



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:42 PM GMT

PDB ID : 4U0D  
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](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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

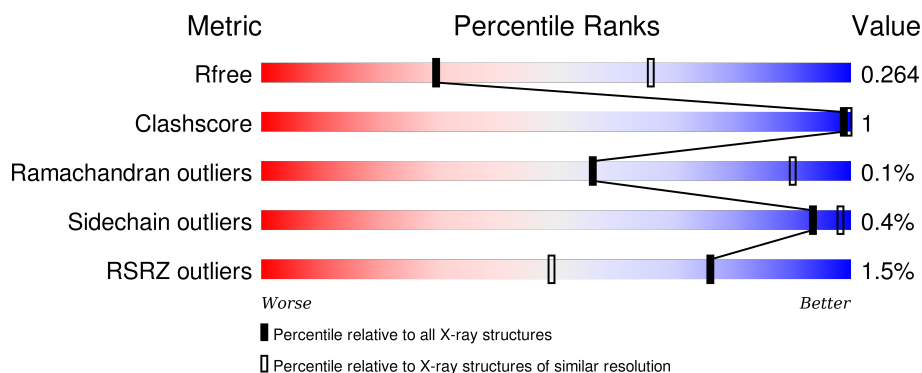
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	
1	B	231	
1	C	231	
1	D	231	
1	E	231	

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Mol	Chain	Length	Quality of chain
1	F	231	 88% 9%
1	G	231	 88% 8%
1	H	231	 86% 12%
1	I	231	 83% 15%
1	J	231	 87% 12%
1	K	231	 87% 12%
1	L	231	 81% 17%
2	M	17	 53% 47%
2	N	17	 53% 47%
2	O	17	 53% 47%
2	P	17	 53% 47%
2	Q	17	 53% 47%
2	R	17	 53% 47%

## 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			

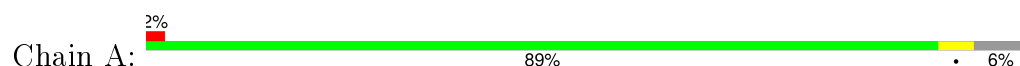
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

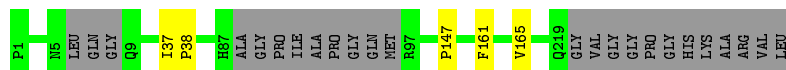
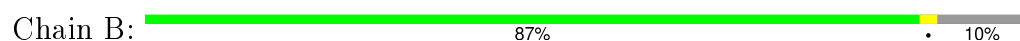
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



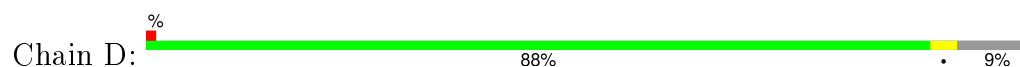
- Molecule 1: Gag polypeptide



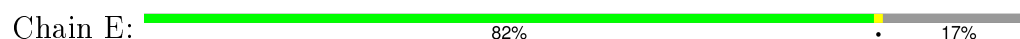
- Molecule 1: Gag polypeptide



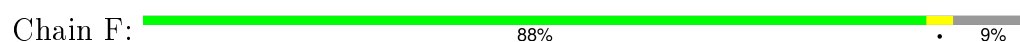
- Molecule 1: Gag polypeptide

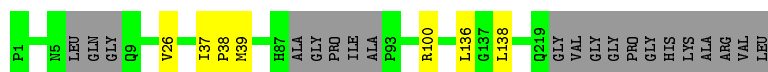


- Molecule 1: Gag polypeptide



- Molecule 1: Gag polypeptide





- Molecule 1: Gag polyprotein

Chain G: 88% 8%



- Molecule 1: Gag polyprotein

Chain H: 86% 2% 12%



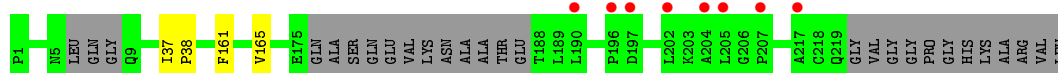
- Molecule 1: Gag polyprotein

Chain I: 83% 2% 15%



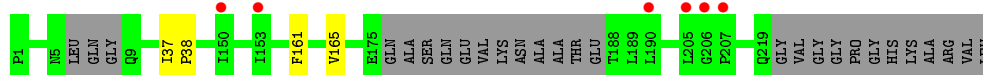
- Molecule 1: Gag polyprotein

Chain J: 87% 3% 12%



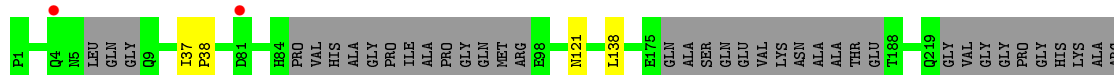
- Molecule 1: Gag polyprotein

Chain K: 87% 3% 12%



- Molecule 1: Gag polyprotein

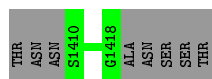
Chain L: 81% 2% 17%



- Molecule 2: Nuclear pore complex protein Nup153

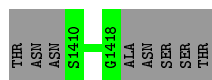


Chain M:  53% 47%



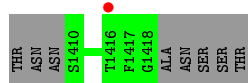
- Molecule 2: Nuclear pore complex protein Nup153

Chain N:  53% 47%



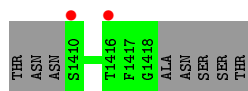
- Molecule 2: Nuclear pore complex protein Nup153

Chain O:  6% 53% 47%



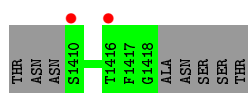
- Molecule 2: Nuclear pore complex protein Nup153

Chain P:  12% 53% 47%



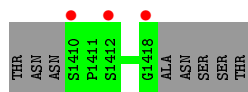
- Molecule 2: Nuclear pore complex protein Nup153

Chain Q:  12% 53% 47%



- Molecule 2: Nuclear pore complex protein Nup153

Chain R:  18% 53% 47%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.38Å 138.06Å 211.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.67 – 3.00 46.07 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (115.67-3.00) 91.2 (46.07-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 11.4	EDS
Estimated twinning fraction	0.136 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 77374 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19269	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.25	0/1699	0.40	0/2312
1	B	0.25	0/1637	0.39	0/2225
1	C	0.25	0/1657	0.39	0/2256
1	D	0.25	0/1642	0.39	0/2235
1	E	0.25	0/1516	0.39	0/2059
1	F	0.25	0/1665	0.40	0/2263
1	G	0.25	0/1672	0.40	0/2273
1	H	0.25	0/1615	0.40	0/2194
1	I	0.25	0/1531	0.38	0/2082
1	J	0.25	0/1600	0.39	0/2177
1	K	0.25	0/1582	0.38	0/2155
1	L	0.25	0/1484	0.38	0/2019
2	M	0.38	0/65	0.38	0/87
2	N	0.37	0/65	0.36	0/87
2	O	0.37	0/65	0.35	0/87
2	P	0.37	0/65	0.34	0/87
2	Q	0.37	0/65	0.34	0/87
2	R	0.37	0/65	0.32	0/87
All	All	0.25	0/19690	0.39	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	5	0
1	B	1602	0	1572	2	0
1	C	1619	0	1583	3	0
1	D	1607	0	1580	4	0
1	E	1484	0	1461	2	0
1	F	1631	0	1599	3	0
1	G	1636	0	1609	3	0
1	H	1580	0	1560	2	0
1	I	1500	0	1451	2	0
1	J	1565	0	1534	2	0
1	K	1548	0	1507	2	0
1	L	1455	0	1417	3	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	32	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 (32) 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: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: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:J:37:ILE:HB	1:J:38:PRO:HD3	1.98	0.46
1:E:37:ILE:HB	1:E:38:PRO:HD3	1.97	0.46
1:D:37:ILE:HB	1:D:38:PRO:HD3	1.97	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:ILE:HB	1:G:38:PRO:HD3	1.99	0.44
1:G:202:LEU:HD22	1:G:214:MET:HG2	2.00	0.44
1:E:37:ILE:HD12	1:E:138:LEU:HB3	2.00	0.43
1:C:26:VAL:HG21	1:C:39:MET:HG2	2.00	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: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:I:161:PHE:O	1:I:165:VAL:HG23	2.21	0.40
1:G:161:PHE:O	1:G:165:VAL:HG23	2.22	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	212/231 (92%)	206 (97%)	6 (3%)	0	100	100
1	B	202/231 (87%)	195 (96%)	6 (3%)	1 (0%)	34	76
1	C	206/231 (89%)	199 (97%)	6 (3%)	1 (0%)	34	76
1	D	204/231 (88%)	199 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	34	76
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%)	56	90

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%)	178 (99%)	2 (1%)	80	94
1	B	174/193 (90%)	174 (100%)	0	100	100
1	C	173/193 (90%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	173/193 (90%)	172 (99%)	1 (1%)	90	97
1	E	161/193 (83%)	161 (100%)	0	100	100
1	F	177/193 (92%)	175 (99%)	2 (1%)	80	94
1	G	177/193 (92%)	175 (99%)	2 (1%)	80	94
1	H	171/193 (89%)	169 (99%)	2 (1%)	78	94
1	I	160/193 (83%)	160 (100%)	0	100	100
1	J	168/193 (87%)	168 (100%)	0	100	100
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%)	2068 (100%)	9 (0%)	93	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	100	ARG
1	D	100	ARG
1	F	100	ARG
1	F	136	LEU
1	G	37	ILE
1	G	136	LEU
1	H	2	ILE
1	H	100	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	179	GLN
1	D	176	GLN

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Mol	Chain	Res	Type
1	F	95	GLN
1	G	95	GLN
1	K	112	GLN
1	L	112	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](#)

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 [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	216/231 (93%)	-0.30	4 (1%) 70 41	36, 64, 140, 159	0
1	B	207/231 (89%)	-0.30	0 100 100	38, 64, 109, 131	0
1	C	211/231 (91%)	-0.30	1 (0%) 91 76	42, 64, 128, 143	0
1	D	210/231 (90%)	-0.33	2 (0%) 84 60	38, 66, 138, 159	0
1	E	192/231 (83%)	-0.40	0 100 100	40, 66, 106, 126	0
1	F	211/231 (91%)	-0.44	0 100 100	34, 58, 99, 139	0
1	G	212/231 (91%)	-0.43	0 100 100	35, 56, 101, 127	0
1	H	204/231 (88%)	-0.20	4 (1%) 68 39	36, 66, 154, 186	0
1	I	196/231 (84%)	-0.18	2 (1%) 84 60	50, 81, 146, 160	0
1	J	204/231 (88%)	-0.06	8 (3%) 43 18	53, 88, 182, 202	0
1	K	204/231 (88%)	-0.09	6 (2%) 55 26	58, 98, 165, 184	0
1	L	191/231 (82%)	-0.25	2 (1%) 84 60	49, 77, 127, 156	0
2	M	9/17 (52%)	-0.58	0 100 100	40, 47, 59, 62	0
2	N	9/17 (52%)	-0.34	0 100 100	42, 45, 67, 70	0
2	O	9/17 (52%)	0.92	1 (11%) 7 3	78, 98, 111, 114	0
2	P	9/17 (52%)	1.15	2 (22%) 1 1	72, 93, 122, 125	0
2	Q	9/17 (52%)	1.16	2 (22%) 1 1	93, 121, 140, 141	0
2	R	9/17 (52%)	1.89	3 (33%) 0 0	94, 111, 157, 158	0
All	All	2512/2874 (87%)	-0.25	37 (1%) 76 49	34, 70, 146, 202	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	207	PRO	7.3
2	R	1410	SER	4.6
1	I	207	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	K	153	ILE	4.4
2	R	1412	SER	4.3
1	K	206	GLY	3.6
1	J	197	ASP	3.5
1	H	205	LEU	3.5
1	J	196	PRO	3.0
1	A	205	LEU	3.0
1	K	190	LEU	2.8
1	A	180	GLU	2.8
1	J	205	LEU	2.8
1	J	207	PRO	2.8
1	L	4[A]	GLN	2.7
2	P	1416	THR	2.7
2	Q	1410	SER	2.7
1	A	208	GLY	2.7
1	H	202	LEU	2.7
1	L	81	ASP	2.7
1	J	204	ALA	2.6
1	I	87	HIS	2.6
1	A	207	PRO	2.6
2	P	1410	SER	2.6
1	H	204	ALA	2.5
1	J	190	LEU	2.5
1	J	202	LEU	2.5
1	K	150	ILE	2.3
2	Q	1416	THR	2.2
1	H	93	PRO	2.2
1	D	184	ALA	2.2
1	K	205	LEU	2.2
1	J	217	ALA	2.1
1	C	192	GLN	2.1
2	O	1416	THR	2.0
1	D	207	PRO	2.0
2	R	1418	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	E	301	1/1	0.88	0.13	-1.76	58,58,58,58	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.