



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:35 am GMT

PDB ID : 4U0B  
Title : Hexamer HIV-1 CA in complex with CPSF6 peptide, P212121 crystal form  
Authors : Price, A.J.; Jacques, D.A.; James, L.C.  
Deposited on : 2014-07-11  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

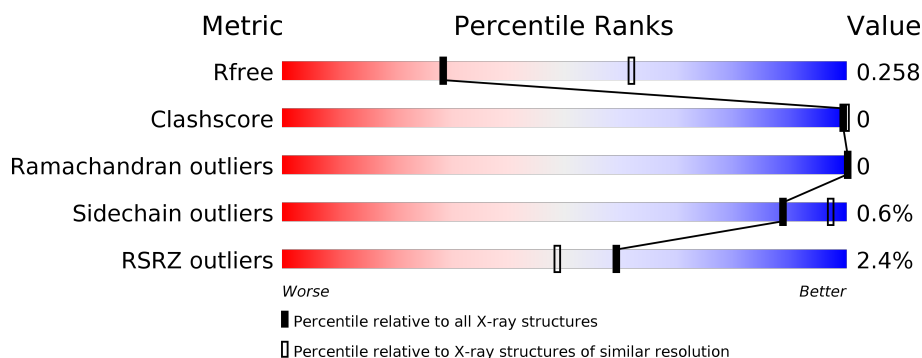
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>90%</div> <div>10%</div> </div>
1	B	231	<div> <div>4%</div> <div>86%</div> <div>13%</div> </div>
1	C	231	<div> <div>3%</div> <div>84%</div> <div>14%</div> </div>
1	D	231	<div> <div>3%</div> <div>87%</div> <div>12%</div> </div>
1	E	231	<div> <div>2%</div> <div>85%</div> <div>14%</div> </div>
1	F	231	<div> <div>2%</div> <div>88%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	231	<div> <div></div> <div>85%</div> <div>14%</div> </div>
1	H	231	<div> <div></div> <div>86%</div> <div>13%</div> </div>
1	I	231	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
1	J	231	<div> <div></div> <div>85%</div> <div>14%</div> </div>
1	K	231	<div> <div>2%</div> <div>85%</div> <div>15%</div> </div>
1	L	231	<div> <div></div> <div>90%</div> <div>10%</div> </div>
2	M	15	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	N	15	<div> <div></div> <div>87%</div> <div>13%</div> </div>
2	O	15	<div> <div>13%</div> <div>93%</div> <div>7%</div> </div>
2	P	15	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	Q	15	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	R	15	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	S	15	<div> <div>13%</div> <div>93%</div> <div>7%</div> </div>
2	T	15	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	U	15	<div> <div></div> <div>93%</div> <div>7%</div> </div>
2	V	15	<div> <div>7%</div> <div>93%</div> <div>7%</div> </div>
2	W	15	<div> <div>20%</div> <div>93%</div> <div>7%</div> </div>
2	X	15	<div> <div>7%</div> <div>93%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19958 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	208	Total	C	N	O	S	0	1	0
			1601	1008	278	301	14			
1	B	201	Total	C	N	O	S	0	0	0
			1554	979	271	290	14			
1	C	198	Total	C	N	O	S	0	1	0
			1527	964	263	286	14			
1	D	203	Total	C	N	O	S	0	1	0
			1577	993	275	294	15			
1	E	198	Total	C	N	O	S	0	1	0
			1533	967	266	286	14			
1	F	207	Total	C	N	O	S	0	0	0
			1585	997	275	300	13			
1	G	198	Total	C	N	O	S	0	1	0
			1533	967	266	286	14			
1	H	202	Total	C	N	O	S	0	1	0
			1555	980	270	291	14			
1	I	211	Total	C	N	O	S	0	1	0
			1627	1025	285	302	15			
1	J	198	Total	C	N	O	S	0	1	0
			1533	967	266	286	14			
1	K	197	Total	C	N	O	S	0	1	0
			1526	962	265	285	14			
1	L	208	Total	C	N	O	S	0	0	0
			1604	1008	279	304	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 Cleavage and polyadenylation specificity factor subunit 6.

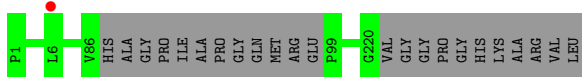
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	N	13	Total	C	N	O	0	0	0
			98	68	15	15			
2	O	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	P	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	Q	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	R	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	S	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	T	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	U	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	V	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	W	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	X	14	Total	C	N	O	0	0	0
			99	69	15	15			

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

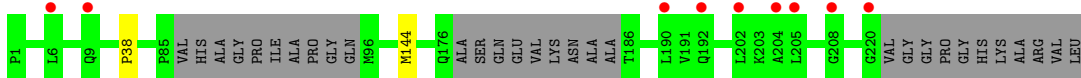
- Molecule 1: Capsid protein p24

Chain A: 




- Molecule 1: Capsid protein p24

Chain B: 




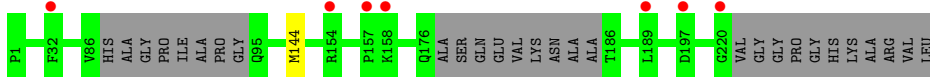
- Molecule 1: Capsid protein p24

Chain C: 




- Molecule 1: Capsid protein p24

Chain D: 

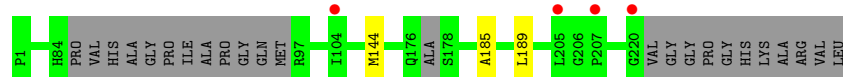
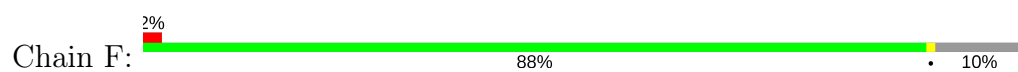


- Molecule 1: Capsid protein p24

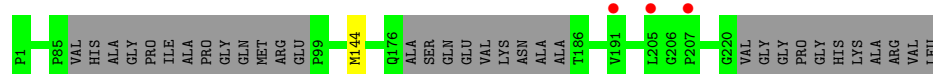
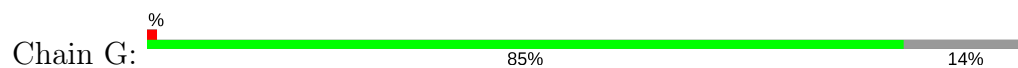
Chain E: 



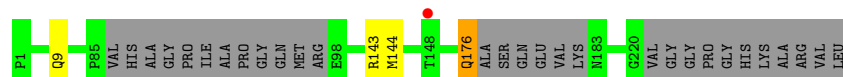
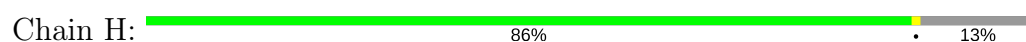
- Molecule 1: Capsid protein p24



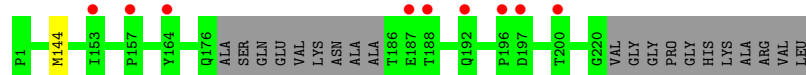
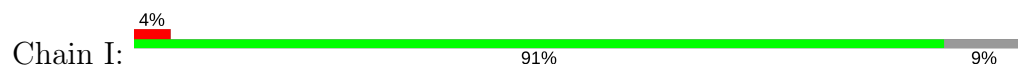
- Molecule 1: Capsid protein p24



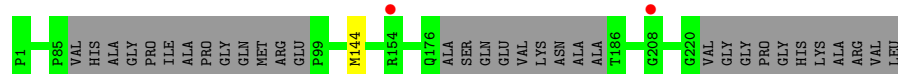
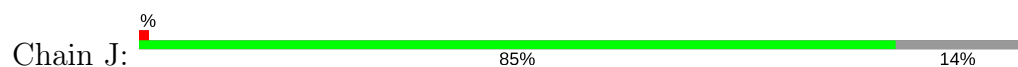
- Molecule 1: Capsid protein p24



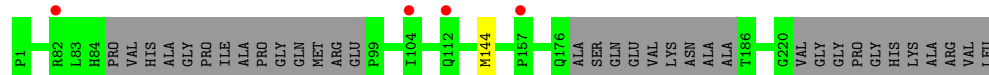
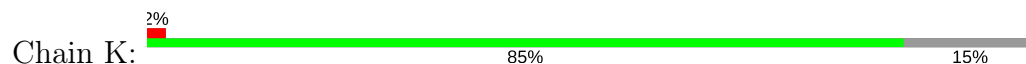
- Molecule 1: Capsid protein p24



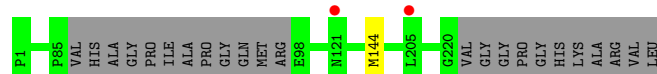
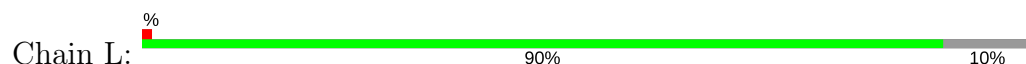
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24




- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

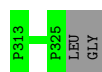


Chain M:  93% 7%



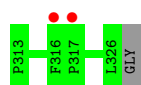
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain N:  87% 13%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain O:  13% 93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain P:  93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain Q:  93% 7%



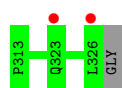
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain R:  93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain S:  13% 93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain T:  93% 7%

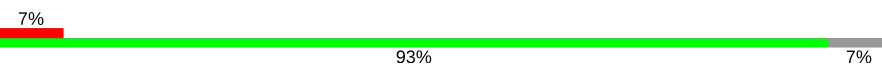


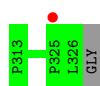
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain U:  93% 7%



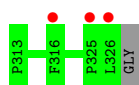
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain V:  7% 93% 7%



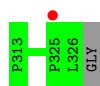
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain W:  20% 93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain X:  7% 93% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.13Å 135.89Å 208.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.80 48.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.60-2.80) 92.7 (48.55-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.230 , 0.262 0.229 , 0.258	Depositor DCC
$R_{free}$ test set	4479 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.8	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.238 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.25	0/1637	0.43	0/2225
1	B	0.25	0/1586	0.41	0/2153
1	C	0.25	0/1562	0.40	0/2122
1	D	0.25	0/1612	0.41	0/2188
1	E	0.25	0/1568	0.41	0/2129
1	F	0.25	0/1616	0.42	0/2196
1	G	0.25	0/1568	0.41	0/2129
1	H	0.25	0/1590	0.41	0/2161
1	I	0.25	0/1666	0.41	0/2265
1	J	0.25	0/1568	0.40	0/2129
1	K	0.25	0/1560	0.41	0/2117
1	L	0.25	0/1637	0.42	0/2225
2	M	0.29	0/105	0.36	0/145
2	N	0.29	0/104	0.39	0/143
2	O	0.30	0/109	0.38	0/150
2	P	0.31	0/105	0.36	0/145
2	Q	0.30	0/109	0.40	0/150
2	R	0.29	0/109	0.35	0/150
2	S	0.29	0/105	0.40	0/145
2	T	0.29	0/105	0.35	0/145
2	U	0.30	0/105	0.35	0/145
2	V	0.30	0/109	0.35	0/150
2	W	0.28	0/105	0.35	0/145
2	X	0.28	0/105	0.34	0/145
All	All	0.25	0/20445	0.41	0/27797

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	1601	0	1588	0	0
1	B	1554	0	1534	1	0
1	C	1527	0	1507	2	0
1	D	1577	0	1562	0	0
1	E	1533	0	1518	0	0
1	F	1585	0	1551	1	0
1	G	1533	0	1518	0	0
1	H	1555	0	1536	2	0
1	I	1627	0	1611	0	0
1	J	1533	0	1518	0	0
1	K	1526	0	1511	0	0
1	L	1604	0	1586	0	0
2	M	99	0	91	0	0
2	N	98	0	95	0	0
2	O	103	0	97	0	0
2	P	99	0	91	0	0
2	Q	103	0	97	0	0
2	R	103	0	97	0	0
2	S	99	0	91	0	0
2	T	99	0	91	0	0
2	U	99	0	91	0	0
2	V	103	0	97	0	0
2	W	99	0	91	0	0
2	X	99	0	91	0	0
All	All	19958	0	19660	4	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 0.

All (4) 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:H:143:ARG:HD3	1:H:176:GLN:HG3	1.91	0.52
1:F:185:ALA:O	1:F:189:LEU:HB3	2.15	0.46
1:C:9:GLN:CD	1:H:9:GLN:HE22	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PRO:HG3	1:C:57:ASN:HB3	2.02	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	205/231 (89%)	200 (98%)	5 (2%)	0	100	100
1	B	195/231 (84%)	191 (98%)	4 (2%)	0	100	100
1	C	193/231 (84%)	189 (98%)	4 (2%)	0	100	100
1	D	198/231 (86%)	193 (98%)	5 (2%)	0	100	100
1	E	193/231 (84%)	189 (98%)	4 (2%)	0	100	100
1	F	201/231 (87%)	198 (98%)	3 (2%)	0	100	100
1	G	193/231 (84%)	189 (98%)	4 (2%)	0	100	100
1	H	197/231 (85%)	193 (98%)	4 (2%)	0	100	100
1	I	208/231 (90%)	205 (99%)	3 (1%)	0	100	100
1	J	193/231 (84%)	188 (97%)	5 (3%)	0	100	100
1	K	192/231 (83%)	190 (99%)	2 (1%)	0	100	100
1	L	204/231 (88%)	202 (99%)	2 (1%)	0	100	100
2	M	12/15 (80%)	12 (100%)	0	0	100	100
2	N	11/15 (73%)	11 (100%)	0	0	100	100
2	O	12/15 (80%)	12 (100%)	0	0	100	100
2	P	12/15 (80%)	12 (100%)	0	0	100	100
2	Q	12/15 (80%)	12 (100%)	0	0	100	100
2	R	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
2	S	12/15 (80%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	12/15 (80%)	12 (100%)	0	0	100	100
2	U	12/15 (80%)	12 (100%)	0	0	100	100
2	V	12/15 (80%)	12 (100%)	0	0	100	100
2	W	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
2	X	12/15 (80%)	12 (100%)	0	0	100	100
All	All	2515/2952 (85%)	2468 (98%)	47 (2%)	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	174/193 (90%)	174 (100%)	0	100	100
1	B	168/193 (87%)	167 (99%)	1 (1%)	89	97
1	C	166/193 (86%)	164 (99%)	2 (1%)	75	94
1	D	172/193 (89%)	171 (99%)	1 (1%)	89	97
1	E	167/193 (86%)	166 (99%)	1 (1%)	89	97
1	F	169/193 (88%)	168 (99%)	1 (1%)	89	97
1	G	167/193 (86%)	166 (99%)	1 (1%)	89	97
1	H	168/193 (87%)	166 (99%)	2 (1%)	75	94
1	I	176/193 (91%)	175 (99%)	1 (1%)	89	97
1	J	167/193 (86%)	166 (99%)	1 (1%)	89	97
1	K	166/193 (86%)	165 (99%)	1 (1%)	89	97
1	L	174/193 (90%)	173 (99%)	1 (1%)	89	97
2	M	10/12 (83%)	10 (100%)	0	100	100
2	N	11/12 (92%)	11 (100%)	0	100	100
2	O	11/12 (92%)	11 (100%)	0	100	100
2	P	10/12 (83%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	11/12 (92%)	11 (100%)	0	100	100
2	R	11/12 (92%)	11 (100%)	0	100	100
2	S	10/12 (83%)	10 (100%)	0	100	100
2	T	10/12 (83%)	10 (100%)	0	100	100
2	U	10/12 (83%)	10 (100%)	0	100	100
2	V	11/12 (92%)	11 (100%)	0	100	100
2	W	10/12 (83%)	10 (100%)	0	100	100
2	X	10/12 (83%)	10 (100%)	0	100	100
All	All	2159/2460 (88%)	2146 (99%)	13 (1%)	89	97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	144	MET
1	C	112	GLN
1	C	144	MET
1	D	144	MET
1	E	144	MET
1	F	144	MET
1	G	144	MET
1	H	144	MET
1	H	176	GLN
1	I	144	MET
1	J	144	MET
1	K	144	MET
1	L	144	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	GLN
1	C	112	GLN
1	D	95	GLN
1	E	121	ASN
1	F	112	GLN
1	F	121	ASN
1	H	9	GLN
2	N	319	GLN



### 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	208/231 (90%)	0.01	1 (0%) 90 88	43, 69, 129, 161	0
1	B	201/231 (87%)	0.37	9 (4%) 34 24	42, 75, 162, 222	0
1	C	198/231 (85%)	0.18	6 (3%) 51 39	57, 86, 131, 145	0
1	D	203/231 (87%)	0.20	7 (3%) 46 34	57, 87, 165, 185	0
1	E	198/231 (85%)	0.13	5 (2%) 58 47	53, 86, 137, 156	0
1	F	207/231 (89%)	0.09	4 (1%) 67 58	48, 72, 128, 158	0
1	G	198/231 (85%)	0.19	3 (1%) 74 67	41, 74, 142, 166	0
1	H	202/231 (87%)	0.06	1 (0%) 90 88	54, 83, 124, 146	0
1	I	211/231 (91%)	0.23	9 (4%) 36 26	52, 83, 149, 165	0
1	J	198/231 (85%)	0.23	2 (1%) 82 77	55, 91, 159, 189	0
1	K	197/231 (85%)	0.15	4 (2%) 65 56	48, 75, 133, 172	0
1	L	208/231 (90%)	0.03	2 (0%) 82 77	41, 72, 132, 163	0
2	M	14/15 (93%)	-0.01	0 100 100	58, 73, 99, 117	0
2	N	13/15 (86%)	0.25	0 100 100	50, 76, 87, 89	0
2	O	14/15 (93%)	0.81	2 (14%) 3 2	64, 87, 114, 116	0
2	P	14/15 (93%)	0.07	0 100 100	72, 89, 109, 118	0
2	Q	14/15 (93%)	0.34	0 100 100	72, 97, 116, 123	0
2	R	14/15 (93%)	0.33	0 100 100	73, 87, 100, 124	0
2	S	14/15 (93%)	0.75	2 (14%) 3 2	65, 81, 95, 102	0
2	T	14/15 (93%)	0.50	0 100 100	65, 85, 108, 113	0
2	U	14/15 (93%)	0.08	0 100 100	70, 92, 118, 126	0
2	V	14/15 (93%)	0.33	1 (7%) 17 9	69, 90, 115, 120	0
2	W	14/15 (93%)	1.30	3 (21%) 1 1	73, 98, 122, 123	0
2	X	14/15 (93%)	0.51	1 (7%) 17 9	63, 82, 109, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2596/2952 (87%)	0.17	62 (2%)	59 49	41, 81, 144, 222	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	LEU	4.9
1	B	204	ALA	4.5
1	K	82	ARG	4.1
1	B	202	LEU	4.0
1	I	188	THR	3.8
1	B	220	GLY	3.7
1	B	208	GLY	3.6
1	I	192	GLN	3.5
1	I	196	PRO	3.4
1	L	121	ASN	3.4
1	F	220	GLY	3.3
1	D	197	ASP	3.2
1	K	104	ILE	3.2
1	D	154	ARG	3.1
2	W	326	LEU	3.0
1	B	190	LEU	2.9
1	C	219	GLN	2.9
1	E	124	ILE	2.9
1	B	9	GLN	2.9
1	C	207	PRO	2.9
2	W	325	PRO	2.8
1	E	144	MET	2.8
1	H	148	THR	2.8
1	D	32	PHE	2.7
2	S	326	LEU	2.7
1	E	203	LYS	2.6
2	O	317	PRO	2.6
1	F	104	ILE	2.6
2	O	316	PHE	2.6
1	K	157	PRO	2.5
2	S	323	GLN	2.5
1	F	207	PRO	2.5
1	I	157	PRO	2.5
1	E	126	VAL	2.5
1	D	220	GLY	2.5
2	X	325	PRO	2.4
1	B	192	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	158	LYS	2.4
1	D	157	PRO	2.3
1	C	202	LEU	2.3
1	C	217	ALA	2.3
1	J	208	GLY	2.3
1	C	220	GLY	2.2
2	V	325	PRO	2.2
1	K	112	GLN	2.2
1	B	6	LEU	2.2
1	G	207	PRO	2.2
1	E	202	LEU	2.2
1	F	205	LEU	2.1
1	G	205	LEU	2.1
1	I	197	ASP	2.1
2	W	316	PHE	2.1
1	J	154	ARG	2.1
1	I	187	GLU	2.1
1	I	200	THR	2.1
1	D	189	LEU	2.1
1	G	191	VAL	2.1
1	I	164	TYR	2.1
1	I	153	ILE	2.0
1	A	6	LEU	2.0
1	C	73	ILE	2.0
1	L	205	LEU	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 carbohydrates 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.