



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:43 AM UTC

PDB ID : 9EDZ / pdb_00009edz
Title : HIV CA - GLFG peptide (4 mM)
Authors : Melcak, I.; Sarafianos, S.G.
Deposited on : 2024-11-18
Resolution : 3.00 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

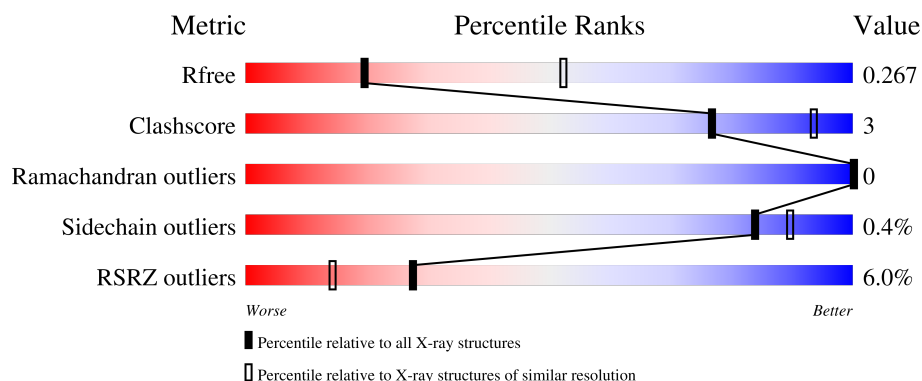
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	231	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	231	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	231	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	E	231	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	
2	M	9	
2	N	9	
2	O	9	
2	P	9	
2	Q	9	
2	R	9	
2	S	9	
2	U	9	
2	V	9	
2	W	9	
2	X	9	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19212 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 Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1578	993	272	299	14			
1	B	211	Total	C	N	O	S	0	0	0
			1594	1004	276	301	13			
1	C	207	Total	C	N	O	S	0	0	0
			1583	993	278	298	14			
1	D	210	Total	C	N	O	S	0	0	0
			1583	994	277	298	14			
1	E	204	Total	C	N	O	S	0	0	0
			1561	986	270	292	13			
1	F	216	Total	C	N	O	S	0	0	0
			1625	1023	284	304	14			
1	G	216	Total	C	N	O	S	0	0	0
			1623	1020	284	305	14			
1	H	210	Total	C	N	O	S	0	0	0
			1543	971	268	290	14			
1	I	212	Total	C	N	O	S	0	0	0
			1573	993	270	297	13			
1	J	214	Total	C	N	O	S	0	0	0
			1621	1015	286	306	14			
1	K	207	Total	C	N	O	S	0	0	0
			1546	973	267	292	14			
1	L	202	Total	C	N	O	S	0	0	0
			1522	960	262	287	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP P12493
A	45	CYS	GLU	engineered mutation	UNP P12493
A	184	ALA	TRP	engineered mutation	UNP P12493
A	185	ALA	MET	engineered mutation	UNP P12493
B	14	CYS	ALA	engineered mutation	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	GLU	engineered mutation	UNP P12493
B	184	ALA	TRP	engineered mutation	UNP P12493
B	185	ALA	MET	engineered mutation	UNP P12493
C	14	CYS	ALA	engineered mutation	UNP P12493
C	45	CYS	GLU	engineered mutation	UNP P12493
C	184	ALA	TRP	engineered mutation	UNP P12493
C	185	ALA	MET	engineered mutation	UNP P12493
D	14	CYS	ALA	engineered mutation	UNP P12493
D	45	CYS	GLU	engineered mutation	UNP P12493
D	184	ALA	TRP	engineered mutation	UNP P12493
D	185	ALA	MET	engineered mutation	UNP P12493
E	14	CYS	ALA	engineered mutation	UNP P12493
E	45	CYS	GLU	engineered mutation	UNP P12493
E	184	ALA	TRP	engineered mutation	UNP P12493
E	185	ALA	MET	engineered mutation	UNP P12493
F	14	CYS	ALA	engineered mutation	UNP P12493
F	45	CYS	GLU	engineered mutation	UNP P12493
F	184	ALA	TRP	engineered mutation	UNP P12493
F	185	ALA	MET	engineered mutation	UNP P12493
G	14	CYS	ALA	engineered mutation	UNP P12493
G	45	CYS	GLU	engineered mutation	UNP P12493
G	184	ALA	TRP	engineered mutation	UNP P12493
G	185	ALA	MET	engineered mutation	UNP P12493
H	14	CYS	ALA	engineered mutation	UNP P12493
H	45	CYS	GLU	engineered mutation	UNP P12493
H	184	ALA	TRP	engineered mutation	UNP P12493
H	185	ALA	MET	engineered mutation	UNP P12493
I	14	CYS	ALA	engineered mutation	UNP P12493
I	45	CYS	GLU	engineered mutation	UNP P12493
I	184	ALA	TRP	engineered mutation	UNP P12493
I	185	ALA	MET	engineered mutation	UNP P12493
J	14	CYS	ALA	engineered mutation	UNP P12493
J	45	CYS	GLU	engineered mutation	UNP P12493
J	184	ALA	TRP	engineered mutation	UNP P12493
J	185	ALA	MET	engineered mutation	UNP P12493
K	14	CYS	ALA	engineered mutation	UNP P12493
K	45	CYS	GLU	engineered mutation	UNP P12493
K	184	ALA	TRP	engineered mutation	UNP P12493
K	185	ALA	MET	engineered mutation	UNP P12493
L	14	CYS	ALA	engineered mutation	UNP P12493
L	45	CYS	GLU	engineered mutation	UNP P12493
L	184	ALA	TRP	engineered mutation	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
L	185	ALA	MET	engineered mutation	UNP P12493

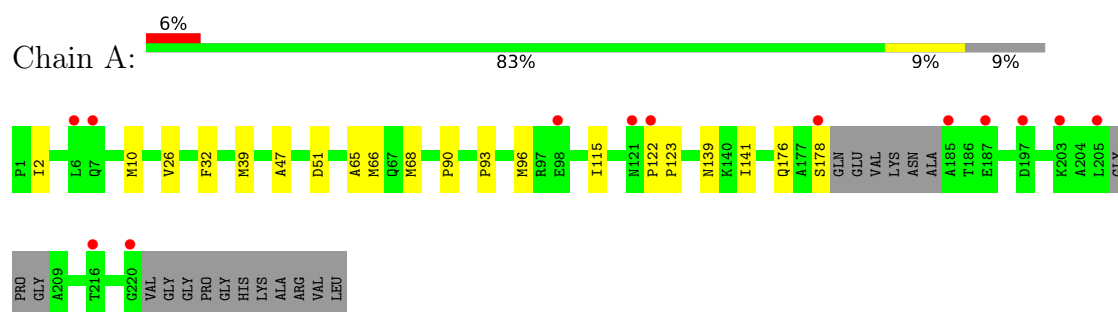
- Molecule 2 is a protein called GLFG peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	2	Total	C	N	O	0	0	0
			15	11	2	2			
2	O	4	Total	C	N	O	0	0	0
			27	19	4	4			
2	P	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	R	5	Total	C	N	O	0	0	0
			33	22	5	6			
2	S	5	Total	C	N	O	0	0	0
			32	22	5	5			
2	V	4	Total	C	N	O	0	0	0
			27	19	4	4			
2	W	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	M	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	Q	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	U	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	X	1	Total	C	N	O	0	0	0
			11	9	1	1			

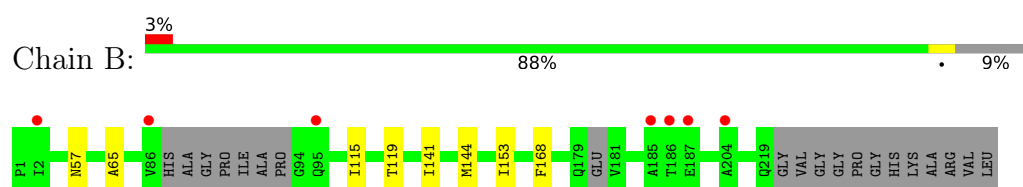
3 Residue-property plots [i](#)

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

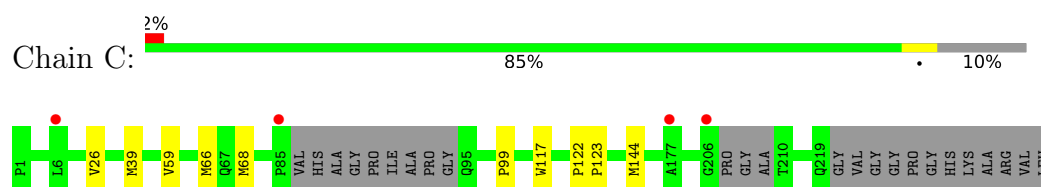
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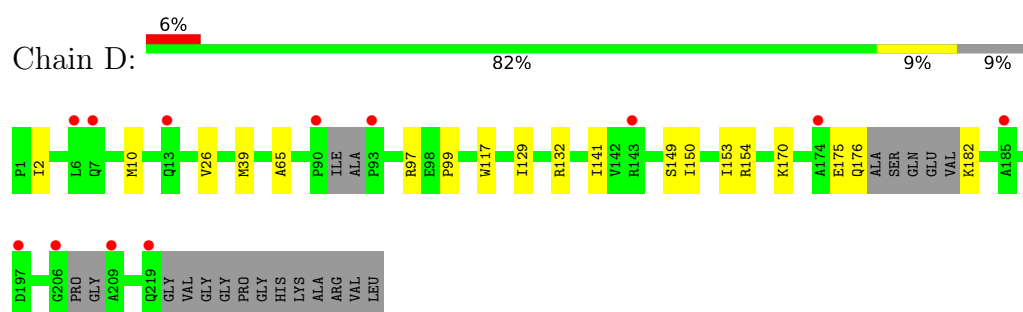
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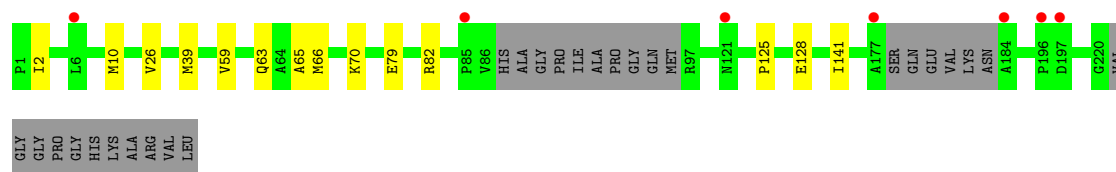
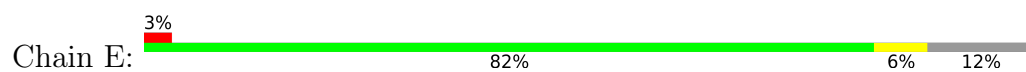
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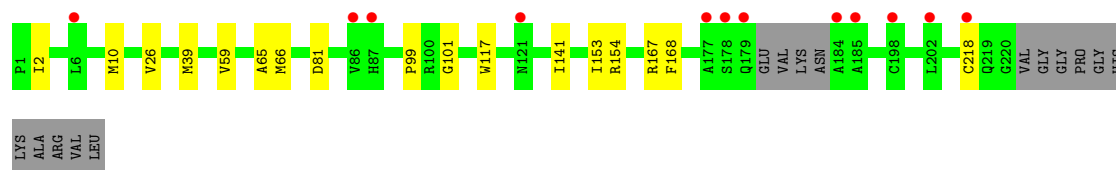
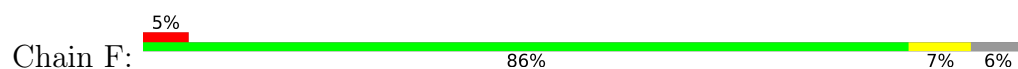
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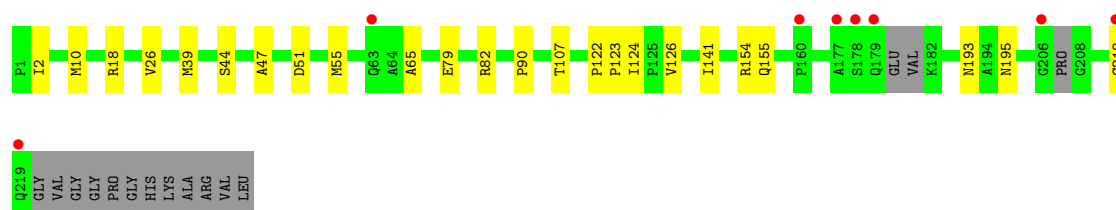
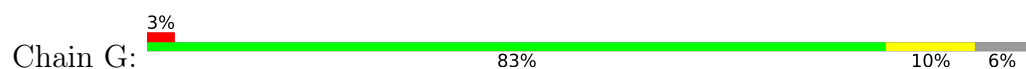
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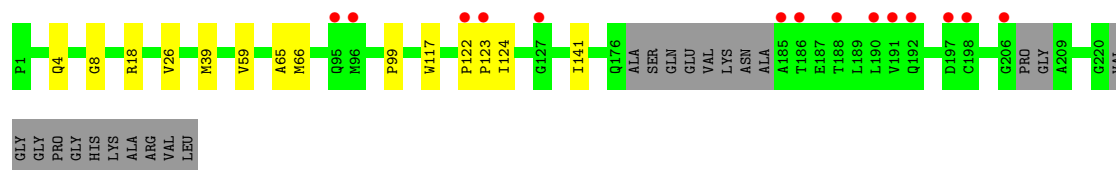
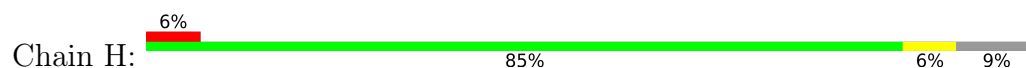
- Molecule 1: Capsid protein p24



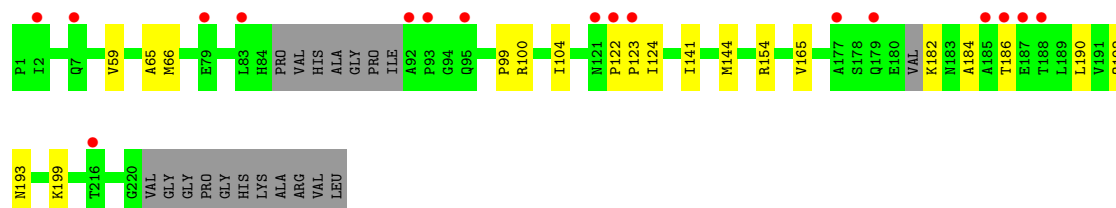
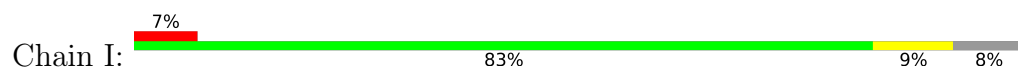
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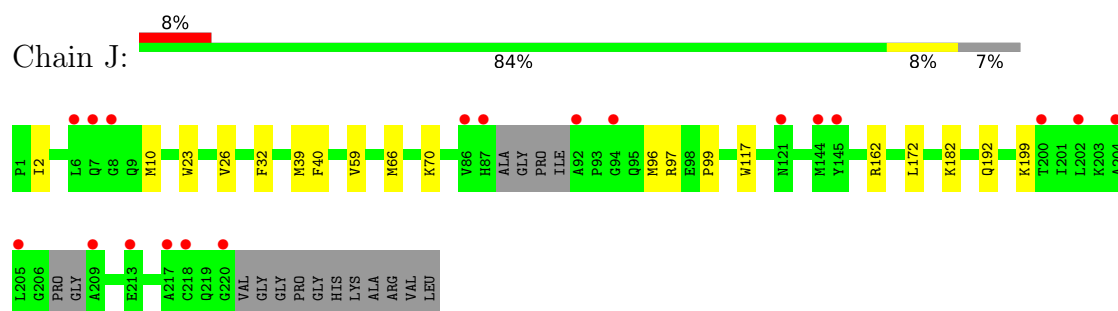
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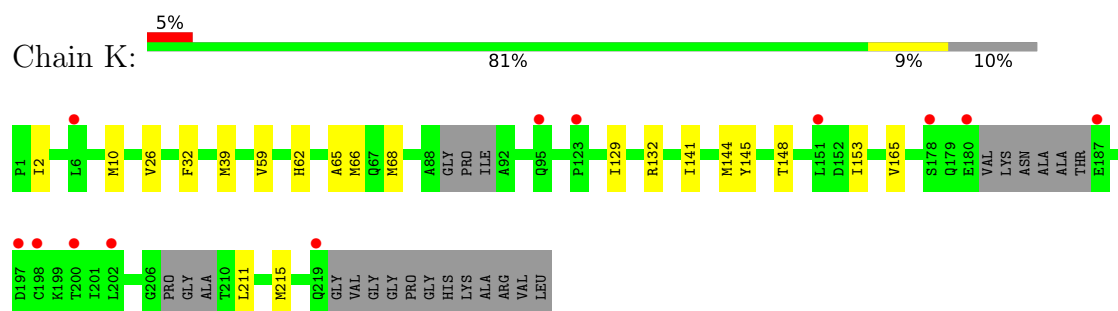
- Molecule 1: Capsid protein p24



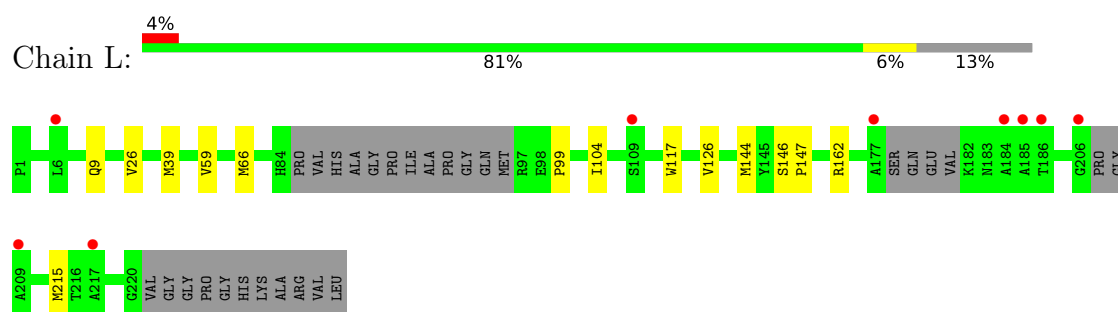
- Molecule 1: Capsid protein p24



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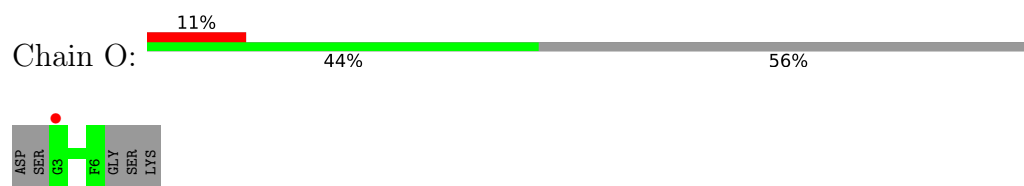
- Molecule 1: Capsid protein p24



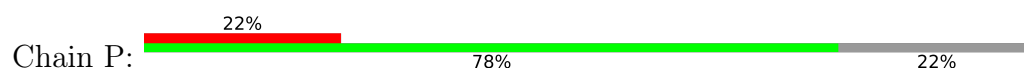
- Molecule 2: GLFG peptide

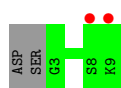


- Molecule 2: GLFG peptide

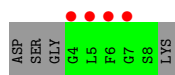
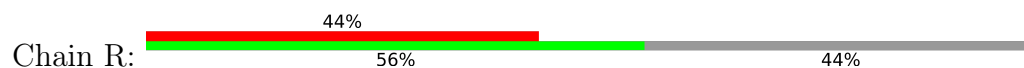


- Molecule 2: GLFG peptide

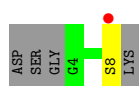
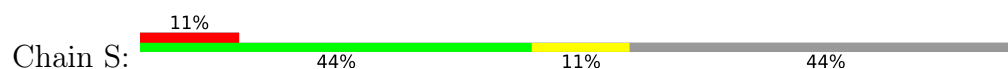




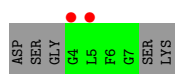
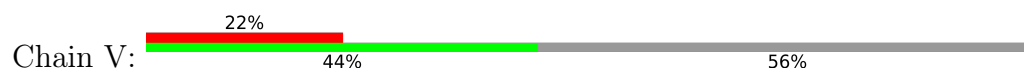
- Molecule 2: GLFG peptide



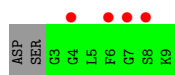
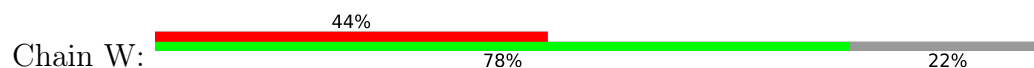
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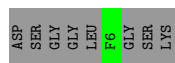
- Molecule 2: GLFG peptide



- Molecule 2: GLFG peptide

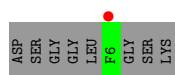


- Molecule 2: GLFG peptide



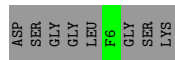
- Molecule 2: GLFG peptide





- Molecule 2: GLFG peptide

Chain X:  11% 89%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.55Å 136.78Å 208.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.70 – 3.00 34.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.70-3.00) 98.6 (34.70-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.236 , 0.267 0.236 , 0.267	Depositor DCC
R_{free} test set	3932 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 21.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19212	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.08	0/1611	0.22	0/2194
1	B	0.08	0/1626	0.21	0/2211
1	C	0.08	0/1614	0.22	0/2193
1	D	0.08	0/1615	0.20	0/2195
1	E	0.07	0/1593	0.21	0/2166
1	F	0.08	0/1660	0.21	0/2260
1	G	0.08	0/1656	0.21	0/2256
1	H	0.08	0/1576	0.19	0/2151
1	I	0.08	0/1605	0.22	0/2187
1	J	0.08	0/1653	0.20	0/2247
1	K	0.08	0/1577	0.20	0/2147
1	L	0.08	0/1551	0.21	0/2109
2	M	0.04	0/11	0.06	0/13
2	N	0.05	0/15	0.13	0/18
2	O	0.05	0/27	0.06	0/34
2	P	0.09	0/41	0.22	0/53
2	Q	0.07	0/11	0.05	0/13
2	R	0.05	0/33	0.11	0/42
2	S	0.04	0/32	0.09	0/41
2	U	0.06	0/11	0.06	0/13
2	V	0.04	0/27	0.09	0/34
2	W	0.05	0/41	0.09	0/53
2	X	0.05	0/11	0.04	0/13
All	All	0.08	0/19597	0.21	0/26643

There are no bond length outliers.

There are no bond angle outliers.

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	A	1578	0	1509	14	0
1	B	1594	0	1544	5	0
1	C	1583	0	1533	6	0
1	D	1583	0	1517	11	0
1	E	1561	0	1540	7	0
1	F	1625	0	1573	8	0
1	G	1623	0	1559	14	0
1	H	1543	0	1451	9	0
1	I	1573	0	1506	10	0
1	J	1621	0	1566	13	0
1	K	1546	0	1463	12	0
1	L	1522	0	1465	7	0
2	M	11	0	8	1	0
2	N	15	0	11	1	0
2	O	27	0	25	0	0
2	P	41	0	32	0	0
2	Q	11	0	8	0	0
2	R	33	0	30	0	0
2	S	32	0	27	1	0
2	U	11	0	8	0	0
2	V	27	0	25	0	0
2	W	41	0	32	0	0
2	X	11	0	8	0	0
All	All	19212	0	18440	108	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 3.

All (108) 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:G:44:SER:HB3	1:G:55:MET:HE1	1.71	0.71
1:C:59:VAL:HG11	1:C:66:MET:HE3	1.75	0.67
1:H:59:VAL:HG11	1:H:66:MET:HE3	1.79	0.64
1:E:59:VAL:HG11	1:E:66:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.81	0.62
1:A:2:ILE:HG22	1:A:10:MET:HE3	1.82	0.61
1:K:59:VAL:HG11	1:K:66:MET:HE3	1.83	0.60
1:I:59:VAL:HG11	1:I:66:MET:HE3	1.83	0.59
1:F:59:VAL:HG11	1:F:66:MET:HE3	1.84	0.59
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.85	0.59
1:L:59:VAL:HG11	1:L:66:MET:HE3	1.85	0.58
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.85	0.58
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.86	0.57
1:G:2:ILE:HG22	1:G:10:MET:HE3	1.87	0.57
1:D:150:ILE:HA	1:D:153:ILE:HD12	1.87	0.56
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.87	0.56
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.85	0.56
1:E:2:ILE:HG22	1:E:10:MET:HE3	1.87	0.56
1:J:26:VAL:HG21	1:J:39:MET:HG2	1.88	0.55
1:D:176:GLN:NE2	1:D:182:LYS:O	2.39	0.55
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.87	0.55
1:I:165:VAL:HG22	1:I:190:LEU:HD11	1.89	0.55
1:J:162:ARG:HH21	1:K:145:TYR:HA	1.72	0.55
1:F:2:ILE:HG22	1:F:10:MET:HE3	1.89	0.54
1:I:154:ARG:HG2	1:I:193:ASN:HB3	1.88	0.54
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.89	0.54
1:G:79:GLU:OE2	1:G:82:ARG:NH2	2.38	0.54
1:J:59:VAL:HG11	1:J:66:MET:HE3	1.88	0.54
1:E:79:GLU:OE2	1:E:82:ARG:NH2	2.39	0.53
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.91	0.52
1:A:139:ASN:HB3	1:A:178:SER:HA	1.90	0.52
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.91	0.52
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.91	0.52
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.92	0.51
1:G:47:ALA:HB1	1:G:51:ASP:HB2	1.93	0.50
1:A:66:MET:HB3	2:M:6:PHE:HZ	1.75	0.50
1:K:65:ALA:HA	1:K:68:MET:HE2	1.92	0.50
1:G:107:THR:HG23	2:S:8:SER:HA	1.93	0.50
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.94	0.50
1:D:99:PRO:HG3	1:D:117:TRP:CE2	2.47	0.50
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.93	0.50
1:J:172:LEU:HD21	1:J:182:LYS:HA	1.94	0.49
1:F:153:ILE:HG21	1:F:168:PHE:HA	1.93	0.49
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.95	0.49
1:G:154:ARG:HG2	1:G:193:ASN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:VAL:HG21	1:E:39:MET:HG2	1.95	0.48
1:G:155:GLN:CD	1:G:195:ASN:HD22	2.22	0.48
1:F:154:ARG:O	1:F:167:ARG:NH2	2.46	0.48
1:H:4:GLN:HE21	1:H:8:GLY:HA2	1.79	0.48
1:D:97:ARG:HB2	1:G:90:PRO:HB2	1.96	0.47
1:I:100:ARG:O	1:I:104:ILE:HG12	2.14	0.47
1:L:144:MET:HE2	1:L:144:MET:HB3	1.81	0.47
1:K:2:ILE:HG22	1:K:10:MET:HE3	1.97	0.47
1:B:57:ASN:HD21	2:N:6:PHE:N	2.13	0.47
1:K:165:VAL:HG11	1:K:215:MET:HE2	1.97	0.46
1:B:115:ILE:O	1:B:119:THR:OG1	2.32	0.46
1:H:99:PRO:HG2	1:H:124:ILE:HG21	1.98	0.46
1:I:99:PRO:HG2	1:I:124:ILE:HG21	1.98	0.45
1:A:93:PRO:HB3	1:J:96:MET:HE2	1.98	0.45
1:D:129:ILE:HG12	1:D:132:ARG:HH12	1.82	0.45
1:F:81:ASP:OD1	1:F:101:GLY:N	2.48	0.45
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.98	0.45
1:A:96:MET:HE2	1:A:96:MET:HB3	1.92	0.45
1:J:32:PHE:HZ	1:J:66:MET:HE2	1.82	0.45
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.99	0.44
1:C:99:PRO:HG3	1:C:117:TRP:CE2	2.52	0.44
1:G:18:ARG:HH22	1:H:18:ARG:NH1	2.15	0.44
1:G:18:ARG:HH22	1:H:18:ARG:HH11	1.66	0.44
1:C:68:MET:HE2	1:C:68:MET:HB3	1.86	0.43
1:E:125:PRO:HB2	1:E:128:GLU:HB2	1.99	0.43
1:L:99:PRO:HG3	1:L:117:TRP:CE2	2.53	0.43
1:A:90:PRO:HB2	1:J:97:ARG:HB2	2.00	0.43
1:G:122:PRO:HA	1:G:123:PRO:HD3	1.90	0.43
1:K:211:LEU:HG	1:K:215:MET:HE3	2.00	0.43
1:K:148:THR:HG21	1:K:153:ILE:HD11	2.00	0.42
1:L:162:ARG:HA	1:L:215:MET:HE3	2.00	0.42
1:K:144:MET:HE2	1:K:144:MET:HB3	1.81	0.42
1:A:26:VAL:HG21	1:A:39:MET:HG2	2.01	0.42
1:A:2:ILE:HD11	1:A:115:ILE:HG12	2.01	0.42
1:C:122:PRO:HA	1:C:123:PRO:HD3	1.89	0.42
1:J:2:ILE:HG22	1:J:10:MET:HE3	2.00	0.42
1:I:182:LYS:C	1:I:184:ALA:H	2.28	0.42
1:I:192:GLN:HA	1:I:199:LYS:HE3	2.02	0.42
1:J:99:PRO:HG3	1:J:117:TRP:CD2	2.55	0.42
1:K:129:ILE:HG12	1:K:132:ARG:HH12	1.85	0.41
1:D:154:ARG:HA	1:D:193:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:32:PHE:HE2	1:K:62:HIS:HB3	1.85	0.41
1:J:99:PRO:HG3	1:J:117:TRP:CE2	2.55	0.41
1:A:32:PHE:HZ	1:A:66:MET:HE2	1.84	0.41
1:H:122:PRO:HA	1:H:123:PRO:HD3	1.92	0.41
1:A:122:PRO:HA	1:A:123:PRO:HD3	1.91	0.41
1:B:153:ILE:HG21	1:B:168:PHE:HA	2.02	0.41
1:A:93:PRO:HG3	1:J:117:TRP:CE2	2.56	0.41
1:G:124:ILE:O	1:G:126:VAL:N	2.52	0.41
1:H:99:PRO:HG3	1:H:117:TRP:CE2	2.56	0.41
1:J:23:TRP:CZ3	1:J:40:PHE:HB2	2.56	0.41
1:J:192:GLN:O	1:J:199:LYS:NZ	2.54	0.41
1:C:144:MET:HE2	1:C:144:MET:HB3	1.88	0.40
1:I:144:MET:HE2	1:I:144:MET:HB3	1.93	0.40
1:L:146:SER:HA	1:L:147:PRO:HD3	1.95	0.40
1:D:149:SER:HA	1:D:175:GLU:OE2	2.21	0.40
1:I:122:PRO:HA	1:I:123:PRO:HD3	1.94	0.40
1:A:68:MET:HE2	1:A:68:MET:HB3	1.89	0.40
1:B:144:MET:HE2	1:B:144:MET:HB3	1.85	0.40
1:D:170:LYS:HA	1:E:63:GLN:HG3	2.03	0.40
1:H:26:VAL:HG21	1:H:39:MET:HG2	2.02	0.40
1:F:99:PRO:HG3	1:F:117:TRP:CE2	2.57	0.40
1:L:104:ILE:HG12	1:L:126:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/231 (89%)	199 (97%)	6 (3%)	0	100	100
1	B	205/231 (89%)	201 (98%)	4 (2%)	0	100	100
1	C	201/231 (87%)	194 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	202/231 (87%)	196 (97%)	6 (3%)	0	100	100
1	E	198/231 (86%)	191 (96%)	7 (4%)	0	100	100
1	F	212/231 (92%)	204 (96%)	8 (4%)	0	100	100
1	G	210/231 (91%)	201 (96%)	9 (4%)	0	100	100
1	H	204/231 (88%)	195 (96%)	9 (4%)	0	100	100
1	I	206/231 (89%)	199 (97%)	7 (3%)	0	100	100
1	J	208/231 (90%)	198 (95%)	10 (5%)	0	100	100
1	K	199/231 (86%)	193 (97%)	6 (3%)	0	100	100
1	L	194/231 (84%)	185 (95%)	9 (5%)	0	100	100
2	O	2/9 (22%)	2 (100%)	0	0	100	100
2	P	5/9 (56%)	5 (100%)	0	0	100	100
2	R	3/9 (33%)	3 (100%)	0	0	100	100
2	S	3/9 (33%)	2 (67%)	1 (33%)	0	100	100
2	V	2/9 (22%)	2 (100%)	0	0	100	100
2	W	5/9 (56%)	5 (100%)	0	0	100	100
All	All	2464/2826 (87%)	2375 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/193 (84%)	161 (99%)	1 (1%)	78	88
1	B	166/193 (86%)	166 (100%)	0	100	100
1	C	167/193 (86%)	167 (100%)	0	100	100
1	D	163/193 (84%)	163 (100%)	0	100	100
1	E	166/193 (86%)	165 (99%)	1 (1%)	78	88
1	F	167/193 (86%)	166 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	166/193 (86%)	165 (99%)	1 (1%)	78	88
1	H	154/193 (80%)	154 (100%)	0	100	100
1	I	160/193 (83%)	159 (99%)	1 (1%)	78	88
1	J	169/193 (88%)	168 (99%)	1 (1%)	78	88
1	K	157/193 (81%)	157 (100%)	0	100	100
1	L	157/193 (81%)	156 (99%)	1 (1%)	78	88
2	M	1/6 (17%)	0	1 (100%)	0	0
2	N	1/6 (17%)	1 (100%)	0	100	100
2	O	2/6 (33%)	2 (100%)	0	100	100
2	P	2/6 (33%)	2 (100%)	0	100	100
2	Q	1/6 (17%)	1 (100%)	0	100	100
2	R	3/6 (50%)	3 (100%)	0	100	100
2	S	2/6 (33%)	2 (100%)	0	100	100
2	U	1/6 (17%)	1 (100%)	0	100	100
2	V	2/6 (33%)	2 (100%)	0	100	100
2	W	2/6 (33%)	2 (100%)	0	100	100
2	X	1/6 (17%)	1 (100%)	0	100	100
All	All	1972/2382 (83%)	1964 (100%)	8 (0%)	84	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	E	70	LYS
1	F	218	CYS
1	G	218	CYS
1	I	186	THR
1	J	70	LYS
1	L	9	GLN
2	M	6	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	ASN

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Mol	Chain	Res	Type
1	C	62	HIS
1	C	74	ASN
1	D	63	GLN
1	D	155	GLN
1	D	193	ASN
1	E	155	GLN
1	F	219	GLN
1	G	4	GLN
1	G	95	GLN
1	G	120	HIS
1	J	4	GLN
1	J	63	GLN
1	K	155	GLN
1	K	193	ASN

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	A	211/231 (91%)	0.23	13 (6%) 26 14	38, 61, 116, 148	0
1	B	211/231 (91%)	0.20	7 (3%) 49 28	39, 66, 116, 171	0
1	C	207/231 (89%)	0.11	4 (1%) 66 43	36, 59, 102, 120	0
1	D	210/231 (90%)	0.32	14 (6%) 24 12	37, 61, 132, 154	0
1	E	204/231 (88%)	0.20	7 (3%) 48 27	38, 64, 104, 148	0
1	F	216/231 (93%)	0.31	12 (5%) 30 15	41, 65, 111, 159	0
1	G	216/231 (93%)	0.31	8 (3%) 45 25	44, 72, 125, 138	0
1	H	210/231 (90%)	0.53	14 (6%) 24 12	46, 74, 141, 178	0
1	I	212/231 (91%)	0.48	17 (8%) 18 9	43, 72, 125, 196	0
1	J	214/231 (92%)	0.24	19 (8%) 15 8	38, 58, 118, 130	0
1	K	207/231 (89%)	0.39	12 (5%) 29 15	41, 66, 132, 188	0
1	L	202/231 (87%)	0.34	9 (4%) 38 20	45, 71, 121, 153	0
2	M	1/9 (11%)	4.64	1 (100%) 0 0	63, 63, 63, 63	1 (100%)
2	N	2/9 (22%)	2.13	1 (50%) 0 0	57, 57, 57, 64	2 (100%)
2	O	4/9 (44%)	2.32	1 (25%) 2 1	75, 91, 108, 132	0
2	P	7/9 (77%)	1.60	2 (28%) 1 1	56, 79, 105, 127	0
2	Q	1/9 (11%)	0.91	0 100 100	83, 83, 83, 83	0
2	R	5/9 (55%)	2.47	4 (80%) 0 0	56, 60, 62, 74	5 (100%)
2	S	5/9 (55%)	1.53	1 (20%) 3 2	62, 66, 69, 72	5 (100%)
2	U	1/9 (11%)	2.07	1 (100%) 0 0	62, 62, 62, 62	1 (100%)
2	V	4/9 (44%)	2.13	2 (50%) 0 0	73, 82, 83, 92	0
2	W	7/9 (77%)	1.93	4 (57%) 0 0	74, 88, 109, 119	0
2	X	1/9 (11%)	0.93	0 100 100	69, 69, 69, 69	0
All	All	2558/2871 (89%)	0.33	153 (5%) 27 14	36, 66, 125, 196	14 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	219	GLN	5.8
2	M	6	PHE	4.6
2	P	8	SER	4.6
2	O	3	GLY	4.4
1	D	6	LEU	4.3
1	L	6	LEU	4.3
1	D	197	ASP	4.2
1	A	7	GLN	4.1
1	A	185	ALA	4.0
1	D	219	GLN	4.0
1	I	177	ALA	4.0
1	I	187	GLU	4.0
1	E	184	ALA	4.0
1	K	202	LEU	4.0
1	I	122	PRO	3.9
1	G	206	GLY	3.9
2	R	4	GLY	3.9
1	I	95	GLN	3.8
1	K	197	ASP	3.8
1	J	218	CYS	3.8
1	J	87	HIS	3.7
1	L	184	ALA	3.7
1	J	220	GLY	3.6
1	G	179	GLN	3.6
1	J	94	GLY	3.6
1	K	6	LEU	3.4
1	K	187	GLU	3.3
1	F	218	CYS	3.3
1	F	86	VAL	3.2
1	A	205	LEU	3.2
1	B	187	GLU	3.2
2	R	5	LEU	3.2
1	J	7	GLN	3.2
1	H	185	ALA	3.2
1	F	177	ALA	3.1
1	I	92	ALA	3.1
1	H	122	PRO	3.1
1	K	219	GLN	3.1
1	F	178	SER	3.1
1	L	209	ALA	3.0
1	A	98	GLU	3.0
1	J	202	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	2.9
1	D	13	GLN	2.9
1	A	220	GLY	2.9
1	C	206	GLY	2.9
1	D	90	PRO	2.8
1	A	121	ASN	2.8
1	L	206	GLY	2.8
1	E	121	ASN	2.8
1	H	190	LEU	2.8
1	H	197	ASP	2.8
1	A	197	ASP	2.8
1	D	206	GLY	2.8
1	H	96	MET	2.8
1	J	86	VAL	2.8
1	A	6	LEU	2.8
1	F	185	ALA	2.7
1	J	204	ALA	2.7
1	I	216	THR	2.7
1	H	206	GLY	2.7
1	J	92	ALA	2.7
2	V	4	GLY	2.7
2	W	7	GLY	2.7
1	B	204	ALA	2.7
1	H	191	VAL	2.7
1	F	179	GLN	2.7
1	J	209	ALA	2.7
1	I	83	LEU	2.7
1	B	186	THR	2.7
1	H	188	THR	2.7
1	G	178	SER	2.7
2	V	5	LEU	2.7
1	D	143	ARG	2.6
2	N	7	GLY	2.6
1	G	218	CYS	2.6
1	I	186	THR	2.6
1	A	178	SER	2.6
1	K	178	SER	2.6
1	A	216	THR	2.6
1	L	186	THR	2.6
1	D	174	ALA	2.6
2	P	9	LYS	2.6
1	A	122	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	6	LEU	2.6
1	L	177	ALA	2.6
1	H	192	GLN	2.6
1	D	209	ALA	2.6
1	I	2	ILE	2.5
1	K	151	LEU	2.5
1	E	196	PRO	2.5
1	J	8	GLY	2.5
1	E	177	ALA	2.5
1	J	144	MET	2.5
1	E	85	PRO	2.5
1	G	160	PRO	2.4
1	I	185	ALA	2.4
1	K	95	GLN	2.4
1	J	200	THR	2.4
1	J	145	TYR	2.4
1	I	179	GLN	2.4
1	F	202	LEU	2.4
1	I	121	ASN	2.4
1	L	185	ALA	2.4
1	H	127	GLY	2.4
1	F	184	ALA	2.4
1	H	95	GLN	2.4
1	L	217	ALA	2.3
2	W	8	SER	2.3
1	A	203	LYS	2.3
1	F	6	LEU	2.3
1	A	187	GLU	2.3
1	I	93	PRO	2.3
1	K	200	THR	2.3
1	D	7	GLN	2.3
1	H	123	PRO	2.3
1	J	6	LEU	2.3
2	W	6	PHE	2.3
1	J	121	ASN	2.3
1	H	186	THR	2.3
1	F	198	CYS	2.3
1	D	188	THR	2.2
1	F	121	ASN	2.2
1	I	188	THR	2.2
1	I	7	GLN	2.2
1	D	93	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	198	CYS	2.2
1	J	217	ALA	2.2
1	G	177	ALA	2.2
1	J	213	GLU	2.2
2	R	7	GLY	2.2
1	F	87	HIS	2.2
1	B	95	GLN	2.1
1	I	79	GLU	2.1
1	I	123	PRO	2.1
2	R	6	PHE	2.1
1	B	86	VAL	2.1
1	B	2	ILE	2.1
1	C	177	ALA	2.1
1	D	185	ALA	2.1
1	K	180	GLU	2.1
2	W	4	GLY	2.1
1	C	6	LEU	2.1
2	U	6	PHE	2.1
1	E	197	ASP	2.1
1	G	63	GLN	2.1
1	C	85	PRO	2.1
1	L	109	SER	2.0
1	J	205	LEU	2.0
2	S	8	SER	2.0
1	K	198	CYS	2.0
1	D	196	PRO	2.0
1	K	123	PRO	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.