



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 04:03 AM UTC

PDB ID : 9EE1 / pdb_00009ee1
Title : HIV CA - GLFG peptide (43 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

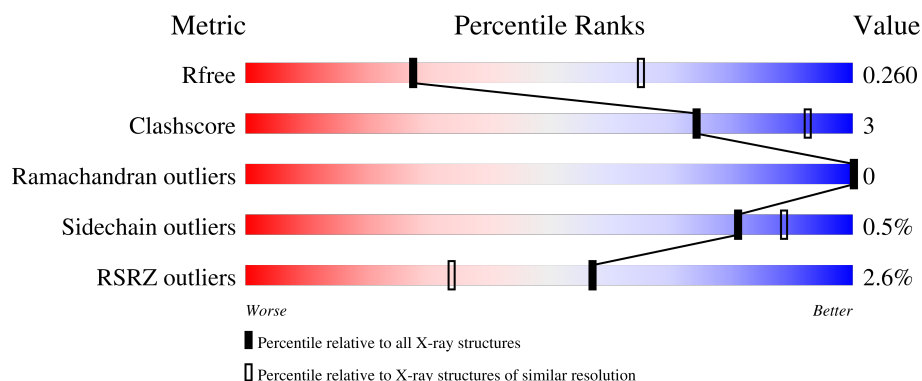
1 Overall quality at a glance

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>3%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>8%</div> </div> </div>
1	B	231	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>
1	C	231	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	D	231	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	E	231	<div> <div></div> <div> <div></div> <div>83%</div> <div>7%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	231	% 84% 8% 8%
1	G	231	% 82% 11% 7%
1	H	231	4% 81% 10% 10%
1	I	231	% 81% 8% 10%
1	J	231	4% 84% 8% 7%
1	K	231	3% 82% 10% 9%
1	L	231	% 80% 9% 11%
2	M	9	11% 78% 22%
2	N	9	11% 89% 11%
2	O	9	11% 67% 11% 22%
2	P	9	78% 22%
2	Q	9	22% 56% 11% 33%
2	R	9	22% 78% 11% 11%
2	S	9	78% 22%
2	T	9	33% 67% 33%
2	U	9	11% 56% 11% 33%
2	V	9	22% 78% 22%
2	W	9	67% 11% 22%
2	X	9	33% 78% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19520 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	212	Total	C	N	O	S	0	0	0
			1572	989	272	297	14			
1	B	216	Total	C	N	O	S	0	0	0
			1639	1032	285	309	13			
1	C	207	Total	C	N	O	S	0	0	0
			1584	993	279	299	13			
1	D	211	Total	C	N	O	S	0	0	0
			1585	994	278	299	14			
1	E	207	Total	C	N	O	S	0	0	0
			1576	995	273	295	13			
1	F	212	Total	C	N	O	S	0	0	0
			1610	1014	281	301	14			
1	G	215	Total	C	N	O	S	0	0	0
			1617	1016	283	304	14			
1	H	208	Total	C	N	O	S	0	0	0
			1559	980	272	293	14			
1	I	208	Total	C	N	O	S	0	0	0
			1554	981	269	291	13			
1	J	214	Total	C	N	O	S	0	0	0
			1629	1020	287	308	14			
1	K	211	Total	C	N	O	S	0	0	0
			1565	985	270	296	14			
1	L	205	Total	C	N	O	S	0	0	0
			1536	969	264	290	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	M	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	N	8	Total	C	N	O	0	0	0
			47	30	8	9			
2	O	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	P	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	Q	6	Total	C	N	O	0	0	0
			38	25	6	7			
2	R	8	Total	C	N	O	0	0	0
			46	30	8	8			
2	S	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	T	6	Total	C	N	O	0	0	0
			34	22	6	6			
2	U	6	Total	C	N	O	0	0	0
			37	24	6	7			
2	V	7	Total	C	N	O	0	0	0
			42	27	7	8			
2	W	7	Total	C	N	O	0	0	0
			41	27	7	7			
2	X	7	Total	C	N	O	0	0	0
			41	27	7	7			

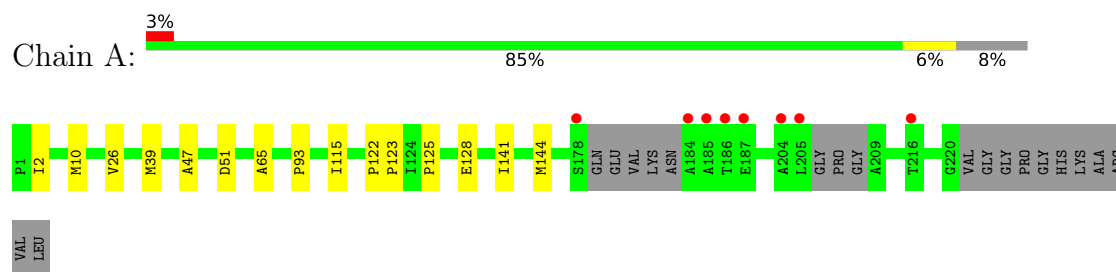
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	K	1	Total	Cl	0	0
			1	1		

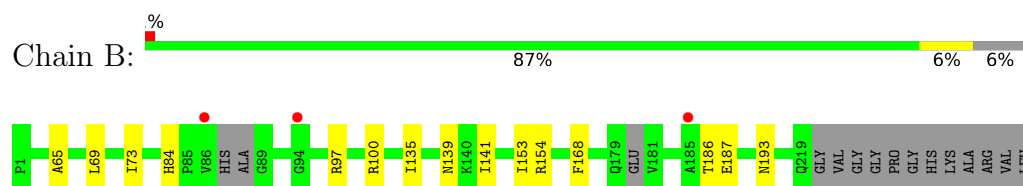
3 Residue-property plots [i](#)

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.

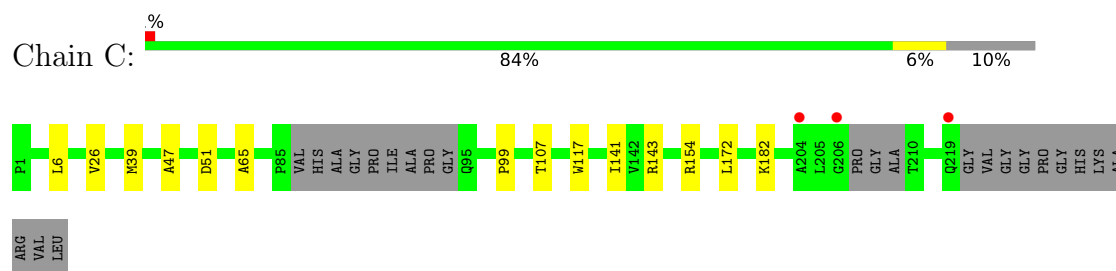
- Molecule 1: Capsid protein p24



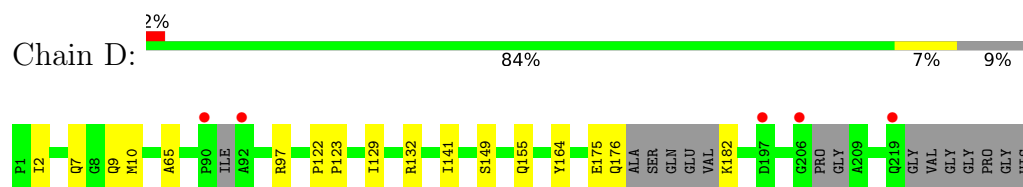
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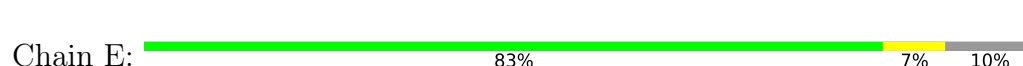
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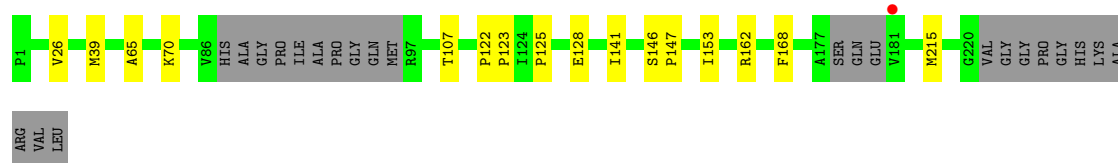


- Molecule 1: Capsid protein p24

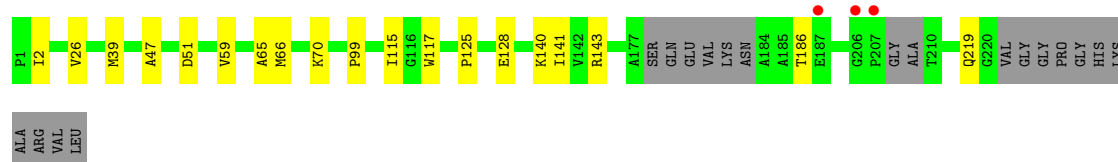
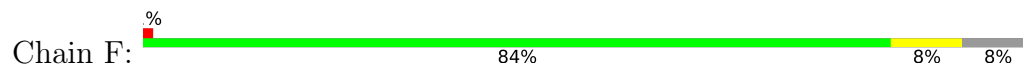


- Molecule 1: Capsid protein p24

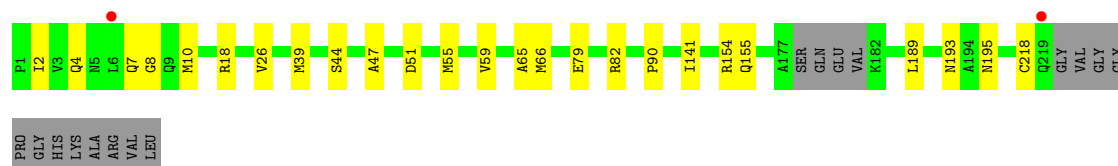
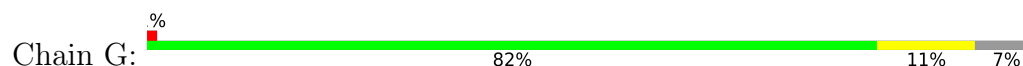




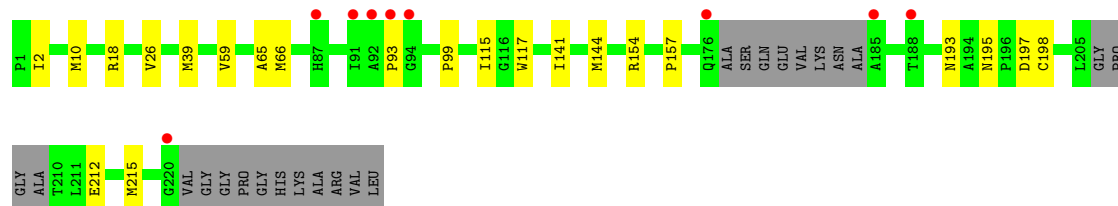
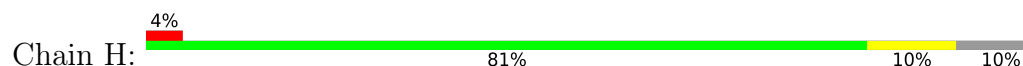
- Molecule 1: Capsid protein p24



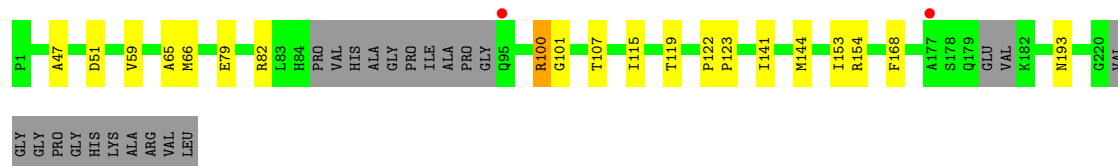
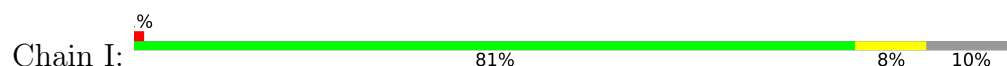
- Molecule 1: Capsid protein p24



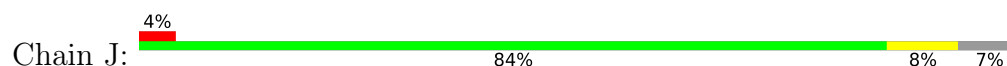
- Molecule 1: Capsid protein p24

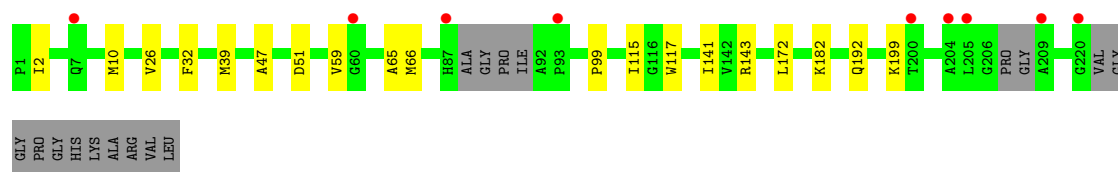


- Molecule 1: Capsid protein p24

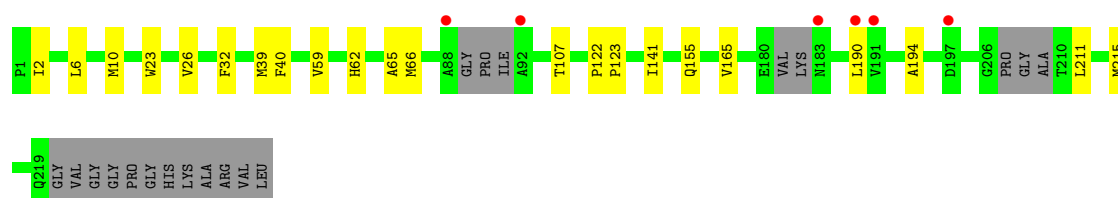
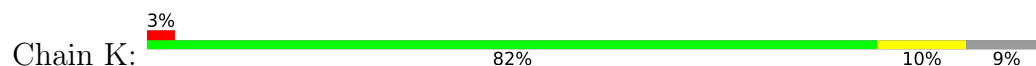


- Molecule 1: Capsid protein p24

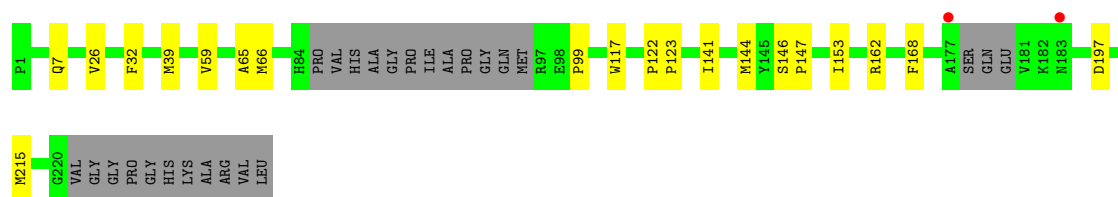
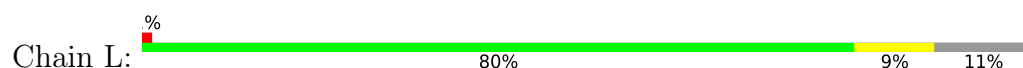




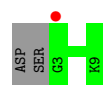
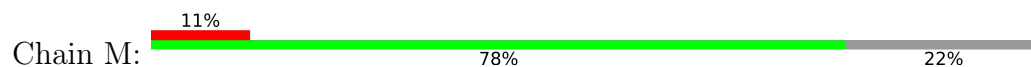
- Molecule 1: Capsid protein p24



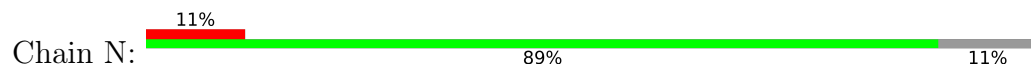
- Molecule 1: Capsid protein p24



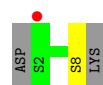
- Molecule 2: GLFG peptide




- Molecule 2: GLFG peptide



- Molecule 2: GLFG peptide



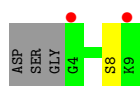
- Molecule 2: GLFG peptide

Chain P:  78% 22%




● Molecule 2: GLFG peptide

Chain Q:  22% 56% 11% 33%




● Molecule 2: GLFG peptide

Chain R:  22% 78% 11% 11%



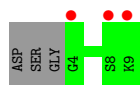
● Molecule 2: GLFG peptide

Chain S:  78% 22%



● Molecule 2: GLFG peptide

Chain T:  33% 67% 33%




● Molecule 2: GLFG peptide

Chain U:  11% 56% 11% 33%



● Molecule 2: GLFG peptide

Chain V:  22% 78% 22%




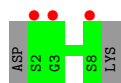
- Molecule 2: GLFG peptide

Chain W:  67% 11% 22%



- Molecule 2: GLFG peptide

Chain X:  33% 78% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.87Å 136.25Å 206.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.20 – 3.00 34.20 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.20-3.00) 99.5 (34.20-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.223 , 0.261 0.223 , 0.260	Depositor DCC
R_{free} test set	3719 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19520	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0/1605	0.21	0/2187
1	B	0.08	0/1673	0.21	0/2276
1	C	0.07	0/1615	0.20	0/2195
1	D	0.07	0/1617	0.19	0/2199
1	E	0.07	0/1608	0.20	0/2187
1	F	0.08	0/1644	0.21	0/2235
1	G	0.07	0/1652	0.20	0/2253
1	H	0.07	0/1592	0.20	0/2168
1	I	0.07	0/1585	0.21	0/2156
1	J	0.08	0/1661	0.20	0/2256
1	K	0.08	0/1596	0.21	0/2174
1	L	0.07	0/1567	0.20	0/2135
2	M	0.04	0/41	0.08	0/53
2	N	0.07	0/47	0.16	0/61
2	O	0.07	0/41	0.16	0/53
2	P	0.07	0/41	0.21	0/53
2	Q	0.05	0/38	0.14	0/49
2	R	0.09	0/46	0.26	0/60
2	S	0.05	0/41	0.11	0/53
2	T	0.10	0/34	0.41	0/44
2	U	0.06	0/37	0.16	0/47
2	V	0.08	0/42	0.23	0/54
2	W	0.05	0/41	0.13	0/53
2	X	0.05	0/41	0.26	0/53
All	All	0.07	0/19905	0.20	0/27054

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	1572	0	1495	9	0
1	B	1639	0	1604	7	0
1	C	1584	0	1532	8	0
1	D	1585	0	1512	10	0
1	E	1576	0	1546	8	0
1	F	1610	0	1565	9	0
1	G	1617	0	1554	14	0
1	H	1559	0	1488	14	0
1	I	1554	0	1493	13	0
1	J	1629	0	1581	11	0
1	K	1565	0	1478	14	0
1	L	1536	0	1474	12	0
2	M	41	0	32	0	0
2	N	47	0	37	0	0
2	O	41	0	32	1	0
2	P	41	0	32	0	0
2	Q	38	0	32	1	0
2	R	46	0	34	1	0
2	S	41	0	32	0	0
2	T	34	0	20	0	0
2	U	37	0	33	1	0
2	V	42	0	35	0	0
2	W	41	0	32	1	0
2	X	41	0	32	0	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	K	1	0	0	0	0
All	All	19520	0	18705	119	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 (119) 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	1.73	0.70
1:H:59:VAL:HG11	1:H:66:MET:HE3	1.75	0.68
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.77	0.67
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.77	0.66
1:I:59:VAL:HG11	1:I:66:MET:HE3	1.77	0.66
1:K:59:VAL:HG11	1:K:66:MET:HE3	1.82	0.60
1:F:70:LYS:NZ	2:R:9:LYS:O	2.34	0.60
1:F:125:PRO:HB2	1:F:128:GLU:HB2	1.84	0.60
1:G:189:LEU:O	1:G:193:ASN:ND2	2.33	0.60
1:J:59:VAL:HG11	1:J:66:MET:HE3	1.84	0.59
1:D:129:ILE:HG12	1:D:132:ARG:HH12	1.68	0.59
1:L:59:VAL:HG11	1:L:66:MET:HE3	1.85	0.59
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.85	0.58
1:A:2:ILE:HG22	1:A:10:MET:HE3	1.85	0.58
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.85	0.57
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.85	0.56
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.86	0.56
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.87	0.56
1:D:97:ARG:HB2	1:G:90:PRO:HB2	1.89	0.55
1:D:176:GLN:NE2	1:D:182:LYS:O	2.36	0.55
1:H:154:ARG:HG2	1:H:193:ASN:HB3	1.89	0.55
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.89	0.54
1:E:125:PRO:HB2	1:E:128:GLU:HB2	1.90	0.54
1:G:59:VAL:HG11	1:G:66:MET:HE3	1.91	0.53
1:I:79:GLU:OE1	1:I:82:ARG:NH1	2.41	0.53
1:K:165:VAL:HG22	1:K:190:LEU:HD11	1.89	0.53
1:C:6:LEU:HB3	1:D:7:GLN:HG3	1.91	0.52
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.92	0.52
1:J:192:GLN:O	1:J:199:LYS:NZ	2.43	0.52
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.91	0.52
1:K:2:ILE:HG22	1:K:10:MET:HE3	1.92	0.52
1:D:9:GLN:NE2	1:G:7:GLN:OE1	2.43	0.51
1:F:59:VAL:HG11	1:F:66:MET:HE3	1.93	0.51
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.91	0.51
1:I:154:ARG:HG2	1:I:193:ASN:HB3	1.92	0.51
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.92	0.50
1:G:79:GLU:OE2	1:G:82:ARG:NH2	2.40	0.50
1:C:99:PRO:HG3	1:C:117:TRP:CE2	2.47	0.50
1:J:172:LEU:HD21	1:J:182:LYS:HA	1.92	0.50
1:K:165:VAL:HG11	1:K:215:MET:HE2	1.94	0.50
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.94	0.50
1:G:2:ILE:HG22	1:G:10:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:PRO:HG3	1:F:117:TRP:CE2	2.48	0.49
1:J:65:ALA:HB1	1:J:141:ILE:HD13	1.94	0.49
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.93	0.49
1:G:155:GLN:CD	1:G:195:ASN:HD22	2.20	0.49
1:K:211:LEU:HG	1:K:215:MET:HE3	1.95	0.48
1:K:215:MET:HB2	1:L:144:MET:HE1	1.95	0.48
1:G:4:GLN:HE21	1:G:8:GLY:HA2	1.78	0.48
1:G:47:ALA:HB1	1:G:51:ASP:HB2	1.94	0.48
1:L:65:ALA:HB1	1:L:141:ILE:HD13	1.96	0.48
1:I:153:ILE:HG21	1:I:168:PHE:HA	1.96	0.47
1:K:107:THR:HG23	2:W:8:SER:HA	1.96	0.47
1:I:107:THR:HG23	2:U:8:SER:HA	1.97	0.47
1:L:99:PRO:HG3	1:L:117:TRP:CE2	2.49	0.47
1:B:84:HIS:O	1:B:100:ARG:NH1	2.48	0.47
1:I:47:ALA:HB1	1:I:51:ASP:HB2	1.94	0.47
1:G:154:ARG:HG2	1:G:193:ASN:HB3	1.96	0.46
1:I:144:MET:HE2	1:I:144:MET:HB3	1.86	0.46
1:L:153:ILE:HG21	1:L:168:PHE:HA	1.97	0.46
1:E:107:THR:HG23	2:Q:8:SER:HA	1.97	0.46
1:I:100:ARG:HG3	1:I:101:GLY:H	1.81	0.46
1:J:99:PRO:HG3	1:J:117:TRP:CE2	2.50	0.46
1:L:144:MET:HE2	1:L:144:MET:HB3	1.87	0.46
1:H:144:MET:HE2	1:H:144:MET:HB3	1.82	0.46
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.97	0.46
1:D:155:GLN:HB2	1:D:164:TYR:CG	2.51	0.46
1:D:122:PRO:HA	1:D:123:PRO:HD3	1.87	0.45
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.98	0.45
1:K:6:LEU:HD13	1:L:7:GLN:HE21	1.81	0.45
1:H:2:ILE:HD11	1:H:115:ILE:HG12	1.98	0.45
1:K:23:TRP:CZ3	1:K:40:PHE:HB2	2.52	0.45
1:B:186:THR:HG23	1:B:187:GLU:H	1.82	0.44
1:G:18:ARG:HH12	1:H:18:ARG:HH11	1.65	0.44
1:H:99:PRO:HG3	1:H:117:TRP:CE2	2.51	0.44
1:F:140:LYS:HG2	1:F:143:ARG:HH21	1.81	0.44
1:H:157:PRO:HA	1:H:195:ASN:HD21	1.82	0.44
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.98	0.44
1:B:153:ILE:HG21	1:B:168:PHE:HA	2.00	0.44
1:J:47:ALA:HB1	1:J:51:ASP:HB2	1.99	0.44
1:B:135:ILE:O	1:B:139:ASN:ND2	2.51	0.44
1:L:122:PRO:HA	1:L:123:PRO:HD3	1.89	0.44
1:H:2:ILE:HG22	1:H:10:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ALA:HB1	1:C:141:ILE:HD13	2.00	0.43
1:B:154:ARG:HA	1:B:193:ASN:HB3	1.99	0.43
1:E:122:PRO:HA	1:E:123:PRO:HD3	1.87	0.43
1:E:153:ILE:HG21	1:E:168:PHE:HA	2.00	0.43
1:H:197:ASP:OD1	1:H:198:CYS:N	2.51	0.43
1:H:212:GLU:HG3	1:I:144:MET:SD	2.59	0.43
1:L:162:ARG:HA	1:L:215:MET:HE3	2.00	0.43
1:E:26:VAL:HG21	1:E:39:MET:HG2	2.01	0.43
1:F:2:ILE:HD11	1:F:115:ILE:HG12	2.00	0.43
1:J:2:ILE:HD11	1:J:115:ILE:HG12	2.00	0.43
1:K:32:PHE:HE2	1:K:62:HIS:HB3	1.83	0.43
1:C:172:LEU:HD21	1:C:182:LYS:HA	2.01	0.43
1:L:32:PHE:HZ	1:L:66:MET:HE2	1.84	0.43
1:A:125:PRO:HB2	1:A:128:GLU:HB2	1.99	0.43
1:K:122:PRO:HA	1:K:123:PRO:HD3	1.86	0.43
1:C:47:ALA:HB1	1:C:51:ASP:HB2	1.99	0.42
1:A:2:ILE:HD11	1:A:115:ILE:HG12	2.01	0.42
1:A:122:PRO:HA	1:A:123:PRO:HD3	1.89	0.42
1:B:69:LEU:O	1:B:73:ILE:HG12	2.20	0.42
1:A:93:PRO:HG3	1:J:117:TRP:CZ2	2.54	0.42
1:J:2:ILE:HG22	1:J:10:MET:HE3	2.01	0.42
1:E:146:SER:HA	1:E:147:PRO:HD3	1.94	0.41
1:F:47:ALA:HB1	1:F:51:ASP:HB2	2.01	0.41
1:I:122:PRO:HA	1:I:123:PRO:HD3	1.86	0.41
1:K:155:GLN:HB3	1:K:194:ALA:HA	2.02	0.41
1:C:107:THR:HG23	2:O:8:SER:HA	2.03	0.41
1:D:149:SER:HA	1:D:175:GLU:OE2	2.21	0.41
1:E:162:ARG:HA	1:E:215:MET:HE3	2.03	0.41
1:H:26:VAL:HG21	1:H:39:MET:HG2	2.02	0.41
1:J:26:VAL:HG21	1:J:39:MET:HG2	2.03	0.41
1:L:146:SER:HA	1:L:147:PRO:HD3	1.97	0.41
1:I:115:ILE:O	1:I:119:THR:OG1	2.34	0.40
1:A:144:MET:HE2	1:A:144:MET:HB3	1.85	0.40
1:C:117:TRP:CZ2	1:H:93:PRO:HG3	2.56	0.40
1:H:215:MET:HB2	1:I:144:MET:HE1	2.02	0.40
1:J:32:PHE:HZ	1:J:66:MET:HE2	1.87	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	A	206/231 (89%)	202 (98%)	4 (2%)	0	100	100
1	B	210/231 (91%)	205 (98%)	5 (2%)	0	100	100
1	C	201/231 (87%)	191 (95%)	10 (5%)	0	100	100
1	D	203/231 (88%)	200 (98%)	3 (2%)	0	100	100
1	E	201/231 (87%)	197 (98%)	4 (2%)	0	100	100
1	F	206/231 (89%)	200 (97%)	6 (3%)	0	100	100
1	G	211/231 (91%)	203 (96%)	8 (4%)	0	100	100
1	H	202/231 (87%)	197 (98%)	5 (2%)	0	100	100
1	I	202/231 (87%)	194 (96%)	8 (4%)	0	100	100
1	J	208/231 (90%)	200 (96%)	8 (4%)	0	100	100
1	K	203/231 (88%)	195 (96%)	8 (4%)	0	100	100
1	L	199/231 (86%)	191 (96%)	8 (4%)	0	100	100
2	M	5/9 (56%)	4 (80%)	1 (20%)	0	100	100
2	N	6/9 (67%)	6 (100%)	0	0	100	100
2	O	5/9 (56%)	5 (100%)	0	0	100	100
2	P	5/9 (56%)	5 (100%)	0	0	100	100
2	Q	4/9 (44%)	4 (100%)	0	0	100	100
2	R	6/9 (67%)	6 (100%)	0	0	100	100
2	S	5/9 (56%)	5 (100%)	0	0	100	100
2	T	4/9 (44%)	4 (100%)	0	0	100	100
2	U	4/9 (44%)	4 (100%)	0	0	100	100
2	V	5/9 (56%)	4 (80%)	1 (20%)	0	100	100
2	W	5/9 (56%)	5 (100%)	0	0	100	100
2	X	5/9 (56%)	5 (100%)	0	0	100	100
All	All	2511/2880 (87%)	2432 (97%)	79 (3%)	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	159/193 (82%)	159 (100%)	0	100	100
1	B	173/193 (90%)	172 (99%)	1 (1%)	78	88
1	C	167/193 (86%)	165 (99%)	2 (1%)	63	82
1	D	162/193 (84%)	162 (100%)	0	100	100
1	E	166/193 (86%)	165 (99%)	1 (1%)	78	88
1	F	167/193 (86%)	165 (99%)	2 (1%)	63	82
1	G	166/193 (86%)	165 (99%)	1 (1%)	78	88
1	H	160/193 (83%)	160 (100%)	0	100	100
1	I	158/193 (82%)	157 (99%)	1 (1%)	78	88
1	J	171/193 (89%)	170 (99%)	1 (1%)	78	88
1	K	157/193 (81%)	157 (100%)	0	100	100
1	L	158/193 (82%)	157 (99%)	1 (1%)	78	88
2	M	2/6 (33%)	2 (100%)	0	100	100
2	N	3/6 (50%)	3 (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	3/6 (50%)	3 (100%)	0	100	100
2	R	2/6 (33%)	2 (100%)	0	100	100
2	S	2/6 (33%)	2 (100%)	0	100	100
2	T	1/6 (17%)	1 (100%)	0	100	100
2	U	3/6 (50%)	3 (100%)	0	100	100
2	V	3/6 (50%)	3 (100%)	0	100	100
2	W	2/6 (33%)	2 (100%)	0	100	100
2	X	2/6 (33%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1991/2388 (83%)	1981 (100%)	10 (0%)	81	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	ARG
1	C	143	ARG
1	C	154	ARG
1	E	70	LYS
1	F	186	THR
1	F	219	GLN
1	G	218	CYS
1	I	100	ARG
1	J	143	ARG
1	L	197	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	C	62	HIS
1	D	9	GLN
1	D	121	ASN
1	D	193	ASN
1	E	67	GLN
1	F	50	GLN
1	F	155	GLN
1	G	4	GLN
1	G	139	ASN
1	H	63	GLN
1	H	195	ASN
1	I	193	ASN
1	J	63	GLN
1	J	219	GLN
1	K	62	HIS

5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	212/231 (91%)	-0.08	8 (3%) 44 24	39, 64, 119, 132	0
1	B	216/231 (93%)	-0.12	3 (1%) 73 51	40, 66, 110, 143	0
1	C	207/231 (89%)	-0.11	3 (1%) 73 51	38, 63, 111, 135	0
1	D	211/231 (91%)	-0.07	5 (2%) 59 36	40, 65, 121, 130	0
1	E	207/231 (89%)	-0.26	1 (0%) 87 72	41, 62, 102, 114	0
1	F	212/231 (91%)	-0.11	3 (1%) 73 51	42, 65, 127, 141	0
1	G	215/231 (93%)	-0.03	2 (0%) 81 61	48, 76, 129, 144	0
1	H	208/231 (90%)	0.14	9 (4%) 40 21	48, 82, 137, 162	0
1	I	208/231 (90%)	-0.07	2 (0%) 79 59	44, 70, 104, 122	0
1	J	214/231 (92%)	-0.13	9 (4%) 40 22	42, 60, 110, 133	0
1	K	211/231 (91%)	0.12	6 (2%) 55 32	44, 69, 143, 159	0
1	L	205/231 (88%)	-0.05	2 (0%) 79 59	49, 76, 113, 142	0
2	M	7/9 (77%)	0.88	1 (14%) 6 3	68, 85, 104, 105	0
2	N	8/9 (88%)	0.77	1 (12%) 8 5	62, 76, 92, 94	0
2	O	7/9 (77%)	1.13	1 (14%) 6 3	61, 77, 88, 91	0
2	P	7/9 (77%)	0.24	0 100 100	51, 60, 78, 80	0
2	Q	6/9 (66%)	1.47	2 (33%) 1 1	55, 69, 80, 81	0
2	R	8/9 (88%)	1.17	2 (25%) 2 1	65, 73, 88, 97	0
2	S	7/9 (77%)	0.34	0 100 100	66, 74, 82, 83	0
2	T	6/9 (66%)	1.63	3 (50%) 0 0	77, 90, 96, 102	0
2	U	6/9 (66%)	0.67	1 (16%) 4 3	66, 83, 87, 87	0
2	V	7/9 (77%)	1.53	2 (28%) 1 1	66, 82, 98, 100	0
2	W	7/9 (77%)	0.85	0 100 100	59, 75, 83, 94	0
2	X	7/9 (77%)	1.76	3 (42%) 0 1	70, 80, 96, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2609/2880 (90%)	-0.03	69 (2%) 57 34	38, 69, 123, 162	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	GLY	4.0
2	X	2	SER	3.7
1	G	219	GLN	3.7
2	Q	4	GLY	3.7
1	H	87	HIS	3.4
2	R	2	SER	3.4
1	F	207	PRO	3.4
1	A	184	ALA	3.3
1	H	93	PRO	3.2
1	K	183	ASN	3.2
1	E	181	VAL	3.1
2	N	2	SER	3.1
2	V	3	GLY	3.1
1	H	92	ALA	3.0
1	K	190	LEU	3.0
1	B	86	VAL	2.9
1	H	91	ILE	2.9
1	J	205	LEU	2.9
1	J	220	GLY	2.8
1	K	197	ASP	2.8
1	H	185	ALA	2.8
2	O	2	SER	2.6
1	A	205	LEU	2.6
1	C	204	ALA	2.6
1	H	188	THR	2.6
2	X	8	SER	2.6
2	T	4	GLY	2.5
1	D	90	PRO	2.5
1	B	94	GLY	2.5
1	A	216	THR	2.5
2	T	9	LYS	2.5
1	G	6	LEU	2.5
1	K	191	VAL	2.5
1	A	185	ALA	2.4
1	I	177	ALA	2.4
1	F	187	GLU	2.4
1	J	60	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	2.4
1	I	95	GLN	2.4
1	A	178	SER	2.4
1	H	94	GLY	2.4
1	J	87	HIS	2.4
2	V	4	GLY	2.4
2	Q	9	LYS	2.4
1	A	187	GLU	2.4
2	X	3	GLY	2.3
2	T	8	SER	2.3
2	R	9	LYS	2.3
1	H	220	GLY	2.3
1	L	177	ALA	2.3
1	H	176	GLN	2.3
1	J	204	ALA	2.3
1	J	200	THR	2.3
1	J	93	PRO	2.2
1	K	88	ALA	2.2
1	D	219	GLN	2.2
1	J	7	GLN	2.2
1	D	206	GLY	2.2
1	C	219	GLN	2.2
1	L	183	ASN	2.2
2	U	3	GLY	2.2
1	D	197	ASP	2.2
1	A	186	THR	2.1
1	J	209	ALA	2.1
2	M	3	GLY	2.1
1	K	92	ALA	2.1
1	F	206	GLY	2.1
1	D	92	ALA	2.0
1	A	204	ALA	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	G	301	1/1	0.85	0.10	81,81,81,81	0
3	CL	A	301	1/1	0.86	0.16	78,78,78,78	0
3	CL	K	301	1/1	0.88	0.09	73,73,73,73	0
3	CL	F	301	1/1	0.95	0.08	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.