:ARG:O	1:OOO:236:MET:HA	2.18	0.44
1:SSS:223:TRP:HA	1:SSS:233:TYR:O	2.17	0.44
1:SSS:94:THR:HA	1:SSS:95:PRO:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SSS:126:LEU:HD22	1:SSS:146:VAL:HG22	2.00	0.44
2:AAA:84:ARG:HD3	2:AAA:252:TYR:CZ	2.53	0.44
2:FFF:160:TYR:N	2:FFF:179:GLN:HE21	1.98	0.44
2:AAA:149:GLU:HG3	3:AAA:384:HOH:O	2.17	0.44
1:LLL:34:ASN:ND2	1:LLL:49:SER:HA	2.33	0.43
1:PPP:36:TYR:HE2	1:PPP:236:MET:O	2.01	0.43
2:AAA:101:MET:CE	2:AAA:287:VAL:HG11	2.48	0.43
1:MMM:55:GLN:O	1:MMM:58:VAL:HG22	2.18	0.43
1:TTT:223:TRP:HA	1:TTT:233:TYR:O	2.17	0.43
1:TTT:0:MET:HE3	1:TTT:93:SER:HB2	2.00	0.43
2:BBB:218:GLY:O	2:BBB:222:VAL:HG11	2.18	0.43
1:KKK:157:TRP:HB3	1:KKK:201:PHE:CZ	2.53	0.43
1:MMM:0:MET:SD	1:MMM:27:GLN:NE2	2.91	0.43
1:MMM:214:ALA:HB3	1:MMM:216:TYR:CE1	2.53	0.43
2:GGG:52:GLU:OE1	2:GGG:52:GLU:HA	2.19	0.43
1:KKK:13:ALA:O	1:KKK:106:ILE:HA	2.19	0.43
1:KKK:162:GLN:HG3	1:KKK:167:GLY:O	2.19	0.43
1:PPP:130:GLY:HA3	1:PPP:142:LEU:HD23	2.00	0.43
1:RRR:128:GLU:HG2	1:RRR:243:THR:OG1	2.17	0.43
1:RRR:145:ALA:HA	1:RRR:200:HIS:CD2	2.53	0.43
2:BBB:160:TYR:N	2:BBB:179:GLN:HE21	1.95	0.43
2:EEE:91:ASN:ND2	2:EEE:99:ILE:HB	2.34	0.43
1:QQQ:227:ASN:HD21	2:GGG:59:LYS:HG3	1.83	0.43
2:GGG:120:VAL:HG21	2:HHH:261:MET:HE1	1.99	0.43
2:BBB:91:ASN:ND2	2:BBB:99:ILE:HB	2.33	0.43
2:DDD:30:LYS:HE2	2:DDD:31:THR:O	2.18	0.43
1:KKK:223:TRP:HA	1:KKK:233:TYR:O	2.18	0.43
2:HHH:218:GLY:O	2:HHH:222:VAL:HG11	2.18	0.43
1:PPP:37:GLN:HB2	1:PPP:47:LEU:HD11	2.01	0.42
1:TTT:140:LEU:HD12	1:TTT:245:VAL:HG11	2.00	0.42
2:AAA:120:VAL:HG21	2:BBB:261:MET:HE1	2.01	0.42
2:AAA:130:ASN:O	2:BBB:268:SER:HA	2.19	0.42
2:GGG:171:PRO:HB3	2:GGG:185:HIS:CG	2.54	0.42
1:OOO:124:VAL:HG22	1:OOO:149:ASP:HB2	2.00	0.42
2:EEE:112:ILE:HD11	2:EEE:277:TYR:HB2	2.01	0.42
2:HHH:112:ILE:CD1	2:III:204:PRO:HG3	2.49	0.42
1:MMM:213:THR:CG2	1:MMM:247:VAL:H	2.31	0.42
2:DDD:154:GLN:CD	2:DDD:181:MET:HE1	2.44	0.42
1:KKK:11:LEU:HD23	1:KKK:104:LEU:CD1	2.49	0.42
1:LLL:223:TRP:HA	1:LLL:233:TYR:O	2.19	0.42
1:QQQ:144:CYS:O	1:QQQ:200[B]:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:66:THR:OG1	2:CCC:68:GLU:HG2	2.20	0.42
2:DDD:30:LYS:HA	2:DDD:30:LYS:HD2	1.74	0.42
2:III:152:GLU:HB3	2:III:206:ARG:CZ	2.50	0.42
1:QQQ:190:VAL:HG22	1:QQQ:205:LEU:CD2	2.50	0.42
2:AAA:68[B]:GLU:HG3	2:AAA:161:ARG:NH1	2.34	0.42
1:LLL:6:GLN:NE2	1:LLL:86:TYR:O	2.47	0.42
1:NNN:11:LEU:HD22	1:NNN:104:LEU:CD1	2.50	0.42
2:EEE:152:GLU:HB3	2:EEE:206[B]:ARG:CZ	2.50	0.42
1:NNN:6:GLN:HG2	1:NNN:102:THR:OG1	2.19	0.42
1:RRR:230:GLY:HA3	2:GGG:130:ASN:HA	2.02	0.42
2:CCC:42[B]:PHE:CD2	2:CCC:112:ILE:HD13	2.54	0.42
2:AAA:105:VAL:HG12	2:AAA:106:THR:HG23	2.02	0.42
2:DDD:47:MET:SD	2:DDD:258:VAL:HG22	2.60	0.42
2:DDD:171:PRO:HB3	2:DDD:185:HIS:CG	2.55	0.42
1:NNN:223:TRP:HA	1:NNN:233:TYR:O	2.20	0.41
2:III:171:PRO:HB3	2:III:185:HIS:CG	2.55	0.41
1:MMM:162:GLN:HB3	1:MMM:215:VAL:CG1	2.50	0.41
1:QQQ:241:GLN:OE1	1:QQQ:241:GLN:N	2.49	0.41
2:AAA:112:ILE:CD1	2:BBB:204:PRO:HG3	2.50	0.41
1:KKK:24:ARG:HA	1:KKK:69:THR:O	2.19	0.41
1:MMM:155:ASN:ND2	1:MMM:220:ARG:HG3	2.35	0.41
1:RRR:170:TRP:CZ2	1:RRR:173:GLU:HG3	2.55	0.41
2:JJJ:152:GLU:OE1	2:JJJ:206[B]:ARG:HD2	2.19	0.41
1:NNN:24:ARG:HA	1:NNN:69:THR:O	2.19	0.41
1:NNN:156:TRP:CE3	1:NNN:173:GLU:HG3	2.55	0.41
1:SSS:208:VAL:HA	1:SSS:212:ASP:OD2	2.21	0.41
2:FFF:52:GLU:O	2:GGG:176:VAL:HG21	2.20	0.41
1:KKK:251:VAL:HA	1:KKK:252:PRO:HD3	1.93	0.41
1:MMM:89:GLN:HB2	1:MMM:98:PHE:CD2	2.56	0.41
1:MMM:24:ARG:HA	1:MMM:69:THR:O	2.20	0.41
1:PPP:220:ARG:O	1:PPP:236:MET:HA	2.20	0.41
1:QQQ:13:ALA:O	1:QQQ:106:ILE:HA	2.20	0.41
2:AAA:30:LYS:HE2	2:AAA:100:LEU:HD21	2.02	0.41
2:DDD:45:PRO:HD2	2:EEE:180:VAL:HB	2.03	0.41
2:FFF:130:ASN:O	2:GGG:268:SER:HA	2.21	0.41
1:OOO:144:CYS:O	1:OOO:200[B]:HIS:HB2	2.21	0.41
1:TTT:67:SER:O	1:TTT:69:THR:N	2.53	0.41
2:JJJ:152:GLU:HB3	2:JJJ:206[B]:ARG:CZ	2.51	0.41
1:SSS:220:ARG:O	1:SSS:236:MET:HA	2.21	0.41
1:LLL:94:THR:HA	1:LLL:95:PRO:C	2.46	0.41
1:MMM:47:LEU:HA	1:MMM:58:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TTT:35:TRP:CZ3	1:TTT:88:CYS:HB3	2.56	0.41
2:BBB:103:GLU:O	2:BBB:282:LEU:HA	2.21	0.41
2:JJJ:217:THR:HG21	2:JJJ:222:VAL:HG21	2.03	0.41
1:KKK:83:PHE:HB3	1:KKK:106:ILE:HD12	2.02	0.41
1:QQQ:106:ILE:N	1:QQQ:106:ILE:HD12	2.36	0.41
1:RRR:60:SER:HB2	1:SSS:189:ARG:CG	2.47	0.40
2:FFF:68[B]:GLU:CD	2:FFF:68[B]:GLU:H	2.30	0.40
1:MMM:162:GLN:HB3	1:MMM:215:VAL:HG13	2.03	0.40
1:PPP:60:SER:OG	1:QQQ:189:ARG:HD3	2.21	0.40
1:QQQ:124:VAL:HG22	1:QQQ:149:ASP:HB2	2.03	0.40
1:SSS:158:SER:CB	1:SSS:173:GLU:HG2	2.52	0.40
1:SSS:176:HIS:O	1:SSS:196:LYS:HE3	2.21	0.40
2:CCC:130:ASN:O	2:DDD:268:SER:HA	2.21	0.40
1:MMM:67:SER:O	1:MMM:69:THR:N	2.54	0.40
1:OOO:195:ASP:OD2	1:OOO:198:LYS:HG3	2.20	0.40
1:RRR:100:GLN:H	1:RRR:100:GLN:CD	2.27	0.40
2:BBB:283:ARG:HH21	2:BBB:285:ARG:HH11	1.69	0.40
2:DDD:160:TYR:HD1	2:DDD:179:GLN:NE2	2.19	0.40
2:JJJ:42:PHE:CD1	2:JJJ:112:ILE:HD13	2.56	0.40
1:MMM:48:ILE:HD13	1:MMM:54:LEU:HA	2.03	0.40
1:QQQ:140:LEU:HD12	1:QQQ:141:SER:H	1.87	0.40
2:BBB:112:ILE:CD1	2:CCC:204:PRO:HG3	2.52	0.40
2:CCC:203:ASP:OD2	2:CCC:206[B]:ARG:HD3	2.22	0.40
2:JJJ:103:GLU:HA	2:JJJ:244:PRO:O	2.22	0.40
1:KKK:130:GLY:HA3	1:KKK:142:LEU:HD23	2.04	0.40
1:TTT:220:ARG:O	1:TTT:236:MET:HA	2.21	0.40
2:CCC:180:VAL:O	2:CCC:181:MET:HG2	2.22	0.40
2:EEE:152:GLU:OE1	2:EEE:206[B]:ARG:HD2	2.22	0.40

There are no symmetry-related clashes.

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	234/253 (92%)	228 (97%)	5 (2%)	1 (0%)	30	22
1	LLL	234/253 (92%)	228 (97%)	5 (2%)	1 (0%)	30	22
1	MMM	226/253 (89%)	218 (96%)	6 (3%)	2 (1%)	14	6
1	NNN	228/253 (90%)	222 (97%)	5 (2%)	1 (0%)	30	22
1	OOO	232/253 (92%)	228 (98%)	3 (1%)	1 (0%)	30	22
1	PPP	227/253 (90%)	215 (95%)	10 (4%)	2 (1%)	14	6
1	QQQ	229/253 (90%)	223 (97%)	5 (2%)	1 (0%)	30	22
1	RRR	232/253 (92%)	228 (98%)	3 (1%)	1 (0%)	30	22
1	SSS	233/253 (92%)	227 (97%)	6 (3%)	0	100	100
1	TTT	234/253 (92%)	227 (97%)	6 (3%)	1 (0%)	30	22
2	AAA	266/272 (98%)	256 (96%)	10 (4%)	0	100	100
2	BBB	258/272 (95%)	248 (96%)	10 (4%)	0	100	100
2	CCC	264/272 (97%)	253 (96%)	10 (4%)	1 (0%)	30	22
2	DDD	260/272 (96%)	251 (96%)	8 (3%)	1 (0%)	30	22
2	EEE	260/272 (96%)	249 (96%)	11 (4%)	0	100	100
2	FFF	260/272 (96%)	251 (96%)	9 (4%)	0	100	100
2	GGG	260/272 (96%)	251 (96%)	9 (4%)	0	100	100
2	HHH	263/272 (97%)	254 (97%)	9 (3%)	0	100	100
2	III	260/272 (96%)	249 (96%)	10 (4%)	1 (0%)	30	22
2	JJJ	262/272 (96%)	251 (96%)	11 (4%)	0	100	100
All	All	4922/5250 (94%)	4757 (97%)	151 (3%)	14 (0%)	36	29

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	OOO	68	GLY
1	QQQ	68	GLY
1	LLL	68	GLY
1	MMM	68	GLY
1	PPP	68	GLY
1	TTT	68	GLY
1	RRR	68	GLY
2	III	92	GLU
1	NNN	68	GLY
2	CCC	92	GLU
2	DDD	92	GLU

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Mol	Chain	Res	Type
1	KKK	68	GLY
1	PPP	131	PRO
1	MMM	131	PRO

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	196/208 (94%)	193 (98%)	3 (2%)	57	56
1	LLL	191/208 (92%)	186 (97%)	5 (3%)	40	35
1	MMM	171/208 (82%)	168 (98%)	3 (2%)	51	50
1	NNN	187/208 (90%)	186 (100%)	1 (0%)	81	84
1	OOO	186/208 (89%)	183 (98%)	3 (2%)	55	54
1	PPP	174/208 (84%)	174 (100%)	0	100	100
1	QQQ	188/208 (90%)	183 (97%)	5 (3%)	39	34
1	RRR	188/208 (90%)	181 (96%)	7 (4%)	30	22
1	SSS	191/208 (92%)	187 (98%)	4 (2%)	47	44
1	TTT	184/208 (88%)	182 (99%)	2 (1%)	65	67
2	AAA	228/237 (96%)	226 (99%)	2 (1%)	70	73
2	BBB	227/237 (96%)	227 (100%)	0	100	100
2	CCC	229/237 (97%)	228 (100%)	1 (0%)	84	87
2	DDD	225/237 (95%)	225 (100%)	0	100	100
2	EEE	230/237 (97%)	230 (100%)	0	100	100
2	FFF	224/237 (94%)	223 (100%)	1 (0%)	84	87
2	GGG	230/237 (97%)	230 (100%)	0	100	100
2	HHH	230/237 (97%)	227 (99%)	3 (1%)	61	61
2	III	223/237 (94%)	222 (100%)	1 (0%)	84	87
2	JJJ	225/237 (95%)	223 (99%)	2 (1%)	70	73
All	All	4127/4450 (93%)	4084 (99%)	43 (1%)	68	70

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	KKK	189	ARG
1	KKK	200	HIS
1	KKK	222	ARG
1	LLL	10	SER
1	LLL	67	SER
1	LLL	166	LYS
1	LLL	222	ARG
1	LLL	241	GLN
1	MMM	200	HIS
1	MMM	221	ASN
1	MMM	222	ARG
1	NNN	222	ARG
1	OOO	60	SER
1	OOO	221	ASN
1	OOO	222	ARG
1	QQQ	7	SER
1	QQQ	63	SER
1	QQQ	67	SER
1	QQQ	188	SER
1	QQQ	222	ARG
1	RRR	9	SER
1	RRR	37	GLN
1	RRR	67	SER
1	RRR	77	SER
1	RRR	100	GLN
1	RRR	122	SER
1	RRR	248	SER
1	SSS	1	ASP
1	SSS	106	ILE
1	SSS	200	HIS
1	SSS	222	ARG
1	TTT	67	SER
1	TTT	200	HIS
2	AAA	21	MET
2	AAA	199	CYS
2	CCC	21	MET
2	FFF	199	CYS
2	HHH	71[A]	SER
2	HHH	71[B]	SER
2	HHH	288	LYS
2	III	199	CYS
2	JJJ	21	MET

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Mol	Chain	Res	Type
2	JJJ	27	LEU

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	KKK	238/253 (94%)	0.39	7 (2%) 53 57	23, 37, 63, 82	0
1	LLL	238/253 (94%)	0.46	10 (4%) 40 43	25, 39, 64, 91	0
1	MMM	230/253 (90%)	1.20	37 (16%) 4 4	32, 58, 79, 95	0
1	NNN	231/253 (91%)	0.60	12 (5%) 33 35	20, 41, 62, 75	1 (0%)
1	OOO	235/253 (92%)	0.66	26 (11%) 10 11	22, 42, 65, 90	1 (0%)
1	PPP	231/253 (91%)	1.17	35 (15%) 5 5	25, 56, 81, 107	1 (0%)
1	QQQ	232/253 (91%)	0.73	16 (6%) 23 24	23, 44, 66, 91	1 (0%)
1	RRR	236/253 (93%)	0.49	15 (6%) 25 27	22, 37, 62, 95	0
1	SSS	237/253 (93%)	0.26	5 (2%) 63 67	22, 35, 58, 75	0
1	TTT	238/253 (94%)	0.38	8 (3%) 48 51	26, 38, 59, 98	0
2	AAA	268/272 (98%)	0.24	11 (4%) 41 44	19, 31, 67, 101	2 (0%)
2	BBB	261/272 (95%)	0.12	7 (2%) 56 60	22, 33, 58, 89	1 (0%)
2	CCC	264/272 (97%)	0.23	8 (3%) 52 56	17, 34, 57, 95	4 (1%)
2	DDD	262/272 (96%)	0.10	8 (3%) 51 55	19, 31, 57, 94	2 (0%)
2	EEE	261/272 (95%)	0.10	12 (4%) 37 40	17, 30, 54, 97	3 (1%)
2	FFF	260/272 (95%)	0.21	6 (2%) 61 65	18, 34, 55, 99	4 (1%)
2	GGG	261/272 (95%)	0.11	7 (2%) 56 60	17, 31, 55, 92	3 (1%)
2	HHH	262/272 (96%)	0.09	8 (3%) 51 55	18, 30, 55, 92	5 (1%)
2	III	263/272 (96%)	0.07	10 (3%) 44 47	20, 30, 56, 90	1 (0%)
2	JJJ	264/272 (97%)	0.23	13 (4%) 35 37	18, 33, 56, 101	2 (0%)
All	All	4972/5250 (94%)	0.38	261 (5%) 33 35	17, 36, 68, 107	31 (0%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	QQQ	23	CYS	6.3
1	PPP	1[A]	ASP	6.2
2	AAA	20	HIS	5.9
1	TTT	107	LYS	4.9
2	AAA	21	MET	4.9
2	FFF	289	ASN	4.6
2	GGG	94	LEU	4.5
2	JJJ	21	MET	4.5
1	QQQ	247	VAL	4.5
1	PPP	123	GLN	4.4
2	JJJ	98	ASN	4.4
2	HHH	24	VAL	4.3
2	HHH	289	ASN	4.3
1	SSS	123	GLN	4.2
1	MMM	124	VAL	4.2
2	AAA	33	VAL	4.2
2	CCC	21	MET	4.2
2	EEE	289	ASN	4.1
1	TTT	106	ILE	4.0
1	NNN	15	VAL	4.0
2	AAA	23	GLY	4.0
1	PPP	78	LEU	4.0
1	NNN	1	ASP	4.0
2	EEE	42	PHE	4.0
2	FFF	99	ILE	4.0
1	SSS	106	ILE	4.0
2	CCC	33	VAL	3.9
1	KKK	123	GLN	3.9
1	OOO	108	GLY	3.9
2	AAA	95	THR	3.8
2	EEE	24	VAL	3.8
1	MMM	123	GLN	3.8
2	GGG	24	VAL	3.8
2	HHH	33	VAL	3.8
1	QQQ	165	GLY	3.7
2	DDD	94	LEU	3.7
2	FFF	24	VAL	3.7
2	GGG	33	VAL	3.7
1	TTT	123	GLN	3.7
2	FFF	33	VAL	3.7
2	CCC	98	ASN	3.7
2	AAA	289	ASN	3.6
2	EEE	33	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	MMM	223	TRP	3.6
2	GGG	52	GLU	3.6
1	QQQ	1	ASP	3.6
2	HHH	93	ASP	3.5
2	III	289	ASN	3.5
2	BBB	33	VAL	3.5
2	DDD	33	VAL	3.5
1	LLL	123	GLN	3.4
1	OOO	14	SER	3.4
1	MMM	131	PRO	3.4
2	III	94	LEU	3.4
1	PPP	40	PRO	3.4
2	AAA	24	VAL	3.3
2	JJJ	42	PHE	3.3
1	MMM	200	HIS	3.3
2	JJJ	289	ASN	3.3
1	PPP	15	VAL	3.3
1	PPP	105	GLU	3.3
2	BBB	42	PHE	3.3
1	OOO	1	ASP	3.3
1	PPP	223	TRP	3.3
1	RRR	14	SER	3.3
1	QQQ	78	LEU	3.2
1	LLL	70	ASP	3.2
1	PPP	21	ILE	3.2
2	BBB	93	ASP	3.2
1	QQQ	164	PRO	3.2
2	BBB	98	ASN	3.2
1	RRR	165	GLY	3.2
2	AAA	42	PHE	3.2
1	MMM	247	VAL	3.2
1	MMM	83	PHE	3.1
1	QQQ	106	ILE	3.1
1	QQQ	15	VAL	3.1
1	RRR	107	LYS	3.1
2	FFF	50	PRO	3.1
1	OOO	59	PRO	3.1
1	OOO	15	VAL	3.0
2	III	24	VAL	3.0
1	NNN	164	PRO	3.0
1	PPP	151	ILE	3.0
1	MMM	1	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	KKK	166	LYS	3.0
1	OOO	123	GLN	3.0
2	EEE	31	THR	3.0
2	GGG	51	ASP	3.0
1	MMM	76	SER	2.9
2	JJJ	24	VAL	2.9
1	KKK	165	GLY	2.9
1	NNN	16	GLY	2.9
1	PPP	124	VAL	2.9
2	JJJ	33	VAL	2.9
1	PPP	164	PRO	2.9
1	OOO	67	SER	2.9
1	PPP	14	SER	2.9
1	SSS	83	PHE	2.8
2	DDD	52	GLU	2.8
1	RRR	100	GLN	2.8
1	RRR	122	SER	2.8
1	OOO	164	PRO	2.8
1	RRR	19	VAL	2.8
2	CCC	22	GLY	2.8
1	PPP	131	PRO	2.8
1	SSS	1	ASP	2.8
1	NNN	248	SER	2.7
1	MMM	86	TYR	2.7
1	MMM	132	GLY	2.7
1	PPP	11	LEU	2.7
1	LLL	1	ASP	2.7
1	OOO	248	SER	2.7
1	NNN	123	GLN	2.7
1	TTT	165	GLY	2.7
1	MMM	145	ALA	2.7
1	PPP	104	LEU	2.7
1	PPP	82	ASP	2.6
1	PPP	56	SER	2.6
1	KKK	164	PRO	2.6
1	NNN	104	LEU	2.6
1	PPP	75	ILE	2.6
2	JJJ	99	ILE	2.6
2	BBB	24	VAL	2.6
1	QQQ	211	ALA	2.6
2	JJJ	92	GLU	2.6
1	OOO	80	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	PPP	80	PRO	2.6
1	LLL	78	LEU	2.6
1	NNN	78	LEU	2.6
1	RRR	15	VAL	2.6
1	RRR	249	SER	2.6
1	OOO	11	LEU	2.6
1	RRR	11	LEU	2.6
2	EEE	98	ASN	2.6
1	QQQ	223	TRP	2.5
1	OOO	106	ILE	2.5
1	OOO	107	LYS	2.5
1	MMM	19	VAL	2.5
1	MMM	40	PRO	2.5
1	PPP	23	CYS	2.5
1	OOO	165	GLY	2.5
2	JJJ	36	ILE	2.5
1	MMM	9	SER	2.5
1	KKK	1	ASP	2.5
2	DDD	30	LYS	2.5
1	MMM	104	LEU	2.5
1	PPP	57	GLY	2.5
1	QQQ	133	LEU	2.5
2	EEE	32	GLY	2.5
1	OOO	75	ILE	2.5
1	PPP	16	GLY	2.4
1	OOO	104	LEU	2.4
1	RRR	79	GLN	2.4
1	RRR	123	GLN	2.4
1	QQQ	122	SER	2.4
1	TTT	1	ASP	2.4
2	CCC	92	GLU	2.4
1	MMM	78	LEU	2.4
2	FFF	42	PHE	2.4
2	CCC	51	ASP	2.4
1	MMM	20	THR	2.4
2	III	33	VAL	2.4
1	OOO	17	ASP	2.4
2	III	239	GLU	2.4
2	GGG	53	HIS	2.4
1	MMM	58	VAL	2.4
1	MMM	68	GLY	2.4
1	OOO	78	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	HHH	42[A]	PHE	2.3
2	JJJ	25	GLU	2.3
2	EEE	99	ILE	2.3
1	OOO	0	MET	2.3
2	JJJ	23	GLY	2.3
2	DDD	166	ASP	2.3
1	LLL	223	TRP	2.3
1	MMM	71	PHE	2.3
1	NNN	71	PHE	2.3
1	MMM	15	VAL	2.3
1	PPP	19	VAL	2.3
2	JJJ	34	ASP	2.3
1	KKK	11	LEU	2.3
1	OOO	16	GLY	2.3
1	OOO	76	SER	2.3
1	MMM	225	ASP	2.3
1	OOO	79	GLN	2.3
1	MMM	213	THR	2.3
1	QQQ	54	LEU	2.3
2	EEE	218	GLY	2.2
2	HHH	218	GLY	2.2
1	PPP	202	SER	2.2
1	MMM	21	ILE	2.2
1	RRR	1	ASP	2.2
2	EEE	34	ASP	2.2
1	PPP	215	VAL	2.2
1	NNN	40	PRO	2.2
2	AAA	22	GLY	2.2
1	PPP	83	PHE	2.2
1	LLL	107	LYS	2.2
2	AAA	239	GLU	2.2
1	MMM	12	SER	2.2
2	III	93	ASP	2.2
2	III	286	ARG	2.2
2	HHH	92	GLU	2.2
1	LLL	15	VAL	2.2
1	PPP	160	VAL	2.2
1	QQQ	79	GLN	2.2
1	SSS	15	VAL	2.2
1	MMM	149	ASP	2.2
1	PPP	17	ASP	2.2
1	TTT	149	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	MMM	14	SER	2.2
1	MMM	165	GLY	2.2
2	CCC	288	LYS	2.2
1	MMM	0	MET	2.1
1	PPP	200	HIS	2.1
1	MMM	62	PHE	2.1
2	III	98	ASN	2.1
2	DDD	34	ASP	2.1
2	DDD	93	ASP	2.1
1	MMM	215	VAL	2.1
1	MMM	99	GLY	2.1
1	OOO	57	GLY	2.1
1	MMM	11	LEU	2.1
1	PPP	126	LEU	2.1
1	PPP	166	LYS	2.1
1	RRR	80	PRO	2.1
1	PPP	145	ALA	2.1
1	KKK	83	PHE	2.1
1	MMM	75	ILE	2.1
1	RRR	21	ILE	2.1
1	TTT	21	ILE	2.1
1	OOO	65	SER	2.1
2	AAA	97	GLY	2.1
2	BBB	193	LYS	2.1
1	PPP	81	GLU	2.1
1	NNN	11	LEU	2.1
2	III	218	GLY	2.1
2	JJJ	22	GLY	2.1
1	TTT	19	VAL	2.1
1	LLL	27	GLN	2.1
2	GGG	177	GLN	2.1
1	LLL	17	ASP	2.1
2	CCC	34	ASP	2.1
1	LLL	106	ILE	2.0
2	EEE	239	GLU	2.0
1	PPP	9	SER	2.0
2	HHH	98	ASN	2.0
1	MMM	164	PRO	2.0
1	PPP	163	PRO	2.0
1	RRR	40	PRO	2.0
2	DDD	24	VAL	2.0
2	EEE	222	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	III	90	LEU	2.0
1	MMM	13	ALA	2.0
1	QQQ	18	ARG	2.0
1	NNN	137	SER	2.0
1	OOO	71	PHE	2.0
1	OOO	68	GLY	2.0
1	QQQ	19	VAL	2.0
2	BBB	222	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.