



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:57 AM UTC

PDB ID : 4U0D / pdb_00004u0d
Title : Hexameric HIV-1 CA in complex with Nup153 peptide, P212121 crystal form
Authors : Price, A.J.; Jacques, D.A.; James, L.C.
Deposited on : 2014-07-11
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

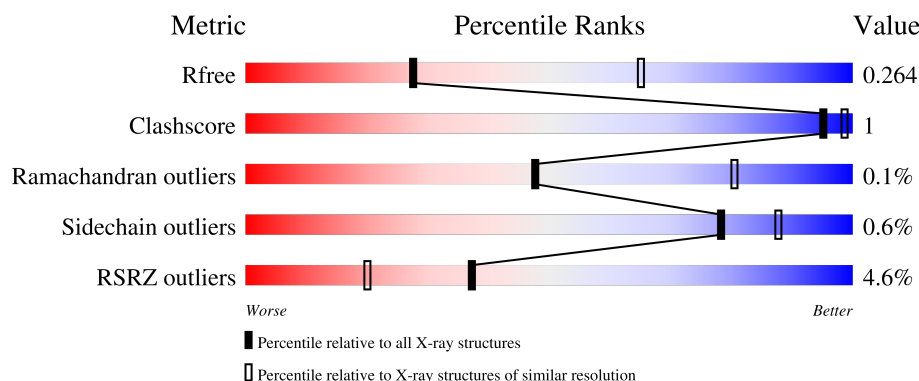
1 Overall quality at a glance

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.



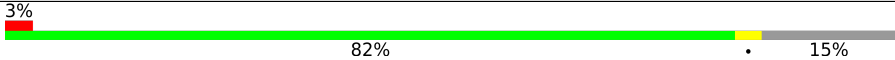
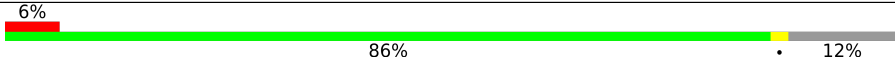
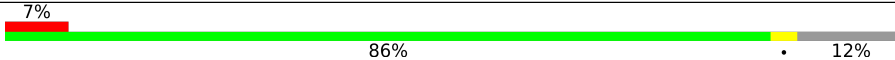
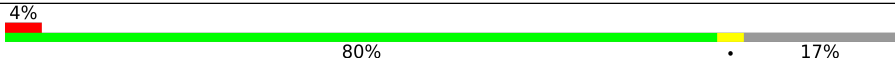
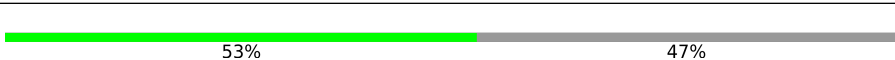
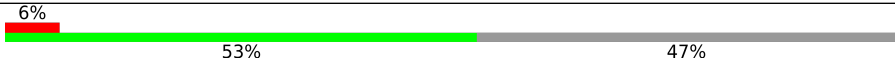
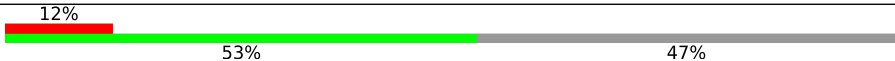
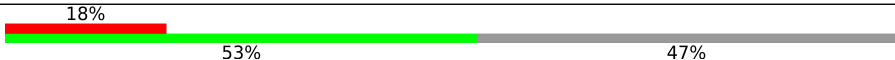
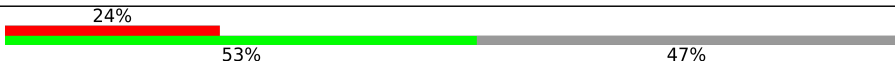
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	3% 87% 6% 6%
1	B	231	2% 87% • 10%
1	C	231	2% 87% • 9%
1	D	231	3% 87% • 9%
1	E	231	3% 80% • 17%

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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	17	
2	N	17	
2	O	17	
2	P	17	
2	Q	17	
2	R	17	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19269 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 Gag polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	2	0
			1663	1046	291	312	14			
1	B	207	Total	C	N	O	S	0	3	0
			1602	1007	279	302	14			
1	C	211	Total	C	N	O	S	0	3	0
			1619	1021	281	302	15			
1	D	210	Total	C	N	O	S	0	2	0
			1607	1015	277	301	14			
1	E	192	Total	C	N	O	S	0	3	0
			1484	941	252	278	13			
1	F	211	Total	C	N	O	S	0	2	0
			1631	1025	285	308	13			
1	G	212	Total	C	N	O	S	0	3	0
			1636	1029	285	308	14			
1	H	204	Total	C	N	O	S	0	2	0
			1580	998	276	292	14			
1	I	196	Total	C	N	O	S	0	2	0
			1500	950	255	282	13			
1	J	204	Total	C	N	O	S	0	2	0
			1565	992	268	291	14			
1	K	204	Total	C	N	O	S	0	2	0
			1548	983	260	291	14			
1	L	191	Total	C	N	O	S	0	2	0
			1455	923	246	274	12			

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 Nuclear pore complex protein Nup153.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	9	Total	C	N	O	0	0	0
			63	42	9	12			
2	N	9	Total	C	N	O	0	0	0
			63	42	9	12			
2	O	9	Total	C	N	O	0	0	0
			63	42	9	12			
2	P	9	Total	C	N	O	0	0	0
			63	42	9	12			
2	Q	9	Total	C	N	O	0	0	0
			63	42	9	12			
2	R	9	Total	C	N	O	0	0	0
			63	42	9	12			

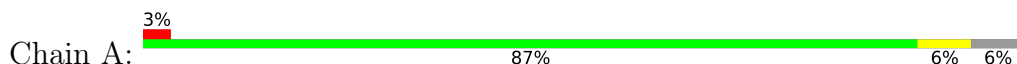
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cl	0	0
			1	1		

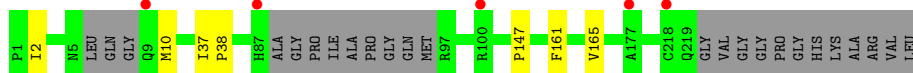
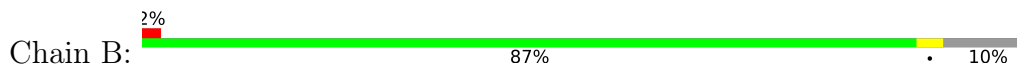
3 Residue-property plots [i](#)

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.

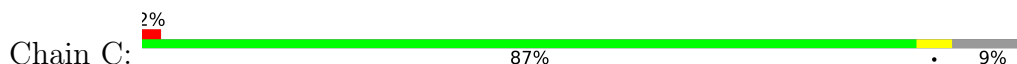
- Molecule 1: Gag polypeptide



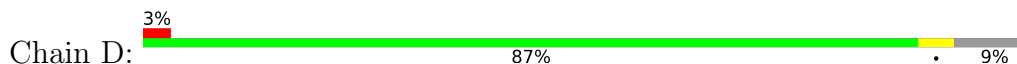
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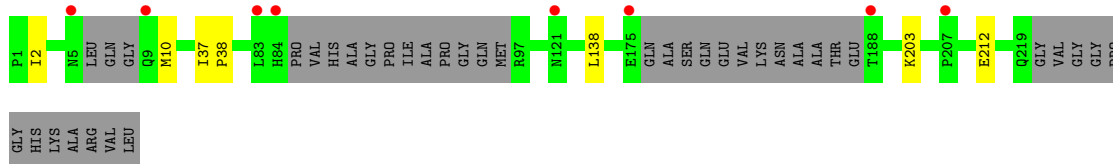
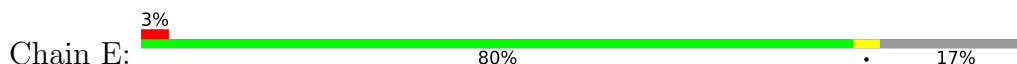
- Molecule 1: Gag polypeptide



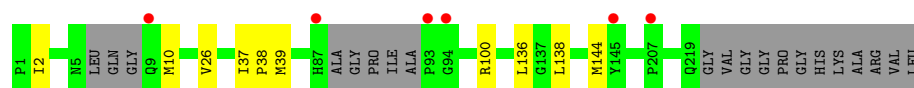
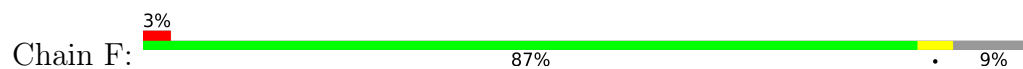
- Molecule 1: Gag polypeptide



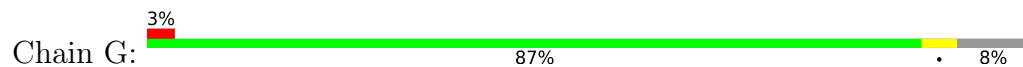
- Molecule 1: Gag polypeptide



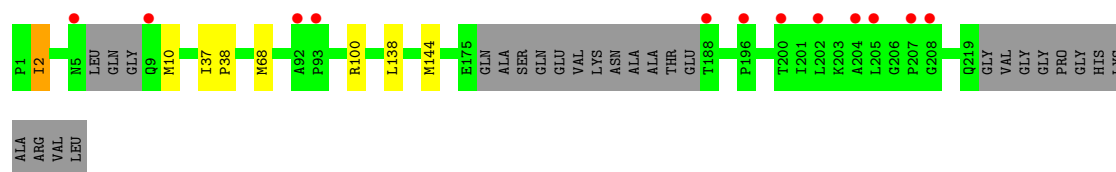
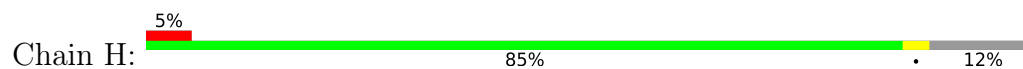
• Molecule 1: Gag polypeptide



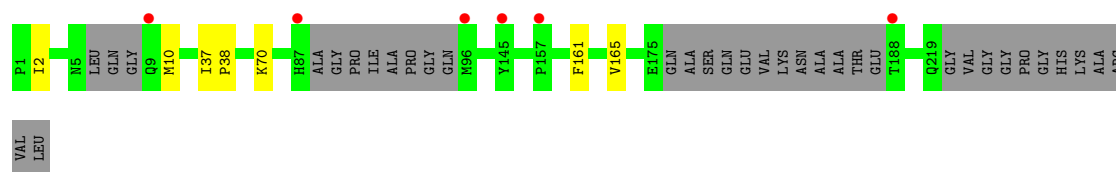
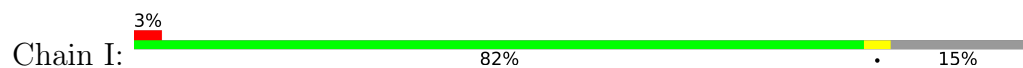
• Molecule 1: Gag polypeptide



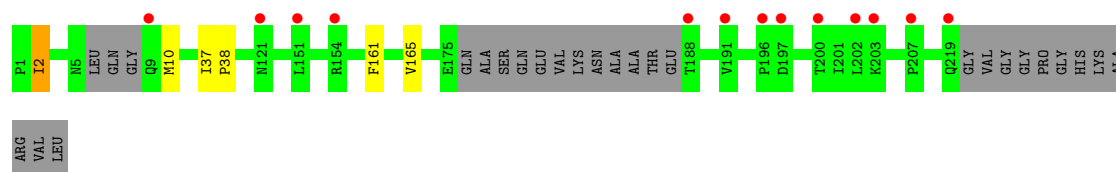
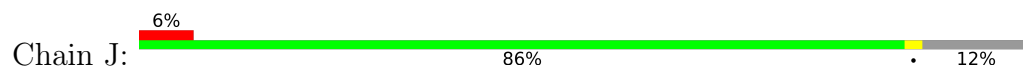
• Molecule 1: Gag polypeptide



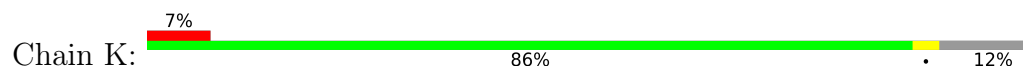
• Molecule 1: Gag polypeptide

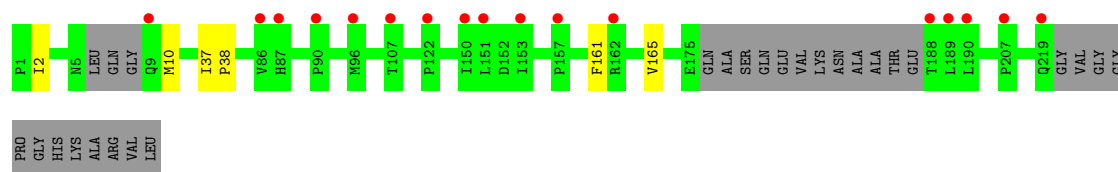


• Molecule 1: Gag polypeptide

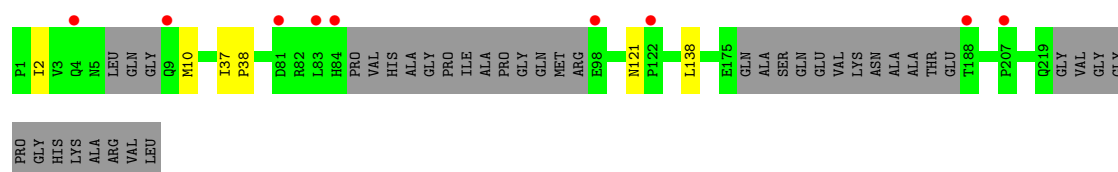
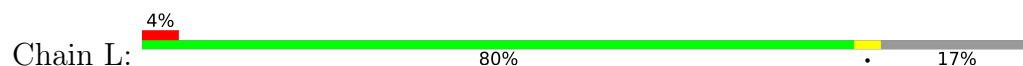


• Molecule 1: Gag polypeptide

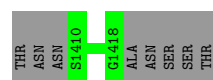




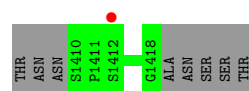
- Molecule 1: Gag polyprotein



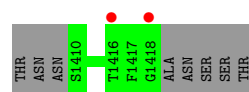
- Molecule 2: Nuclear pore complex protein Nup153



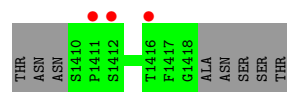
- Molecule 2: Nuclear pore complex protein Nup153



- Molecule 2: Nuclear pore complex protein Nup153



- Molecule 2: Nuclear pore complex protein Nup153



- Molecule 2: Nuclear pore complex protein Nup153



THR	ASN	ASN	S1410	P1411	S1412	G1413	V1414	F1415	T1416	F1417	G1418	ALA	ASN	SER	SER	THR

- Molecule 2: Nuclear pore complex protein Nup153



THR	ASN	ASN	S1410	P1411	S1412	G1413	V1414	F1415	T1416	F1417	G1418	ALA	ASN	SER	SER	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.38Å 138.06Å 211.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.67 – 3.00 115.67 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (115.67-3.00) 96.6 (115.67-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.246 , 0.267 0.244 , 0.264	Depositor DCC
R_{free} test set	3884 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.136 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19269	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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](#)

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	0.39	0/1699	0.68	0/2312
1	B	0.38	0/1637	0.67	0/2225
1	C	0.38	0/1657	0.67	0/2256
1	D	0.39	0/1642	0.67	0/2235
1	E	0.38	0/1516	0.67	0/2059
1	F	0.38	0/1665	0.67	0/2263
1	G	0.38	0/1672	0.67	0/2273
1	H	0.38	0/1615	0.66	0/2194
1	I	0.38	0/1531	0.67	0/2082
1	J	0.39	0/1600	0.66	0/2177
1	K	0.39	0/1582	0.67	0/2155
1	L	0.38	0/1484	0.67	0/2019
2	M	0.50	0/65	0.60	0/87
2	N	0.46	0/65	0.58	0/87
2	O	0.47	0/65	0.51	0/87
2	P	0.46	0/65	0.49	0/87
2	Q	0.43	0/65	0.49	0/87
2	R	0.43	0/65	0.46	0/87
All	All	0.38	0/19690	0.67	0/26772

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 [i](#)

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	1663	0	1639	7	0
1	B	1602	0	1572	3	0
1	C	1619	0	1583	4	0
1	D	1607	0	1580	5	0
1	E	1484	0	1461	4	0
1	F	1631	0	1599	5	0
1	G	1636	0	1609	4	0
1	H	1580	0	1560	4	0
1	I	1500	0	1451	3	0
1	J	1565	0	1534	3	0
1	K	1548	0	1507	3	0
1	L	1455	0	1417	4	0
2	M	63	0	56	0	0
2	N	63	0	56	0	0
2	O	63	0	56	0	0
2	P	63	0	56	0	0
2	Q	63	0	56	0	0
2	R	63	0	56	0	0
3	E	1	0	0	0	0
All	All	19269	0	18848	47	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 1.

All (47) 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:A:92:ALA:HB3	1:A:93:PRO:HD3	1.79	0.65
1:H:68:MET:SD	1:H:144:MET:HE1	2.48	0.53
1:A:93:PRO:N	1:A:94:GLY:HA2	2.24	0.53
1:A:37:ILE:HB	1:A:38:PRO:HD3	1.95	0.48
1:C:37:ILE:HB	1:C:38:PRO:HD3	1.95	0.47
1:F:37:ILE:HB	1:F:38:PRO:HD3	1.96	0.47
1:B:2:ILE:HG22	1:B:10:MET:HE3	1.97	0.47
1:L:37:ILE:HB	1:L:38:PRO:HD3	1.97	0.47
1:A:161:PHE:O	1:A:165:VAL:HG23	2.15	0.47
1:E:37:ILE:HB	1:E:38:PRO:HD3	1.97	0.46
1:J:37:ILE:HB	1:J:38:PRO:HD3	1.98	0.46
1:A:2:ILE:HG22	1:A:10:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:ILE:HG22	1:K:10:MET:HE3	1.98	0.46
1:D:37:ILE:HB	1:D:38:PRO:HD3	1.97	0.46
1:J:2:ILE:HG22	1:J:10:MET:HE3	1.97	0.46
1:A:96:MET:HE3	1:A:124:ILE:HD12	1.97	0.45
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.98	0.45
1:K:37:ILE:HB	1:K:38:PRO:HD3	1.98	0.45
1:E:2:ILE:HG22	1:E:10:MET:HE3	1.99	0.45
1:H:37:ILE:HB	1:H:38:PRO:HD3	1.99	0.45
1:J:161:PHE:O	1:J:165:VAL:HG23	2.17	0.45
1:A:37:ILE:CD1	1:A:138:LEU:HB3	2.47	0.44
1:B:37:ILE:HB	1:B:38:PRO:HD3	1.99	0.44
1:G:2:ILE:HG22	1:G:10:MET:HE3	1.99	0.44
1:G:37:ILE:HB	1:G:38:PRO:HD3	1.99	0.44
1:H:2:ILE:HG22	1:H:10:MET:HE3	1.99	0.44
1:L:2:ILE:HG22	1:L:10:MET:HE3	2.00	0.44
1:G:202:LEU:HD22	1:G:214:MET:HG2	2.00	0.44
1:C:2:ILE:HG22	1:C:10:MET:HE3	2.00	0.44
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.99	0.44
1:E:37:ILE:HD12	1:E:138:LEU:HB3	2.00	0.43
1:F:2:ILE:HG22	1:F:10:MET:HE3	1.99	0.43
1:C:26:VAL:HG21	1:C:39:MET:HG2	2.00	0.43
1:I:2:ILE:HG22	1:I:10:MET:HE3	1.99	0.43
1:K:161:PHE:O	1:K:165:VAL:HG23	2.18	0.43
1:C:161:PHE:O	1:C:165:VAL:HG23	2.18	0.43
1:E:212:GLU:HG3	1:F:144:MET:HE1	2.01	0.42
1:I:37:ILE:HB	1:I:38:PRO:HD3	2.00	0.42
1:L:37:ILE:HD12	1:L:138:LEU:HB3	2.02	0.42
1:H:37:ILE:HD12	1:H:138:LEU:HB3	2.01	0.42
1:D:161:PHE:O	1:D:165:VAL:HG23	2.19	0.42
1:D:37:ILE:HD12	1:D:138:LEU:HB3	2.01	0.41
1:F:37:ILE:HD12	1:F:138:LEU:HB3	2.03	0.41
1:B:161:PHE:O	1:B:165:VAL:HG23	2.20	0.41
1:D:123:PRO:HD3	1:L:121:ASN:HD21	1.85	0.41
1:G:161:PHE:O	1:G:165:VAL:HG23	2.22	0.40
1:I:161:PHE:O	1:I:165:VAL:HG23	2.21	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	212/231 (92%)	206 (97%)	6 (3%)	0	100	100
1	B	202/231 (87%)	195 (96%)	6 (3%)	1 (0%)	24	60
1	C	206/231 (89%)	199 (97%)	6 (3%)	1 (0%)	24	60
1	D	204/231 (88%)	199 (98%)	5 (2%)	0	100	100
1	E	185/231 (80%)	178 (96%)	7 (4%)	0	100	100
1	F	205/231 (89%)	199 (97%)	6 (3%)	0	100	100
1	G	207/231 (90%)	200 (97%)	6 (3%)	1 (0%)	24	60
1	H	198/231 (86%)	187 (94%)	11 (6%)	0	100	100
1	I	188/231 (81%)	182 (97%)	6 (3%)	0	100	100
1	J	198/231 (86%)	190 (96%)	8 (4%)	0	100	100
1	K	198/231 (86%)	192 (97%)	6 (3%)	0	100	100
1	L	183/231 (79%)	176 (96%)	7 (4%)	0	100	100
2	M	7/17 (41%)	7 (100%)	0	0	100	100
2	N	7/17 (41%)	7 (100%)	0	0	100	100
2	O	7/17 (41%)	5 (71%)	2 (29%)	0	100	100
2	P	7/17 (41%)	6 (86%)	1 (14%)	0	100	100
2	Q	7/17 (41%)	6 (86%)	1 (14%)	0	100	100
2	R	7/17 (41%)	6 (86%)	1 (14%)	0	100	100
All	All	2428/2874 (84%)	2340 (96%)	85 (4%)	3 (0%)	48	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	93	PRO
1	B	147	PRO
1	C	147	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/193 (93%)	177 (98%)	3 (2%)	53	78
1	B	174/193 (90%)	174 (100%)	0	100	100
1	C	173/193 (90%)	173 (100%)	0	100	100
1	D	173/193 (90%)	172 (99%)	1 (1%)	78	88
1	E	161/193 (83%)	160 (99%)	1 (1%)	78	88
1	F	177/193 (92%)	175 (99%)	2 (1%)	65	83
1	G	177/193 (92%)	175 (99%)	2 (1%)	65	83
1	H	171/193 (89%)	169 (99%)	2 (1%)	63	82
1	I	160/193 (83%)	159 (99%)	1 (1%)	78	88
1	J	168/193 (87%)	167 (99%)	1 (1%)	78	88
1	K	165/193 (86%)	165 (100%)	0	100	100
1	L	156/193 (81%)	156 (100%)	0	100	100
2	M	7/14 (50%)	7 (100%)	0	100	100
2	N	7/14 (50%)	7 (100%)	0	100	100
2	O	7/14 (50%)	7 (100%)	0	100	100
2	P	7/14 (50%)	7 (100%)	0	100	100
2	Q	7/14 (50%)	7 (100%)	0	100	100
2	R	7/14 (50%)	7 (100%)	0	100	100
All	All	2077/2400 (86%)	2064 (99%)	13 (1%)	78	88

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

Mol	Chain	Res	Type
1	A	2	ILE
1	A	100	ARG
1	A	136	LEU
1	D	100	ARG
1	E	203	LYS
1	F	100	ARG

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Mol	Chain	Res	Type
1	F	136	LEU
1	G	37	ILE
1	G	136	LEU
1	H	2	ILE
1	H	100	ARG
1	I	70	LYS
1	J	2	ILE

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

Mol	Chain	Res	Type
1	A	112	GLN
1	A	179	GLN
1	B	112	GLN
1	B	179	GLN
1	C	21	ASN
1	D	176	GLN
1	E	21	ASN
1	F	21	ASN
1	H	12	HIS
1	J	12	HIS
1	K	84	HIS
1	K	112	GLN
1	L	21	ASN
1	L	112	GLN
1	L	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/231 (93%)	0.25	6 (2%) 55 32	36, 64, 140, 159	0
1	B	207/231 (89%)	0.19	5 (2%) 59 36	38, 64, 109, 131	1 (0%)
1	C	211/231 (91%)	0.29	4 (1%) 66 43	42, 64, 127, 143	1 (0%)
1	D	210/231 (90%)	0.22	6 (2%) 53 31	38, 66, 138, 159	0
1	E	192/231 (83%)	0.17	8 (4%) 40 22	35, 66, 106, 126	1 (0%)
1	F	211/231 (91%)	0.13	6 (2%) 55 32	34, 58, 99, 139	0
1	G	212/231 (91%)	0.10	7 (3%) 49 28	30, 56, 101, 127	1 (0%)
1	H	204/231 (88%)	0.39	12 (5%) 28 14	36, 66, 154, 186	0
1	I	196/231 (84%)	0.35	6 (3%) 51 30	50, 81, 146, 160	0
1	J	204/231 (88%)	0.56	13 (6%) 25 13	53, 88, 182, 202	0
1	K	204/231 (88%)	0.72	17 (8%) 17 9	58, 98, 165, 184	0
1	L	191/231 (82%)	0.40	9 (4%) 36 19	49, 77, 127, 156	0
2	M	9/17 (52%)	0.03	0 100 100	40, 47, 59, 62	0
2	N	9/17 (52%)	0.60	1 (11%) 10 6	42, 45, 67, 70	0
2	O	9/17 (52%)	1.87	2 (22%) 2 1	78, 98, 111, 114	0
2	P	9/17 (52%)	1.93	3 (33%) 1 1	72, 93, 122, 125	0
2	Q	9/17 (52%)	2.34	6 (66%) 0 0	93, 121, 140, 141	0
2	R	9/17 (52%)	2.11	4 (44%) 0 1	94, 111, 157, 158	0
All	All	2512/2874 (87%)	0.34	115 (4%) 37 20	30, 70, 146, 202	4 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	188	THR	5.9
1	L	98	GLU	4.8
1	H	188	THR	4.6

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Mol	Chain	Res	Type	RSRZ
2	R	1411	PRO	4.2
2	O	1416	THR	4.2
1	L	83	LEU	4.1
1	L	84	HIS	3.9
1	F	93	PRO	3.9
1	K	219	GLN	3.9
1	D	186	THR	3.9
1	C	183	ASN	3.7
2	P	1416	THR	3.7
1	K	188	THR	3.6
1	L	188	THR	3.6
1	C	177	ALA	3.6
1	G	93	PRO	3.5
1	H	93	PRO	3.5
1	K	207	PRO	3.5
1	G	92	ALA	3.4
1	I	96	MET	3.4
2	P	1411	PRO	3.4
2	Q	1416	THR	3.4
2	Q	1411	PRO	3.4
1	B	177	ALA	3.2
1	J	9	GLN	3.2
2	R	1416	THR	3.2
2	R	1412	SER	3.2
2	P	1412	SER	3.1
1	F	145	TYR	3.1
1	I	188	THR	3.1
1	G	198	CYS	3.1
1	I	87	HIS	3.0
1	L	207	PRO	2.8
1	K	86	VAL	2.8
1	F	94	GLY	2.8
1	F	9	GLN	2.8
1	A	93	PRO	2.8
1	D	157	PRO	2.8
1	E	188	THR	2.8
1	L	9	GLN	2.7
1	D	151	LEU	2.7
1	J	203	LYS	2.7
1	K	122	PRO	2.7
1	D	177	ALA	2.7
1	K	87	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	87	HIS	2.7
1	H	202	LEU	2.6
1	K	190	LEU	2.6
1	I	157	PRO	2.6
1	C	9	GLN	2.6
1	A	205	LEU	2.6
1	H	92	ALA	2.6
1	J	196	PRO	2.6
1	B	9	GLN	2.6
2	Q	1414	VAL	2.6
2	Q	1415	PHE	2.5
1	I	9	GLN	2.5
1	J	202	LEU	2.5
1	K	151	LEU	2.4
1	E	175	GLU	2.4
1	J	154	ARG	2.4
1	D	185	ALA	2.4
1	L	4[A]	GLN	2.4
1	H	200	THR	2.4
1	K	189	LEU	2.4
2	N	1412	SER	2.4
2	Q	1412	SER	2.4
1	B	218	CYS	2.4
1	E	84	HIS	2.4
2	O	1418	GLY	2.3
1	E	207	PRO	2.3
1	J	207	PRO	2.3
1	L	122	PRO	2.3
1	J	197	ASP	2.3
2	R	1414	VAL	2.3
1	H	207	PRO	2.2
1	A	91	ILE	2.2
1	K	150	ILE	2.2
1	K	90	PRO	2.2
1	E	9	GLN	2.2
1	A	208	GLY	2.2
1	H	204	ALA	2.2
1	J	151	LEU	2.2
1	G	9	GLN	2.2
1	A	92	ALA	2.2
1	B	87	HIS	2.2
1	C	186	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	200	THR	2.1
1	K	107	THR	2.1
1	I	145	TYR	2.1
1	E	83	LEU	2.1
2	Q	1410	SER	2.1
1	G	207	PRO	2.1
1	L	81	ASP	2.1
1	J	191	VAL	2.1
1	K	153	ILE	2.1
1	K	9	GLN	2.1
1	K	96	MET	2.1
1	A	180	GLU	2.1
1	G	94	GLY	2.1
1	H	208	GLY	2.1
1	K	162	ARG	2.1
1	K	157	PRO	2.1
1	E	121	ASN	2.1
1	F	87	HIS	2.1
1	E	5	ASN	2.1
1	J	121	ASN	2.1
1	D	162	ARG	2.1
1	H	205	LEU	2.1
1	B	100	ARG	2.0
1	H	5	ASN	2.0
1	H	9	GLN	2.0
1	F	207	PRO	2.0
1	H	196	PRO	2.0
1	J	219	GLN	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($\text{\AA}^2$)	Q<0.9
3	CL	E	301	1/1	0.95	0.08	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.