



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:20 PM UTC

PDB ID : 9EE3 / pdb\_00009ee3  
Title : HIV CA - FG peptide (14 mM)  
Authors : Melcak, I.; Sarafianos, S.G.  
Deposited on : 2024-11-18  
Resolution : 3.10 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

<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>.

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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

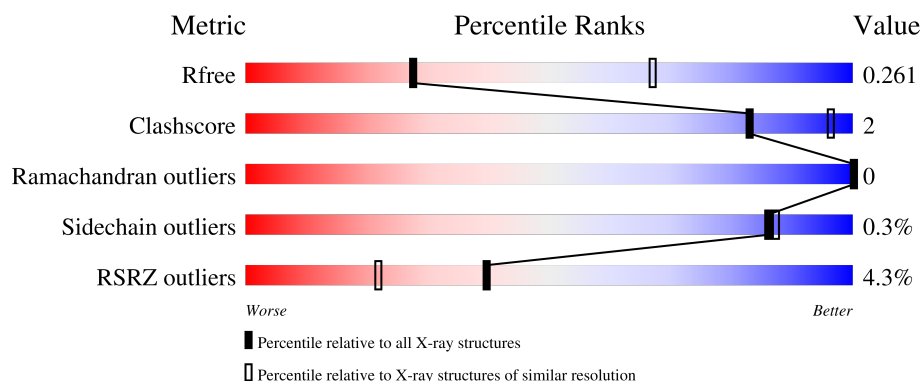
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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  $\geq 3$ , 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% 88% 6% 6%
1	B	231	 2% 83% 7% 10%
1	C	231	 3% 87% 8% 2%
1	D	231	 6% 80% 8% 13%
1	E	231	 4% 84% 8% 8%

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Mol	Chain	Length	Quality of chain
1	F	231	 91% 5%
1	G	231	 88% 6% 6%
1	H	231	 84% 6% 10%
1	I	231	 85% 7% 8%
1	J	231	 84% 8% 8%
1	K	231	 80% 7% 13%
1	L	231	 83% 6% 11%
2	M	9	 11% 89%
2	O	9	 11% 89%
2	P	9	 11% 89%
2	Q	9	 11% 89%
2	S	9	 11% 89%
2	W	9	 22% 78%
2	X	9	 22% 78%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19261 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	218	Total	C	N	O	S	0	0	0
			1628	1026	284	304	14			
1	B	208	Total	C	N	O	S	0	0	0
			1591	1001	276	300	14			
1	C	212	Total	C	N	O	S	0	0	0
			1622	1018	284	306	14			
1	D	202	Total	C	N	O	S	0	0	0
			1534	962	268	290	14			
1	E	213	Total	C	N	O	S	0	0	0
			1606	1012	279	301	14			
1	F	219	Total	C	N	O	S	0	0	0
			1656	1041	290	311	14			
1	G	218	Total	C	N	O	S	0	0	0
			1657	1040	290	313	14			
1	H	209	Total	C	N	O	S	0	0	0
			1588	1000	278	296	14			
1	I	212	Total	C	N	O	S	0	0	0
			1595	1010	274	297	14			
1	J	214	Total	C	N	O	S	0	0	0
			1634	1025	287	308	14			
1	K	201	Total	C	N	O	S	0	0	0
			1521	957	264	286	14			
1	L	205	Total	C	N	O	S	0	0	0
			1543	972	266	292	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 FG peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	2	Total	C	N	O	0	0	0
			15	11	2	2			
2	X	2	Total	C	N	O	0	0	0
			15	11	2	2			
2	M	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	O	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	P	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	Q	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	S	1	Total	C	N	O	0	0	0
			11	9	1	1			

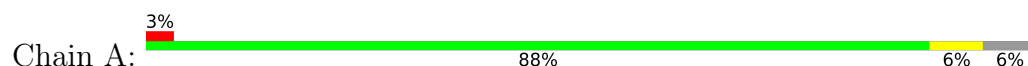
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

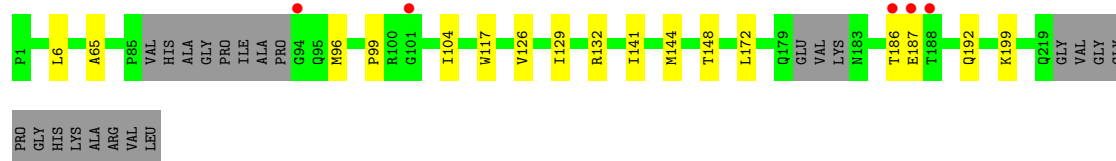
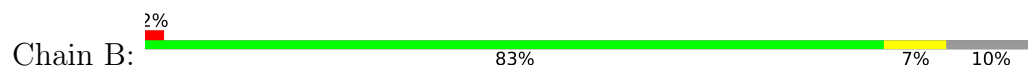
### 3 Residue-property plots [i](#)

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.

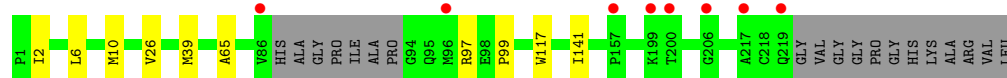
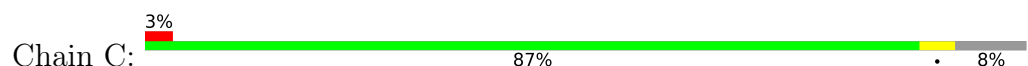
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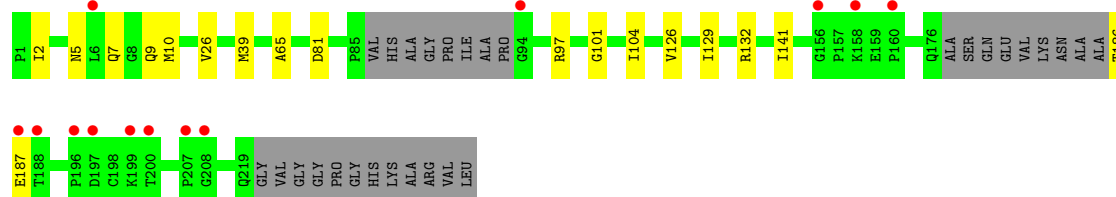
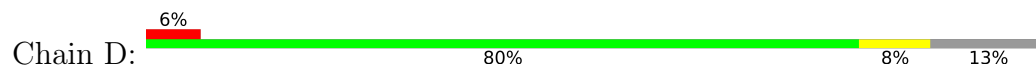
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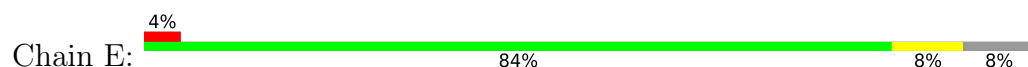
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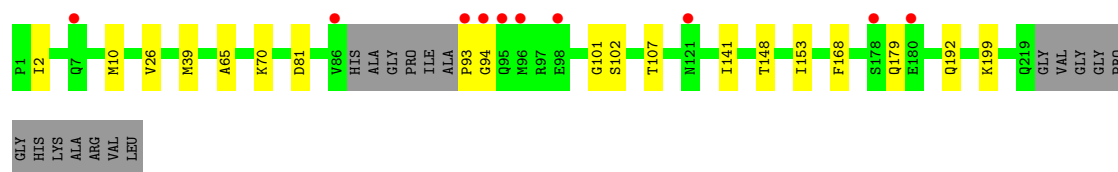


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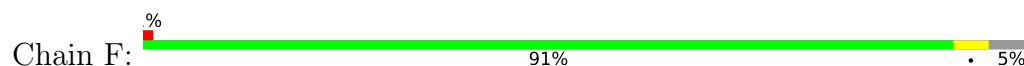


- Molecule 1: Capsid protein p24

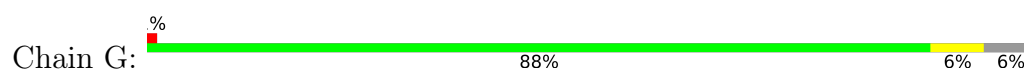




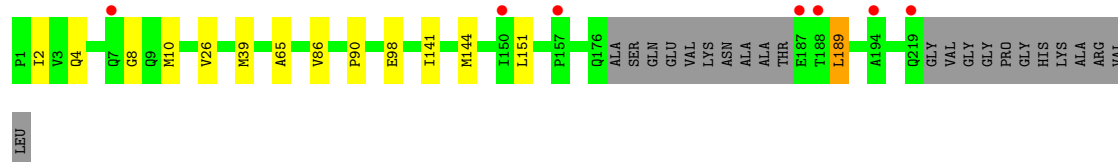
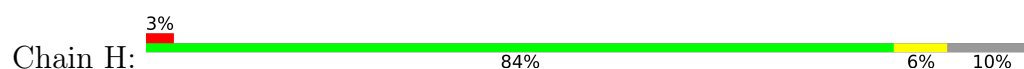
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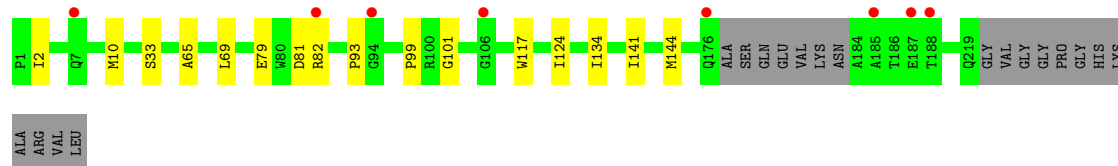
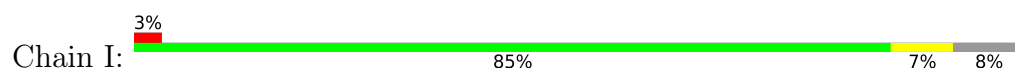
- Molecule 1: Capsid protein p24



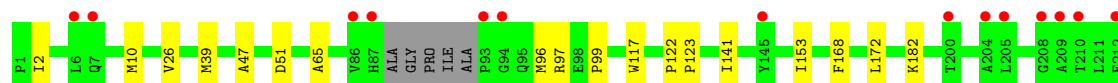
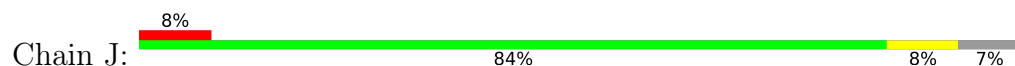
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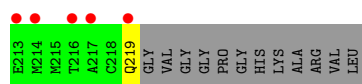
- Molecule 1: Capsid protein p24



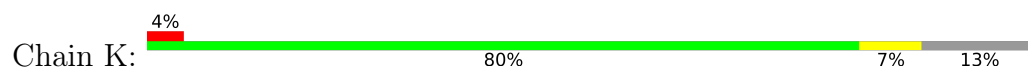
- Molecule 1: Capsid protein p24



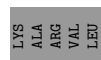
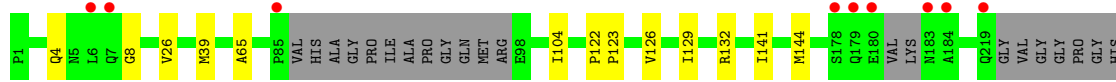
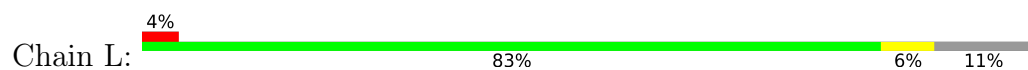




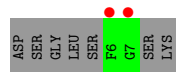
- Molecule 1: Capsid protein p24



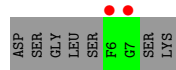
- Molecule 1: Capsid protein p24



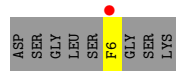
- Molecule 2: FG peptide



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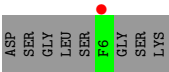


- Molecule 2: FG peptide

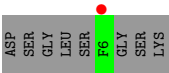


- Molecule 2: FG peptide





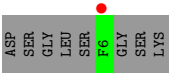
● Molecule 2: FG peptide



● Molecule 2: FG peptide



● Molecule 2: FG peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.59Å 135.86Å 206.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.01 – 3.10 34.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (34.01-3.10) 96.0 (34.01-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.228 , 0.261 0.228 , 0.261	Depositor DCC
$R_{free}$ test set	3393 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 21.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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

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	0.09	0/1664	0.21	0/2268
1	B	0.08	0/1623	0.20	0/2205
1	C	0.08	0/1655	0.21	0/2250
1	D	0.09	0/1566	0.21	0/2129
1	E	0.09	0/1640	0.21	0/2232
1	F	0.09	0/1692	0.21	0/2304
1	G	0.08	0/1693	0.20	0/2305
1	H	0.08	0/1624	0.20	0/2212
1	I	0.08	0/1631	0.19	0/2223
1	J	0.09	0/1668	0.21	0/2267
1	K	0.09	0/1554	0.20	0/2115
1	L	0.08	0/1575	0.21	0/2147
2	M	0.05	0/11	0.07	0/13
2	O	0.05	0/11	0.05	0/13
2	P	0.04	0/11	0.06	0/13
2	Q	0.05	0/11	0.06	0/13
2	S	0.04	0/11	0.06	0/13
2	W	0.04	0/15	0.09	0/18
2	X	0.04	0/15	0.09	0/18
All	All	0.08	0/19670	0.20	0/26758

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	1628	0	1571	9	0
1	B	1591	0	1558	10	0
1	C	1622	0	1584	6	0
1	D	1534	0	1464	11	0
1	E	1606	0	1559	9	0
1	F	1656	0	1606	5	0
1	G	1657	0	1609	10	0
1	H	1588	0	1542	8	0
1	I	1595	0	1553	9	0
1	J	1634	0	1594	11	0
1	K	1521	0	1454	8	0
1	L	1543	0	1479	7	0
2	M	11	0	8	1	0
2	O	11	0	8	0	0
2	P	11	0	8	0	0
2	Q	11	0	8	0	0
2	S	11	0	8	0	0
2	W	15	0	11	0	0
2	X	15	0	11	0	0
3	E	1	0	0	0	0
All	All	19261	0	18635	92	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 2.

All (92) 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:C:2:ILE:HG22	1:C:10:MET:HE3	1.80	0.62
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.81	0.61
1:B:172:LEU:HD21	1:B:186:THR:HG22	1.83	0.60
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.85	0.59
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.83	0.59
1:H:151:LEU:HD23	1:H:189:LEU:HD21	1.85	0.59
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:GLN:NE2	1:K:146:SER:O	2.38	0.57
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.88	0.56
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.86	0.56
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.87	0.56
1:D:5:ASN:OD1	1:D:9:GLN:N	2.39	0.56
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.87	0.55
1:E:2:ILE:HG22	1:E:10:MET:HE3	1.87	0.55
1:D:9:GLN:NE2	1:G:7:GLN:OE1	2.40	0.55
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.88	0.54
1:D:97:ARG:HB2	1:G:90:PRO:HB2	1.90	0.54
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.90	0.53
1:I:79:GLU:OE2	1:I:82:ARG:NH2	2.35	0.53
1:L:65:ALA:HB1	1:L:141:ILE:HD13	1.89	0.53
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.90	0.53
1:B:96:MET:HE2	1:I:93:PRO:HA	1.90	0.52
1:G:2:ILE:HG22	1:G:10:MET:HE3	1.92	0.52
1:H:4:GLN:HE21	1:H:8:GLY:HA2	1.75	0.52
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.92	0.51
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.93	0.51
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.92	0.50
1:A:53:ASN:OD1	2:M:6:PHE:N	2.44	0.50
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.92	0.50
1:I:81:ASP:OD1	1:I:101:GLY:N	2.45	0.50
1:B:6:LEU:HB3	1:C:6:LEU:HG	1.93	0.50
1:C:97:ARG:HB2	1:H:90:PRO:HB2	1.94	0.50
1:L:129:ILE:HG12	1:L:132:ARG:HH12	1.76	0.50
1:C:65:ALA:HB1	1:C:141:ILE:HD13	1.95	0.49
1:J:65:ALA:HB1	1:J:141:ILE:HD13	1.94	0.49
1:K:154:ARG:HA	1:K:193:ASN:HB3	1.94	0.49
1:G:81:ASP:OD1	1:G:101:GLY:N	2.44	0.49
1:J:153:ILE:HG21	1:J:168:PHE:HA	1.95	0.49
1:I:69:LEU:HD21	1:I:134:ILE:HG23	1.95	0.48
1:J:26:VAL:HG21	1:J:39:MET:HG2	1.95	0.48
1:B:99:PRO:HG3	1:B:117:TRP:CE2	2.47	0.48
1:L:4:GLN:HE21	1:L:8:GLY:HA2	1.77	0.48
1:D:104:ILE:HG12	1:D:126:VAL:HG12	1.96	0.48
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.95	0.48
1:C:99:PRO:HG3	1:C:117:TRP:CE2	2.48	0.48
1:D:81:ASP:OD1	1:D:101:GLY:N	2.47	0.47
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.95	0.47
1:A:90:PRO:HB2	1:J:97:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:PRO:HG3	1:I:117:TRP:CE2	2.49	0.47
1:E:153:ILE:HG21	1:E:168:PHE:HA	1.95	0.47
1:E:192:GLN:HA	1:E:199:LYS:HE3	1.97	0.47
1:B:104:ILE:HG12	1:B:126:VAL:HG12	1.97	0.47
1:J:99:PRO:HG3	1:J:117:TRP:CE2	2.50	0.46
1:E:26:VAL:HG21	1:E:39:MET:HG2	1.97	0.46
1:G:215:MET:HB2	1:H:144:MET:HE1	1.98	0.46
1:K:99:PRO:HG3	1:K:117:TRP:CE2	2.51	0.46
1:K:60:GLY:O	1:K:63:GLN:NE2	2.47	0.46
1:L:104:ILE:HG12	1:L:126:VAL:HG12	1.96	0.46
1:H:26:VAL:HG21	1:H:39:MET:HG2	1.97	0.45
1:A:93:PRO:HB3	1:J:96:MET:HE2	1.98	0.45
1:B:144:MET:HE2	1:B:144:MET:HB3	1.89	0.45
1:I:117:TRP:HB3	1:I:124:ILE:HB	1.98	0.45
1:D:129:ILE:HG12	1:D:132:ARG:HH12	1.82	0.45
1:F:2:ILE:HG22	1:F:10:MET:HE3	1.98	0.45
1:B:186:THR:OG1	1:B:187:GLU:N	2.49	0.45
1:H:86:VAL:HG13	1:H:98:GLU:HB2	1.98	0.45
1:B:192:GLN:HA	1:B:199:LYS:HE3	1.98	0.44
1:J:2:ILE:HG22	1:J:10:MET:HE3	1.98	0.44
1:K:129:ILE:HG12	1:K:132:ARG:HH12	1.82	0.44
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.99	0.43
1:A:2:ILE:HG22	1:A:10:MET:HE3	2.00	0.43
1:E:93:PRO:HB2	1:E:94:GLY:H	1.67	0.43
1:D:186:THR:OG1	1:D:187:GLU:N	2.52	0.42
1:G:122:PRO:HA	1:G:123:PRO:HD3	1.93	0.42
1:D:7:GLN:HB3	1:G:7:GLN:NE2	2.35	0.42
1:J:47:ALA:HB1	1:J:51:ASP:HB2	2.01	0.42
1:E:102:SER:HB2	1:E:107:THR:HB	2.02	0.42
1:I:144:MET:HE2	1:I:144:MET:HB3	1.89	0.41
1:J:172:LEU:HD21	1:J:182:LYS:HA	2.02	0.41
1:B:129:ILE:HG12	1:B:132:ARG:HH12	1.86	0.41
1:F:146:SER:HA	1:F:147:PRO:HD3	1.89	0.41
1:L:122:PRO:HA	1:L:123:PRO:HD3	1.89	0.41
1:A:144:MET:HE2	1:A:144:MET:HB3	1.85	0.41
1:L:144:MET:HE2	1:L:144:MET:HB3	1.95	0.41
1:E:179:GLN:HB3	1:F:70:LYS:HE3	2.02	0.41
1:J:122:PRO:HA	1:J:123:PRO:HD3	1.94	0.41
1:K:23:TRP:CZ3	1:K:40:PHE:HB2	2.56	0.41
1:G:124:ILE:O	1:G:126:VAL:N	2.52	0.40
1:E:81:ASP:OD1	1:E:101:GLY:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:ILE:HG22	1:H:10:MET:HE3	2.02	0.40
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.95	0.40
1:I:2:ILE:HG22	1:I:10:MET:HE3	2.03	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	214/231 (93%)	211 (99%)	3 (1%)	0	100	100
1	B	202/231 (87%)	198 (98%)	4 (2%)	0	100	100
1	C	208/231 (90%)	205 (99%)	3 (1%)	0	100	100
1	D	196/231 (85%)	189 (96%)	7 (4%)	0	100	100
1	E	209/231 (90%)	202 (97%)	7 (3%)	0	100	100
1	F	217/231 (94%)	208 (96%)	9 (4%)	0	100	100
1	G	214/231 (93%)	206 (96%)	8 (4%)	0	100	100
1	H	205/231 (89%)	200 (98%)	5 (2%)	0	100	100
1	I	208/231 (90%)	201 (97%)	7 (3%)	0	100	100
1	J	210/231 (91%)	201 (96%)	9 (4%)	0	100	100
1	K	195/231 (84%)	188 (96%)	7 (4%)	0	100	100
1	L	199/231 (86%)	193 (97%)	6 (3%)	0	100	100
All	All	2477/2772 (89%)	2402 (97%)	75 (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	167/193 (86%)	167 (100%)	0	100	100
1	B	169/193 (88%)	168 (99%)	1 (1%)	78	83
1	C	172/193 (89%)	172 (100%)	0	100	100
1	D	159/193 (82%)	159 (100%)	0	100	100
1	E	167/193 (86%)	165 (99%)	2 (1%)	63	78
1	F	171/193 (89%)	171 (100%)	0	100	100
1	G	174/193 (90%)	174 (100%)	0	100	100
1	H	167/193 (86%)	166 (99%)	1 (1%)	78	83
1	I	166/193 (86%)	165 (99%)	1 (1%)	78	83
1	J	173/193 (90%)	173 (100%)	0	100	100
1	K	158/193 (82%)	157 (99%)	1 (1%)	78	83
1	L	160/193 (83%)	160 (100%)	0	100	100
2	M	1/7 (14%)	1 (100%)	0	100	100
2	O	1/7 (14%)	1 (100%)	0	100	100
2	P	1/7 (14%)	1 (100%)	0	100	100
2	Q	1/7 (14%)	1 (100%)	0	100	100
2	S	1/7 (14%)	1 (100%)	0	100	100
2	W	1/7 (14%)	1 (100%)	0	100	100
2	X	1/7 (14%)	1 (100%)	0	100	100
All	All	2010/2365 (85%)	2004 (100%)	6 (0%)	86	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	148	THR
1	E	70	LYS
1	E	148	THR
1	H	189	LEU

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Mol	Chain	Res	Type
1	I	33	SER
1	K	144	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	13	GLN
1	A	155	GLN
1	B	7	GLN
1	B	9	GLN
1	C	4	GLN
1	C	62	HIS
1	C	179	GLN
1	E	63	GLN
1	E	155	GLN
1	F	155	GLN
1	G	62	HIS
1	G	84	HIS
1	I	95	GLN
1	J	13	GLN
1	J	63	GLN
1	J	179	GLN
1	K	155	GLN
1	L	4	GLN
1	L	9	GLN

### 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, 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	218/231 (94%)	0.15	8 (3%) 45 25	33, 51, 94, 113	0
1	B	208/231 (90%)	0.14	5 (2%) 59 38	34, 56, 82, 135	0
1	C	212/231 (91%)	0.18	8 (3%) 44 25	31, 52, 101, 129	0
1	D	202/231 (87%)	0.29	13 (6%) 25 14	32, 54, 123, 142	0
1	E	213/231 (92%)	0.24	10 (4%) 36 19	32, 53, 93, 126	0
1	F	219/231 (94%)	0.12	3 (1%) 73 53	33, 54, 97, 115	0
1	G	218/231 (94%)	0.14	3 (1%) 73 53	38, 59, 98, 125	0
1	H	209/231 (90%)	0.32	7 (3%) 49 29	38, 59, 110, 145	0
1	I	212/231 (91%)	0.34	8 (3%) 44 25	38, 62, 91, 144	0
1	J	214/231 (92%)	0.31	19 (8%) 15 8	34, 51, 110, 145	0
1	K	201/231 (87%)	0.33	9 (4%) 38 20	37, 56, 118, 148	0
1	L	205/231 (88%)	0.27	9 (4%) 39 21	38, 61, 103, 140	0
2	M	1/9 (11%)	3.41	1 (100%) 0 0	87, 87, 87, 87	0
2	O	1/9 (11%)	2.91	1 (100%) 0 0	69, 69, 69, 69	0
2	P	1/9 (11%)	2.81	1 (100%) 0 0	44, 44, 44, 44	1 (100%)
2	Q	1/9 (11%)	1.27	0 100 100	77, 77, 77, 77	0
2	S	1/9 (11%)	2.11	1 (100%) 0 0	60, 60, 60, 60	1 (100%)
2	W	2/9 (22%)	3.58	2 (100%) 0 0	46, 46, 46, 54	2 (100%)
2	X	2/9 (22%)	2.54	2 (100%) 0 0	66, 66, 66, 84	0
All	All	2540/2835 (89%)	0.24	110 (4%) 40 22	31, 56, 104, 148	4 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	217	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	98	GLU	5.2
1	J	87	HIS	4.4
1	I	187	GLU	4.3
1	E	94	GLY	4.2
1	C	219	GLN	4.1
1	J	213	GLU	4.0
2	W	7	GLY	4.0
1	A	6	LEU	3.9
1	B	187	GLU	3.9
1	L	180	GLU	3.9
1	D	188	THR	3.9
1	H	187	GLU	3.9
1	D	197	ASP	3.8
1	E	95	GLN	3.7
1	K	188	THR	3.7
1	J	94	GLY	3.4
2	M	6	PHE	3.4
1	D	187	GLU	3.3
1	L	85	PRO	3.3
1	J	93	PRO	3.2
1	L	184	ALA	3.2
1	H	157	PRO	3.2
1	E	86	VAL	3.2
2	W	6	PHE	3.2
1	J	216	THR	3.2
1	I	188	THR	3.0
1	J	219	GLN	3.0
1	B	188	THR	3.0
1	I	94	GLY	3.0
1	A	121	ASN	3.0
1	L	219	GLN	2.9
2	O	6	PHE	2.9
1	A	7	GLN	2.9
1	B	186	THR	2.9
1	J	200	THR	2.9
1	J	209	ALA	2.9
1	J	6	LEU	2.9
1	J	145	TYR	2.8
1	G	220	GLY	2.8
2	P	6	PHE	2.8
1	L	6	LEU	2.8
1	H	219	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	82	ARG	2.7
1	J	214	MET	2.7
1	A	184	ALA	2.7
1	E	121	ASN	2.7
1	A	220	GLY	2.7
2	X	7	GLY	2.7
1	E	7	GLN	2.6
1	A	216	THR	2.6
1	E	178	SER	2.6
1	H	150	ILE	2.6
1	B	94	GLY	2.6
1	K	6	LEU	2.6
1	K	93	PRO	2.6
1	K	95	GLN	2.6
1	C	96	MET	2.5
1	K	191	VAL	2.5
1	C	157	PRO	2.5
1	A	219	GLN	2.5
1	L	178	SER	2.5
1	D	199	LYS	2.5
1	C	217	ALA	2.5
1	J	212	GLU	2.5
1	I	7	GLN	2.4
2	X	6	PHE	2.4
1	J	210	THR	2.4
1	E	93	PRO	2.4
1	J	205	LEU	2.4
1	I	106	GLY	2.4
1	F	200	THR	2.4
1	J	204	ALA	2.4
1	J	7	GLN	2.4
1	L	7	GLN	2.4
1	E	180	GLU	2.3
1	C	200	THR	2.3
1	C	206	GLY	2.3
1	K	189	LEU	2.3
1	A	181	VAL	2.3
1	D	6	LEU	2.3
1	F	208	GLY	2.3
1	J	86	VAL	2.3
1	G	188	THR	2.2
1	C	86	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	179	GLN	2.2
1	H	7	GLN	2.2
1	I	185	ALA	2.2
1	K	219	GLN	2.2
1	D	207	PRO	2.2
1	E	96	MET	2.2
1	D	156	GLY	2.1
1	D	196	PRO	2.1
2	S	6	PHE	2.1
1	D	160	PRO	2.1
1	L	183	ASN	2.1
1	D	158	LYS	2.1
1	K	197	ASP	2.1
1	H	188	THR	2.1
1	K	198	CYS	2.1
1	B	101	GLY	2.1
1	D	94	GLY	2.1
1	D	208	GLY	2.1
1	I	176	GLN	2.1
1	H	194	ALA	2.0
1	J	208	GLY	2.0
1	L	179	GLN	2.0
1	G	160	PRO	2.0
1	C	199	LYS	2.0
1	D	200	THR	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 ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	E	301	1/1	0.90	0.10	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.