



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:56 AM UTC

PDB ID : 9EE2 / pdb_00009ee2
Title : HIV CA - FSFG peptide (14 mM)
Authors : Melcak, I.; Sarafianos, S.G.
Deposited on : 2024-11-18
Resolution : 2.99 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

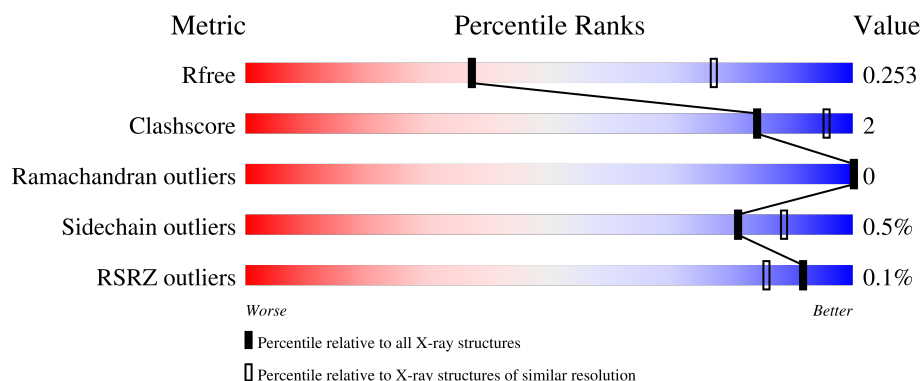
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.99 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.



















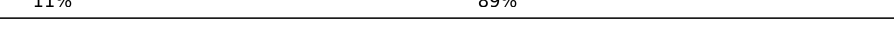
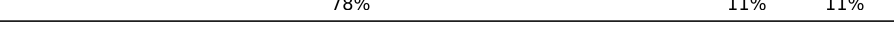
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	 88% 5% 7%
1	B	231	 85% 6% 9%
1	C	231	 88% 5% 7%
1	D	231	 81% 7% 11%
1	E	231	 84% 6% 10%

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Mol	Chain	Length	Quality of chain
1	F	231	 88%7%5%
1	G	231	 89%6%6%
1	H	231	 85%6%9%
1	I	231	 86%7%7%
1	J	231	 86%7%6%
1	K	231	 80%6%14%
1	L	231	 86%•11%
2	M	9	 11%89%
2	N	9	 11%89%
2	O	9	 11%89%
2	P	9	 67%11%22%
2	Q	9	 11%89%
2	R	9	 11%89%
2	S	9	 11%89%
2	U	9	 11%89%
2	V	9	 11%89%
2	W	9	 78%11%11%
2	X	9	 11%89%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19425 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	215	Total	C	N	O	S	0	0	0
			1613	1017	281	301	14			
1	B	211	Total	C	N	O	S	0	0	0
			1607	1013	279	301	14			
1	C	214	Total	C	N	O	S	0	0	0
			1634	1026	286	308	14			
1	D	205	Total	C	N	O	S	0	0	0
			1549	972	271	292	14			
1	E	208	Total	C	N	O	S	0	0	0
			1581	996	274	298	13			
1	F	219	Total	C	N	O	S	0	0	0
			1661	1044	291	312	14			
1	G	218	Total	C	N	O	S	0	0	0
			1657	1040	290	313	14			
1	H	211	Total	C	N	O	S	0	0	0
			1602	1008	281	299	14			
1	I	215	Total	C	N	O	S	0	0	0
			1619	1024	280	301	14			
1	J	216	Total	C	N	O	S	0	0	0
			1640	1028	288	310	14			
1	K	198	Total	C	N	O	S	0	0	0
			1509	950	262	283	14			
1	L	206	Total	C	N	O	S	0	0	0
			1555	977	267	298	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 FSFG peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			47	31	7	9			
2	W	8	Total	C	N	O	0	0	0
			51	34	8	9			
2	M	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	N	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	Q	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	R	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			
2	U	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	V	1	Total	C	N	O	0	0	0
			11	9	1	1			
2	X	1	Total	C	N	O	0	0	0
			11	9	1	1			

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

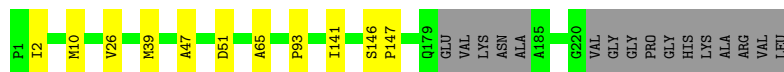
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cl	0	0
			1	1		

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.

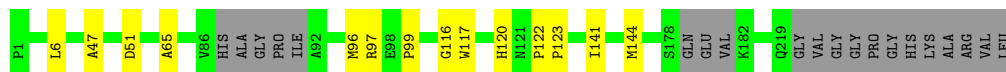
- Molecule 1: Capsid protein p24

Chain A: 




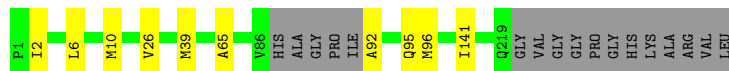
- Molecule 1: Capsid protein p24

Chain B: 




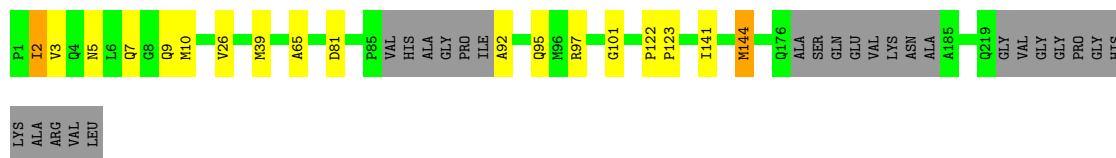
- Molecule 1: Capsid protein p24

Chain C: 




- Molecule 1: Capsid protein p24

Chain D: 




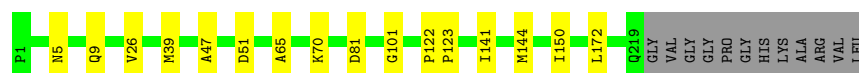
- Molecule 1: Capsid protein p24

Chain E: 




- Molecule 1: Capsid protein p24

Chain F:  88% 7% 5%




- Molecule 1: Capsid protein p24

Chain G:  89% 6% 6%




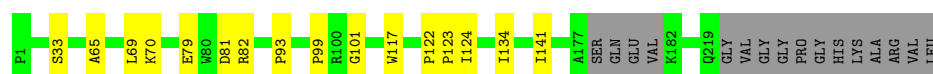
- Molecule 1: Capsid protein p24

Chain H:  85% 6% 9%



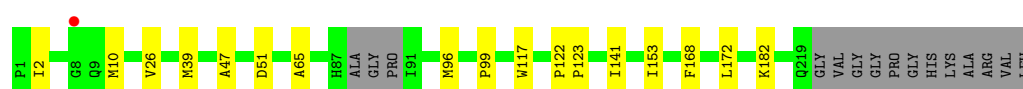
- Molecule 1: Capsid protein p24

Chain I:  86% 7% 7%



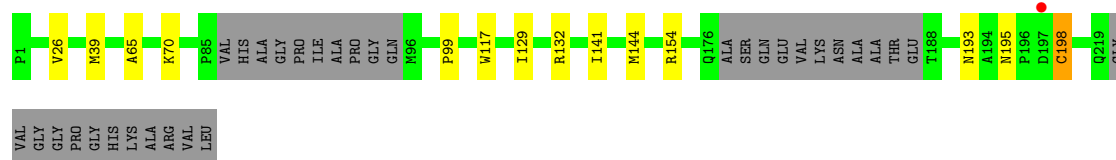
- Molecule 1: Capsid protein p24

Chain J:  86% 7% 6%




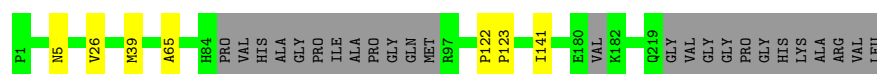
- Molecule 1: Capsid protein p24

Chain K:  80% 6% 14%



- Molecule 1: Capsid protein p24


Chain L:  86% 11%



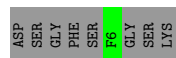
● Molecule 2: FSFG peptide

Chain P:  67% 11% 22%

● Molecule 2: FSFG peptide

Chain W:  78% 11% 11%

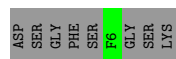
● Molecule 2: FSFG peptide

Chain M:  11% 89%

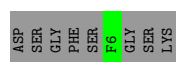
● Molecule 2: FSFG peptide

Chain N:  11% 89%

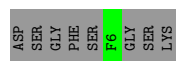
● Molecule 2: FSFG peptide

Chain O:  11% 89%

● Molecule 2: FSFG peptide

Chain Q:  11% 89%

● Molecule 2: FSFG peptide

Chain R:  11% 89%

● Molecule 2: FSFG peptide

Chain S:  11% 89%

ASP	SER	GLY	PHE	SER	F6	GLY	SER	LYS
-----	-----	-----	-----	-----	----	-----	-----	-----

● Molecule 2: FSFG peptide



ASP	SER	GLY	PHE	SER	F6	GLY	SER	LYS
-----	-----	-----	-----	-----	----	-----	-----	-----

● Molecule 2: FSFG peptide



ASP	SER	GLY	PHE	SER	F6	GLY	SER	LYS
-----	-----	-----	-----	-----	----	-----	-----	-----

● Molecule 2: FSFG peptide



ASP	SER	GLY	PHE	SER	F6	GLY	SER	LYS
-----	-----	-----	-----	-----	----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.41Å 136.45Å 208.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.47 – 2.99 34.47 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.8 (34.47-2.99) 98.7 (34.47-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.233 , 0.253 0.233 , 0.253	Depositor DCC
R_{free} test set	3961 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.196 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19425	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.08	0/1649	0.19	0/2247
1	B	0.07	0/1640	0.19	0/2230
1	C	0.07	0/1668	0.20	0/2269
1	D	0.08	0/1582	0.21	0/2152
1	E	0.07	0/1614	0.19	0/2197
1	F	0.07	0/1698	0.20	0/2312
1	G	0.08	0/1693	0.18	0/2305
1	H	0.07	0/1638	0.21	0/2231
1	I	0.07	0/1655	0.21	0/2253
1	J	0.08	0/1674	0.20	0/2278
1	K	0.08	0/1541	0.19	0/2096
1	L	0.07	0/1586	0.18	0/2160
2	M	0.05	0/11	0.10	0/13
2	N	0.05	0/11	0.07	0/13
2	O	0.07	0/11	0.08	0/13
2	P	0.09	0/48	0.19	0/62
2	Q	0.05	0/11	0.05	0/13
2	R	0.05	0/11	0.06	0/13
2	S	0.07	0/11	0.05	0/13
2	U	0.04	0/11	0.05	0/13
2	V	0.04	0/11	0.07	0/13
2	W	0.08	0/52	0.33	0/68
2	X	0.07	0/11	0.07	0/13
All	All	0.07	0/19837	0.20	0/26977

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	1613	0	1562	6	0
1	B	1607	0	1571	10	0
1	C	1634	0	1596	7	0
1	D	1549	0	1474	12	0
1	E	1581	0	1539	7	0
1	F	1661	0	1609	9	0
1	G	1657	0	1609	9	0
1	H	1602	0	1555	8	0
1	I	1619	0	1579	10	0
1	J	1640	0	1589	10	0
1	K	1509	0	1452	7	0
1	L	1555	0	1487	3	0
2	M	11	0	8	0	0
2	N	11	0	8	0	0
2	O	11	0	8	0	0
2	P	47	0	35	0	0
2	Q	11	0	8	0	0
2	R	11	0	8	0	0
2	S	11	0	8	0	0
2	U	11	0	8	0	0
2	V	11	0	8	0	0
2	W	51	0	34	1	0
2	X	11	0	8	0	0
3	E	1	0	0	1	0
All	All	19425	0	18763	87	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 (87) 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:96:MET:HE2	1:H:93:PRO:HA	1.81	0.62
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.82	0.62
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:HB3	1:I:93:PRO:HD3	1.82	0.61
1:I:79:GLU:OE2	1:I:82:ARG:NH2	2.28	0.60
1:A:93:PRO:HA	1:J:96:MET:HE2	1.83	0.60
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.84	0.59
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.84	0.59
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.84	0.59
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.84	0.58
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.85	0.57
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.87	0.57
1:D:5:ASN:OD1	1:D:9:GLN:N	2.39	0.54
1:E:2:ILE:HG22	1:E:10:MET:HE3	1.90	0.54
1:J:26:VAL:HG21	1:J:39:MET:HG2	1.90	0.54
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.88	0.53
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.89	0.53
1:B:99:PRO:HG3	1:B:117:TRP:CE2	2.45	0.52
1:E:179:GLN:HB3	1:F:70:LYS:HE3	1.91	0.52
1:D:81:ASP:OD1	1:D:101:GLY:N	2.43	0.51
1:I:99:PRO:HG3	1:I:117:TRP:CE2	2.45	0.51
1:J:2:ILE:HG22	1:J:10:MET:HE3	1.93	0.51
1:C:65:ALA:HB1	1:C:141:ILE:HD13	1.92	0.51
1:C:92:ALA:HB3	1:C:95:GLN:HB2	1.93	0.51
1:D:92:ALA:HB3	1:D:95:GLN:HB2	1.93	0.50
1:C:2:ILE:HG22	1:C:10:MET:HE3	1.94	0.49
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.94	0.49
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.95	0.49
1:L:65:ALA:HB1	1:L:141:ILE:HD13	1.94	0.49
1:B:96:MET:HE2	1:I:93:PRO:HA	1.96	0.48
1:G:81:ASP:OD1	1:G:101:GLY:N	2.45	0.47
1:I:81:ASP:OD1	1:I:101:GLY:N	2.45	0.47
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.95	0.47
1:K:70:LYS:HE3	2:W:5:SER:HB2	1.97	0.47
1:A:2:ILE:HG22	1:A:10:MET:HE3	1.96	0.47
1:H:26:VAL:HG21	1:H:39:MET:HG2	1.97	0.47
1:K:99:PRO:HG3	1:K:117:TRP:CE2	2.50	0.47
1:K:129:ILE:HG12	1:K:132:ARG:HH12	1.80	0.47
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.97	0.46
1:B:6:LEU:HB3	1:C:6:LEU:HG	1.97	0.46
1:D:97:ARG:HB2	1:G:90:PRO:HB2	1.97	0.46
1:J:99:PRO:HG3	1:J:117:TRP:CE2	2.52	0.45
1:I:117:TRP:HB3	1:I:124:ILE:HB	1.99	0.45
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ALA:HB1	1:H:51:ASP:HB2	1.99	0.45
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.98	0.45
1:I:69:LEU:HD21	1:I:134:ILE:HG23	1.98	0.45
1:I:122:PRO:HA	1:I:123:PRO:HD3	1.89	0.44
1:F:5:ASN:OD1	1:F:9:GLN:N	2.44	0.44
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.98	0.44
1:E:192:GLN:HA	1:E:199:LYS:HE3	2.00	0.43
1:G:2:ILE:HG22	1:G:10:MET:HE3	2.00	0.43
1:L:122:PRO:HA	1:L:123:PRO:HD3	1.89	0.43
1:D:122:PRO:HA	1:D:123:PRO:HD3	1.88	0.43
1:J:153:ILE:HG21	1:J:168:PHE:HA	2.00	0.43
1:E:18:ARG:NH2	3:E:301:CL:CL	2.88	0.43
1:H:86:VAL:HG21	1:H:100:ARG:HG2	2.01	0.43
1:K:195:ASN:OD1	1:K:198:CYS:HB3	2.18	0.43
1:B:122:PRO:HA	1:B:123:PRO:HD3	1.88	0.43
1:G:158:LYS:HD3	1:G:158:LYS:H	1.84	0.43
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.99	0.42
1:J:65:ALA:HB1	1:J:141:ILE:HD13	2.01	0.42
1:G:5:ASN:OD1	1:G:9:GLN:N	2.43	0.42
1:D:9:GLN:NE2	1:G:7:GLN:OE1	2.52	0.42
1:H:144:MET:HE2	1:H:144:MET:HB3	1.88	0.42
1:F:81:ASP:OD1	1:F:101:GLY:N	2.49	0.42
1:B:47:ALA:HB1	1:B:51:ASP:HB2	2.01	0.42
1:F:122:PRO:HA	1:F:123:PRO:HD3	1.94	0.42
1:B:117:TRP:CZ2	1:I:93:PRO:HG2	2.55	0.42
1:D:144:MET:HE2	1:D:144:MET:HB3	1.87	0.42
1:K:154:ARG:HA	1:K:193:ASN:HB3	2.02	0.42
1:B:116:GLY:O	1:B:120:HIS:HB2	2.19	0.41
1:B:144:MET:HE2	1:B:144:MET:HB3	1.93	0.41
1:E:102:SER:HB2	1:E:107:THR:HB	2.03	0.41
1:F:150:ILE:HD13	1:F:172:LEU:HB2	2.03	0.41
1:J:99:PRO:HG3	1:J:117:TRP:CD2	2.55	0.41
1:H:153:ILE:HG21	1:H:168:PHE:HA	2.02	0.41
1:J:172:LEU:HD21	1:J:182:LYS:HA	2.02	0.41
1:D:7:GLN:HB3	1:G:7:GLN:NE2	2.35	0.41
1:E:172:LEU:HD21	1:E:186:THR:HG21	2.02	0.41
1:J:47:ALA:HB1	1:J:51:ASP:HB2	2.02	0.41
1:F:47:ALA:HB1	1:F:51:ASP:HB2	2.03	0.41
1:F:144:MET:HE2	1:F:144:MET:HB3	1.92	0.41
1:C:6:LEU:O	1:D:7:GLN:NE2	2.49	0.40
1:A:146:SER:HA	1:A:147:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:PRO:HA	1:J:123:PRO:HD3	1.93	0.40
1:H:37:ILE:HB	1:H:38:PRO:HD3	2.04	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	211/231 (91%)	209 (99%)	2 (1%)	0	100	100
1	B	205/231 (89%)	201 (98%)	4 (2%)	0	100	100
1	C	210/231 (91%)	206 (98%)	4 (2%)	0	100	100
1	D	199/231 (86%)	197 (99%)	2 (1%)	0	100	100
1	E	204/231 (88%)	196 (96%)	8 (4%)	0	100	100
1	F	217/231 (94%)	211 (97%)	6 (3%)	0	100	100
1	G	214/231 (93%)	207 (97%)	7 (3%)	0	100	100
1	H	207/231 (90%)	203 (98%)	4 (2%)	0	100	100
1	I	211/231 (91%)	207 (98%)	4 (2%)	0	100	100
1	J	212/231 (92%)	205 (97%)	7 (3%)	0	100	100
1	K	192/231 (83%)	187 (97%)	5 (3%)	0	100	100
1	L	200/231 (87%)	196 (98%)	4 (2%)	0	100	100
2	P	5/9 (56%)	5 (100%)	0	0	100	100
2	W	6/9 (67%)	6 (100%)	0	0	100	100
All	All	2493/2790 (89%)	2436 (98%)	57 (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	167/193 (86%)	167 (100%)	0	100	100
1	B	169/193 (88%)	169 (100%)	0	100	100
1	C	173/193 (90%)	173 (100%)	0	100	100
1	D	159/193 (82%)	156 (98%)	3 (2%)	50	76
1	E	166/193 (86%)	165 (99%)	1 (1%)	78	88
1	F	172/193 (89%)	172 (100%)	0	100	100
1	G	174/193 (90%)	174 (100%)	0	100	100
1	H	168/193 (87%)	167 (99%)	1 (1%)	78	88
1	I	168/193 (87%)	166 (99%)	2 (1%)	63	82
1	J	172/193 (89%)	172 (100%)	0	100	100
1	K	158/193 (82%)	156 (99%)	2 (1%)	61	81
1	L	162/193 (84%)	161 (99%)	1 (1%)	78	88
2	M	1/7 (14%)	1 (100%)	0	100	100
2	N	1/7 (14%)	1 (100%)	0	100	100
2	O	1/7 (14%)	1 (100%)	0	100	100
2	P	4/7 (57%)	3 (75%)	1 (25%)	0	3
2	Q	1/7 (14%)	1 (100%)	0	100	100
2	R	1/7 (14%)	1 (100%)	0	100	100
2	S	1/7 (14%)	1 (100%)	0	100	100
2	U	1/7 (14%)	1 (100%)	0	100	100
2	V	1/7 (14%)	1 (100%)	0	100	100
2	W	3/7 (43%)	3 (100%)	0	100	100
2	X	1/7 (14%)	1 (100%)	0	100	100
All	All	2024/2393 (85%)	2013 (100%)	11 (0%)	81	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	ILE
1	D	3	VAL
1	D	144	MET
1	E	70	LYS
1	H	189	LEU
1	I	33	SER
1	I	70	LYS
1	K	144	MET
1	K	198	CYS
1	L	5	ASN
2	P	8	SER

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	13	GLN
1	A	62	HIS
1	A	155	GLN
1	B	120	HIS
1	B	121	ASN
1	C	4	GLN
1	D	95	GLN
1	G	4	GLN
1	H	95	GLN
1	H	176	GLN
1	I	13	GLN
1	J	121	ASN
1	J	179	GLN
1	K	155	GLN
1	L	139	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 [i](#)

There are no oligosaccharides 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, 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	215/231 (93%)	-1.05	0	100	100	56, 82, 134, 158	0
1	B	211/231 (91%)	-1.15	0	100	100	53, 80, 129, 182	0
1	C	214/231 (92%)	-1.16	0	100	100	48, 73, 124, 169	0
1	D	205/231 (88%)	-0.96	0	100	100	48, 82, 164, 201	0
1	E	208/231 (90%)	-0.96	0	100	100	56, 86, 140, 203	0
1	F	219/231 (94%)	-0.91	0	100	100	58, 91, 149, 172	0
1	G	218/231 (94%)	-0.92	0	100	100	62, 94, 143, 169	0
1	H	211/231 (91%)	-0.82	1 (0%)	87	72	60, 94, 153, 188	0
1	I	215/231 (93%)	-1.06	0	100	100	54, 87, 140, 177	0
1	J	216/231 (93%)	-1.10	1 (0%)	87	72	48, 74, 135, 175	0
1	K	198/231 (85%)	-0.89	1 (0%)	87	72	52, 82, 162, 203	0
1	L	206/231 (89%)	-0.82	0	100	100	62, 94, 146, 164	0
2	M	1/9 (11%)	-0.29	0	100	100	76, 76, 76, 76	1 (100%)
2	N	1/9 (11%)	-0.00	0	100	100	98, 98, 98, 98	0
2	O	1/9 (11%)	-0.83	0	100	100	72, 72, 72, 72	0
2	P	7/9 (77%)	0.44	0	100	100	76, 102, 109, 119	0
2	Q	1/9 (11%)	-0.22	0	100	100	92, 92, 92, 92	0
2	R	1/9 (11%)	-0.62	0	100	100	69, 69, 69, 69	1 (100%)
2	S	1/9 (11%)	-0.64	0	100	100	72, 72, 72, 72	1 (100%)
2	U	1/9 (11%)	-0.57	0	100	100	84, 84, 84, 84	0
2	V	1/9 (11%)	-0.43	0	100	100	59, 59, 59, 59	1 (100%)
2	W	8/9 (88%)	-0.08	0	100	100	74, 112, 136, 140	0
2	X	1/9 (11%)	-0.19	0	100	100	86, 86, 86, 86	0
All	All	2560/2871 (89%)	-0.98	3 (0%)	92	86	48, 85, 147, 203	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	197	ASP	2.5
1	H	150	ILE	2.3
1	J	8	GLY	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	E	301	1/1	0.98	0.03	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.