Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 06:22 AM EDT

PDB ID	:	7T12
Title	:	Hexameric HIV-1 (O-group) CA
Authors	:	Jacques, D.A.; James, L.C.
Deposited on	:	2021-12-01
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 (i) 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 (i)) were used in the production of this report:

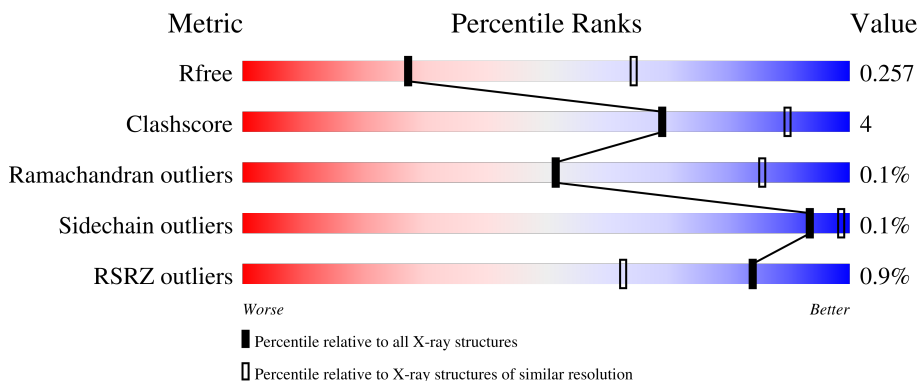|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.257
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		0.1%
RSRZ outliers		0.9%

Worse ... *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	232	78% 12% 11%
1	B	232	82% 8% 9%
1	C	232	75% 12% 13%
1	D	232	78% 8% 15%
1	E	232	75% 10% 15%

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Mol	Chain	Length	Quality of chain
1	F	232	74%　　15%　　11%
1	G	232	80%　　9%　　12%
1	H	232	81%　　·　　16%
1	I	232	3%　84%　　·　　12%
1	J	232	2%　80%　　7%　　13%
1	K	232	2%　72%　　12%　　16%
1	L	232	%　75%　　9%　　15%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 18744 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	207	Total	C	N	O	S	0	5	0
			1604	1012	277	303	12			
1	B	210	Total	C	N	O	S	0	6	0
			1616	1019	280	304	13			
1	C	202	Total	C	N	O	S	0	6	0
			1564	989	270	292	13			
1	D	198	Total	C	N	O	S	0	6	0
			1537	975	262	287	13			
1	E	198	Total	C	N	O	S	0	6	0
			1543	978	265	287	13			
1	F	206	Total	C	N	O	S	0	5	0
			1589	1003	275	299	12			
1	G	205	Total	C	N	O	S	0	6	0
			1583	1004	272	294	13			
1	H	196	Total	C	N	O	S	0	6	0
			1530	970	262	285	13			
1	I	205	Total	C	N	O	S	0	6	0
			1579	998	272	296	13			
1	J	201	Total	C	N	O	S	0	6	0
			1560	987	267	293	13			
1	K	194	Total	C	N	O	S	0	6	0
			1509	957	257	282	13			
1	L	197	Total	C	N	O	S	0	5	0
			1530	968	264	286	12			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ILE	VAL	conflict	UNP Q79665
A	14	CYS	ALA	engineered mutation	UNP Q79665
A	45	CYS	GLU	engineered mutation	UNP Q79665
A	185	ALA	TRP	engineered mutation	UNP Q79665
A	186	ALA	MET	engineered mutation	UNP Q79665

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Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	GLU	conflict	UNP Q79665
B	11	ILE	VAL	conflict	UNP Q79665
B	14	CYS	ALA	engineered mutation	UNP Q79665
B	45	CYS	GLU	engineered mutation	UNP Q79665
B	185	ALA	TRP	engineered mutation	UNP Q79665
B	186	ALA	MET	engineered mutation	UNP Q79665
B	209	GLY	GLU	conflict	UNP Q79665
C	11	ILE	VAL	conflict	UNP Q79665
C	14	CYS	ALA	engineered mutation	UNP Q79665
C	45	CYS	GLU	engineered mutation	UNP Q79665
C	185	ALA	TRP	engineered mutation	UNP Q79665
C	186	ALA	MET	engineered mutation	UNP Q79665
C	209	GLY	GLU	conflict	UNP Q79665
D	11	ILE	VAL	conflict	UNP Q79665
D	14	CYS	ALA	engineered mutation	UNP Q79665
D	45	CYS	GLU	engineered mutation	UNP Q79665
D	185	ALA	TRP	engineered mutation	UNP Q79665
D	186	ALA	MET	engineered mutation	UNP Q79665
D	209	GLY	GLU	conflict	UNP Q79665
E	11	ILE	VAL	conflict	UNP Q79665
E	14	CYS	ALA	engineered mutation	UNP Q79665
E	45	CYS	GLU	engineered mutation	UNP Q79665
E	185	ALA	TRP	engineered mutation	UNP Q79665
E	186	ALA	MET	engineered mutation	UNP Q79665
E	209	GLY	GLU	conflict	UNP Q79665
F	11	ILE	VAL	conflict	UNP Q79665
F	14	CYS	ALA	engineered mutation	UNP Q79665
F	45	CYS	GLU	engineered mutation	UNP Q79665
F	185	ALA	TRP	engineered mutation	UNP Q79665
F	186	ALA	MET	engineered mutation	UNP Q79665
F	209	GLY	GLU	conflict	UNP Q79665
G	11	ILE	VAL	conflict	UNP Q79665
G	14	CYS	ALA	engineered mutation	UNP Q79665
G	45	CYS	GLU	engineered mutation	UNP Q79665
G	185	ALA	TRP	engineered mutation	UNP Q79665
G	186	ALA	MET	engineered mutation	UNP Q79665
G	209	GLY	GLU	conflict	UNP Q79665
H	11	ILE	VAL	conflict	UNP Q79665
H	14	CYS	ALA	engineered mutation	UNP Q79665
H	45	CYS	GLU	engineered mutation	UNP Q79665
H	185	ALA	TRP	engineered mutation	UNP Q79665
H	186	ALA	MET	engineered mutation	UNP Q79665

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| Chain	Residue	Modelled	Actual	Comment	Reference
H	209	GLY	GLU	conflict	UNP Q79665
I	11	ILE	VAL	conflict	UNP Q79665
I	14	CYS	ALA	engineered mutation	UNP Q79665
I	45	CYS	GLU	engineered mutation	UNP Q79665
I	185	ALA	TRP	engineered mutation	UNP Q79665
I	186	ALA	MET	engineered mutation	UNP Q79665
I	209	GLY	GLU	conflict	UNP Q79665
J	11	ILE	VAL	conflict	UNP Q79665
J	14	CYS	ALA	engineered mutation	UNP Q79665
J	45	CYS	GLU	engineered mutation	UNP Q79665
J	185	ALA	TRP	engineered mutation	UNP Q79665
J	186	ALA	MET	engineered mutation	UNP Q79665
J	209	GLY	GLU	conflict	UNP Q79665
K	11	ILE	VAL	conflict	UNP Q79665
K	14	CYS	ALA	engineered mutation	UNP Q79665
K	45	CYS	GLU	engineered mutation	UNP Q79665
K	185	ALA	TRP	engineered mutation	UNP Q79665
K	186	ALA	MET	engineered mutation	UNP Q79665
K	209	GLY	GLU	conflict	UNP Q79665
L	11	ILE	VAL	conflict	UNP Q79665
L	14	CYS	ALA	engineered mutation	UNP Q79665
L	45	CYS	GLU	engineered mutation	UNP Q79665
L	185	ALA	TRP	engineered mutation	UNP Q79665
L	186	ALA	MET	engineered mutation	UNP Q79665
L	209	GLY	GLU	conflict	UNP Q79665

3 Residue-property plots ⓘ

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
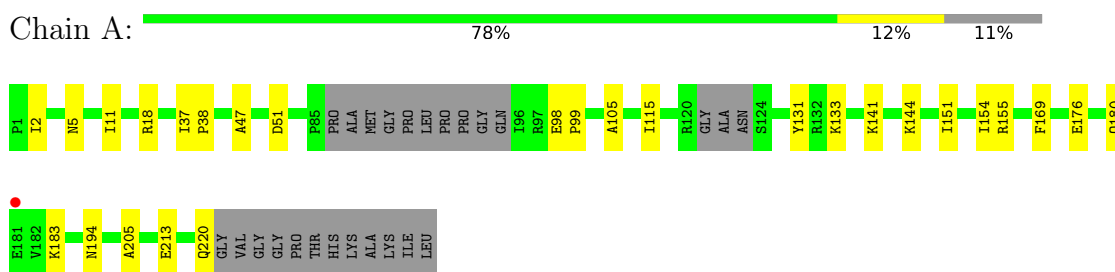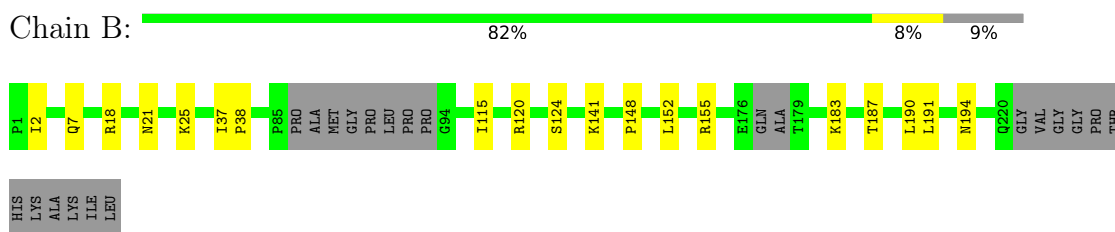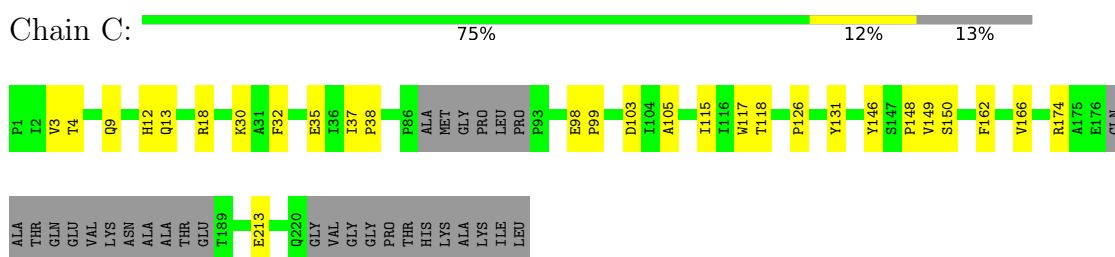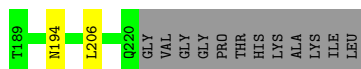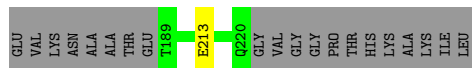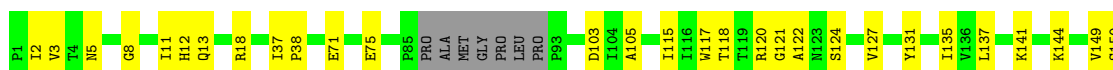
Chain A:

• Molecule 1: Capsid protein p24

Chain B:

• Molecule 1: Capsid protein p24

Chain C:

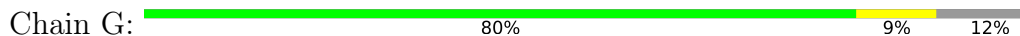• Molecule 1: Capsid protein p24

Chain D:

• Molecule 1: Capsid protein p24

Chain E:

• Molecule 1: Capsid protein p24
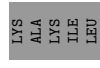
Chain F:

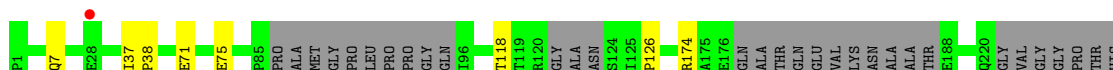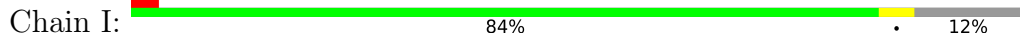• Molecule 1: Capsid protein p24

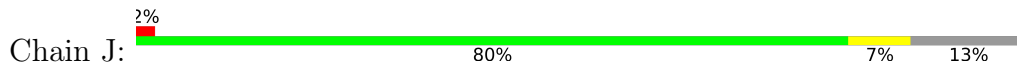Chain G:

• Molecule 1: Capsid protein p24

Chain H:

• Molecule 1: Capsid protein p24

Chain I:

GLY GLY PRO THR HIS LYS ALA LYS ILE LEU

● Molecule 1: Capsid protein p24

Chain J:

2%

80% 7% 13%

P1 H12 R18 I37 P38 A47 D51 E79 R82 P85 PRO ALA MET GLY PRO LEU PRO PRO G94 I115 T118 T119 R120 GLY ALA ASN S124 V127 E176 Q177 A178 T179 Q180 GLU VAL LYS ASN ALA ALA THR GLU T189 G207 P208 G209 A210

E213 E214 Q220 GLY VAL GLY GLY PRO THR HIS LYS ALA LYS ILE LEU

● Molecule 1: Capsid protein p24

Chain K:

2%

72% 12% 16%

P1 I2 N5 A6 Q7 G8 Q9 M10 I11 H12 N21 K25 K30 E35 I36 I37 P38 P85 PRO ALA MET GLY PRO LEU PRO PRO GLY GLN ILE R97 E98 P99 A105 I115 T118 T119 R120 GLY ALA ASN S124 I125 P126 Y131 K141 P148 V149 S150
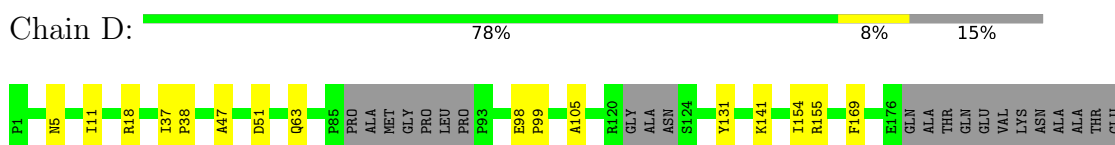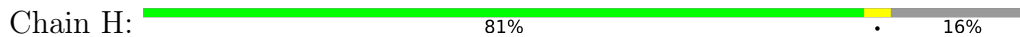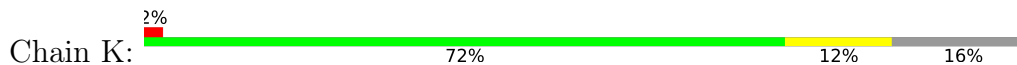
I154 R155 F169 E176 GLN ALA THR GLN GLU VAL LYS ASN ALA ALA THR GLU T189 N194 C199 L203 M215 Q220 GLY VAL GLY GLY PRO THR HIS LYS ALA LYS ILE LEU
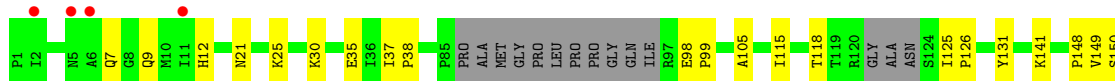
● Molecule 1: Capsid protein p24

Chain L:

%

75% 9% 15%

P1 I2 V3 Q7 Q13 R18 N21 K25 I37 P38 A47 D51 P85 PRO ALA MET GLY PRO LEU PRO PRO G94 R97 E98 P99 A105 E113 I116 R120 GLY ALA ASN S124 Y131 R163 F169 E176 GLN ALA THR GLN GLU
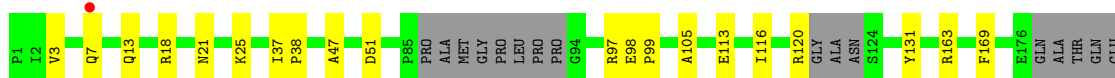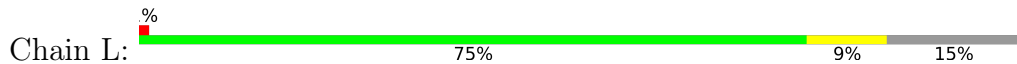
VAL LYS ASN ALA ALA THR GLU T189 L190 L191 Q201 E213 Q220 GLY VAL GLY GLY PRO THR HIS LYS ALA LYS ILE LEU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.20Å 151.73Å 120.42Å 90.00° 105.03° 90.00°	Depositor
Resolution (Å)	75.86 – 3.00 75.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (75.86-3.00) 97.1 (75.87-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.214 , 0.259 0.213 , 0.257	Depositor DCC
R_{free} test set	2944 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	79.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18744	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.27	0/1634	0.44	0/2219
1	B	0.25	0/1649	0.43	0/2240
1	C	0.25	0/1599	0.43	0/2171
1	D	0.25	0/1570	0.43	0/2130
1	E	0.25	0/1576	0.42	0/2137
1	F	0.25	0/1620	0.43	0/2200
1	G	0.25	0/1620	0.43	0/2203
1	H	0.25	0/1562	0.41	0/2119
1	I	0.25	0/1612	0.43	0/2189
1	J	0.25	0/1592	0.43	0/2160
1	K	0.25	0/1541	0.42	0/2091
1	L	0.25	0/1559	0.42	0/2114
All	All	0.25	0/19134	0.43	0/25973

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	1604	0	1591	19	1
1	B	1616	0	1596	17	0
1	C	1564	0	1549	17	0
1	D	1537	0	1525	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1543	0	1536	15	0
1	F	1589	0	1577	24	0
1	G	1583	0	1569	12	0
1	H	1530	0	1524	5	0
1	I	1579	0	1565	6	0
1	J	1560	0	1545	9	1
1	K	1509	0	1496	17	1
1	L	1530	0	1517	13	0
All	All	18744	0	18590	139	2

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 4.

All (139) 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:K:7:GLN:NE2	1:K:9:GLN:OE1	2.21	0.73
1:B:7:GLN:OE1	1:H:7:GLN:NE2	2.25	0.70
1:B:152:LEU:HD23	1:B:190:LEU:HD21	1.74	0.69
1:G:145:MET:O	1:L:163:ARG:NH2	2.26	0.68
1:A:180:GLN:O	1:A:183:LYS:NZ	2.29	0.66
1:A:220:GLN:HE21	1:B:148:PRO:HB3	1.63	0.64
1:K:7:GLN:HE21	1:K:9:GLN:HB2	1.61	0.64
1:F:152:LEU:HD23	1:F:190:LEU:HD21	1.82	0.62
1:K:155:ARG:HG2	1:K:194:ASN:HB3	1.81	0.61
1:E:213:GLU:OE2	1:F:141:LYS:HD3	2.03	0.59
1:F:121:GLY:N	1:K:7:GLN:OE1	2.22	0.58
1:A:18:ARG:NH2	1:B:18:ARG:HH11	2.04	0.56
1:L:37:ILE:HB	1:L:38[A]:PRO:HD3	1.86	0.56
1:B:37:ILE:HB	1:B:38[A]:PRO:HD3	1.88	0.56
1:G:37:ILE:HB	1:G:38[A]:PRO:HD3	1.88	0.56
1:I:37:ILE:HB	1:I:38[A]:PRO:HD3	1.88	0.55
1:B:120:ARG:O	1:B:124:SER:OG	2.23	0.55
1:A:144:LYS:HD2	1:A:176:GLU:HA	1.89	0.55
1:C:37:ILE:HB	1:C:38[A]:PRO:HD3	1.90	0.54
1:J:47:ALA:HB1	1:J:51:ASP:HB2	1.89	0.54
1:B:18:ARG:HH21	1:C:18:ARG:HG2	1.72	0.54
1:H:37:ILE:HB	1:H:38[A]:PRO:HD3	1.87	0.54
1:G:154:ILE:HG21	1:G:169:PHE:HA	1.90	0.54
1:K:118:THR:HG22	1:K:126:PRO:HA	1.89	0.54
1:A:220:GLN:NE2	1:B:148:PRO:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ILE:HB	1:D:38[A]:PRO:HD3	1.89	0.53
1:L:47:ALA:HB1	1:L:51:ASP:HB2	1.90	0.53
1:D:98:GLU:HG3	1:D:99:PRO:HD2	1.91	0.52
1:E:37:ILE:HB	1:E:38[A]:PRO:HD3	1.92	0.52
1:A:151[A]:ILE:HB	1:A:176:GLU:OE2	2.08	0.52
1:B:155:ARG:HA	1:B:194:ASN:HB3	1.91	0.52
1:K:37:ILE:HB	1:K:38[A]:PRO:HD3	1.90	0.52
1:G:18:ARG:HG2	1:L:18:ARG:NH2	2.24	0.52
1:A:213:GLU:OE1	1:B:141:LYS:HD3	2.09	0.52
1:G:141:LYS:HD3	1:L:213:GLU:OE2	2.10	0.51
1:A:18:ARG:HH22	1:B:18:ARG:HH11	1.57	0.51
1:E:5:ASN:HB3	1:E:11:ILE:HD13	1.93	0.50
1:A:2:ILE:HG12	1:A:115:ILE:HG12	1.94	0.50
1:G:5:ASN:HB3	1:G:11:ILE:HD13	1.94	0.50
1:E:18:ARG:NH2	1:F:18:ARG:HH11	2.10	0.49
1:J:37:ILE:HB	1:J:38[A]:PRO:HD3	1.94	0.49
1:E:116:ILE:O	1:E:120:ARG:HG3	2.12	0.49
1:A:141:LYS:HD3	1:F:213:GLU:OE1	2.13	0.49
1:G:116:ILE:O	1:G:120:ARG:HG3	2.12	0.49
1:H:174:ARG:HD2	1:I:63:GLN:NE2	2.27	0.49
1:J:79:GLU:OE2	1:J:82:ARG:NH2	2.35	0.49
1:I:5:ASN:HB3	1:I:11:ILE:HD13	1.94	0.48
1:C:98:GLU:HG3	1:C:99:PRO:HD2	1.96	0.48
1:F:3:VAL:HG11	1:F:13:GLN:OE1	2.13	0.48
1:A:154:ILE:HG21	1:A:169:PHE:HA	1.96	0.47
1:A:155:ARG:HA	1:A:194:ASN:HB3	1.97	0.47
1:K:30:LYS:HD2	1:K:35:GLU:OE2	2.13	0.47
1:D:105:ALA:HA	1:D:131:TYR:CD1	2.49	0.47
1:F:118:THR:HG23	1:F:127:VAL:HG22	1.97	0.47
1:A:5:ASN:HB3	1:A:11:ILE:HD13	1.97	0.47
1:K:154:ILE:HG21	1:K:169:PHE:HA	1.96	0.46
1:F:154:ILE:HG21	1:F:169:PHE:HA	1.98	0.46
1:A:37:ILE:HB	1:A:38[A]:PRO:HD3	1.98	0.46
1:F:8:GLY:HA3	1:L:7:GLN:HG2	1.98	0.46
1:K:98:GLU:OE2	1:K:125:ILE:HD11	2.16	0.45
1:C:149:VAL:HG12	1:C:150:SER:O	2.16	0.45
1:D:5:ASN:HB3	1:D:11:ILE:HD13	1.99	0.45
1:C:213:GLU:OE1	1:D:141:LYS:HD3	2.17	0.45
1:F:141:LYS:HA	1:F:144:LYS:HE3	1.99	0.45
1:F:120:ARG:HD3	1:F:122:ALA:O	2.16	0.44
1:G:34:PRO:HG3	1:G:175:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ILE:HG21	1:E:169:PHE:HA	2.00	0.44
1:F:120:ARG:O	1:F:124:SER:HB3	2.17	0.44
1:L:169:PHE:CD2	1:L:191:LEU:HD13	2.52	0.44
1:A:18:ARG:HH22	1:B:18:ARG:NH1	2.16	0.44
1:A:105:ALA:HA	1:A:131:TYR:CE1	2.53	0.44
1:B:21:ASN:O	1:B:25:LYS:HG2	2.17	0.44
1:E:18:ARG:HH21	1:F:18:ARG:HG2	1.83	0.44
1:C:12:HIS:HB2	1:C:115:ILE:HD11	1.99	0.44
1:F:12:HIS:HB2	1:F:115:ILE:HD11	2.00	0.44
1:C:32:PHE:HD2	1:C:146:TYR:CE2	2.35	0.44
1:E:98:GLU:HG3	1:E:99:PRO:HD2	1.99	0.44
1:D:154:ILE:HG21	1:D:169:PHE:HA	1.98	0.44
1:F:37:ILE:HB	1:F:38[A]:PRO:HD3	1.99	0.44
1:I:131:TYR:CE2	1:I:135:ILE:HD11	2.53	0.44
1:K:149:VAL:HG12	1:K:150:SER:O	2.18	0.44
1:E:149:VAL:HG12	1:E:150:SER:O	2.18	0.43
1:C:105:ALA:HA	1:C:131:TYR:CD1	2.53	0.43
1:C:105:ALA:HA	1:C:131:TYR:CE1	2.53	0.43
1:F:105:ALA:HA	1:F:131:TYR:CD1	2.54	0.43
1:A:98:GLU:HG3	1:A:99:PRO:HD2	2.00	0.43
1:G:3:VAL:HG11	1:G:13:GLN:OE1	2.18	0.43
1:J:176:GLU:HA	1:J:176:GLU:OE1	2.19	0.43
1:J:213:GLU:OE1	1:K:141:LYS:HD3	2.18	0.43
1:C:3:VAL:HG11	1:C:13:GLN:OE1	2.19	0.43
1:D:155:ARG:HA	1:D:194:ASN:HB3	1.98	0.43
1:C:118:THR:HG22	1:C:126:PRO:HA	2.01	0.43
1:K:7:GLN:HE21	1:K:9:GLN:CB	2.31	0.43
1:D:47:ALA:HB1	1:D:51:ASP:HB2	2.00	0.43
1:F:2:ILE:HG12	1:F:115:ILE:HG12	2.01	0.43
1:C:103:ASP:HB3	1:C:117:TRP:CZ3	2.54	0.42
1:E:96:ILE:HD12	1:E:116:ILE:HG21	2.00	0.42
1:L:105:ALA:HA	1:L:131:TYR:CD1	2.54	0.42
1:F:149:VAL:HG12	1:F:150:SER:O	2.18	0.42
1:K:105:ALA:HA	1:K:131:TYR:CD1	2.54	0.42
1:L:116:ILE:O	1:L:120:ARG:HG3	2.18	0.42
1:A:18:ARG:HG2	1:F:18:ARG:NH2	2.35	0.42
1:B:2:ILE:HG12	1:B:115:ILE:HG12	2.02	0.42
1:E:161:PRO:HG2	1:E:164:ASP:OD2	2.20	0.42
1:I:18:ARG:NH2	1:J:18:ARG:HG2	2.35	0.42
1:C:174:ARG:HD2	1:D:63:GLN:NE2	2.35	0.42
1:F:5:ASN:HB3	1:F:11:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:VAL:HG11	1:L:13:GLN:OE1	2.19	0.42
1:F:137:LEU:HD23	1:F:141:LYS:HE2	2.02	0.42
1:F:131:TYR:CE2	1:F:135:ILE:HD11	2.55	0.42
1:H:71:GLU:O	1:H:75:GLU:HG3	2.19	0.42
1:L:98:GLU:HG3	1:L:99:PRO:HD2	2.00	0.42
1:I:71:GLU:O	1:I:75:GLU:HG3	2.19	0.41
1:L:21:ASN:O	1:L:25:LYS:HG2	2.19	0.41
1:L:97:ARG:NH2	1:L:113:GLU:OE1	2.48	0.41
1:F:103:ASP:HB3	1:F:117:TRP:CZ3	2.55	0.41
1:E:47:ALA:HB1	1:E:51:ASP:HB2	2.01	0.41
1:J:118:THR:HG23	1:J:127:VAL:HG22	2.02	0.41
1:B:183:LYS:O	1:B:187:THR:HG23	2.21	0.41
1:G:35:GLU:O	1:G:39:MET:HG2	2.20	0.41
1:H:118:THR:HG22	1:H:126:PRO:HA	2.03	0.41
1:K:98:GLU:HG3	1:K:99:PRO:HD2	2.02	0.41
1:K:12:HIS:HB2	1:K:115:ILE:HD11	2.02	0.41
1:B:187:THR:O	1:B:191:LEU:HB3	2.21	0.41
1:C:4:THR:HA	1:C:9:GLN:O	2.21	0.41
1:D:18:ARG:NH2	1:E:18:ARG:HG2	2.35	0.41
1:G:149:VAL:HG12	1:G:150:SER:O	2.20	0.41
1:J:177:GLN:HG2	1:J:180:GLN:OE1	2.20	0.41
1:K:203:LEU:HD22	1:K:215[A]:MET:HG2	2.03	0.41
1:E:4:THR:HA	1:E:9:GLN:O	2.21	0.41
1:C:162:PHE:O	1:C:166:VAL:HG23	2.22	0.40
1:F:71:GLU:O	1:F:75:GLU:HG3	2.21	0.40
1:G:144:LYS:HD3	1:G:144:LYS:C	2.41	0.40
1:J:12:HIS:HB2	1:J:115:ILE:HD11	2.03	0.40
1:B:18:ARG:NH2	1:C:18:ARG:HG2	2.36	0.40
1:E:2:ILE:HG12	1:E:115:ILE:HG12	2.03	0.40
1:C:30:LYS:HD2	1:C:35:GLU:OE2	2.22	0.40
1:K:21:ASN:O	1:K:25:LYS:HG2	2.21	0.40
1:A:47:ALA:HB1	1:A:51:ASP:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LEU:O	1:K:155:ARG:NH2[2_556]	2.07	0.13
1:A:205:ALA:O	1:J:179:THR:OG1[1_556]	2.14	0.06

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	201/232 (87%)	199 (99%)	2 (1%)	0	100	100
1	B	205/232 (88%)	202 (98%)	3 (2%)	0	100	100
1	C	197/232 (85%)	195 (99%)	1 (0%)	1 (0%)	29	68
1	D	191/232 (82%)	189 (99%)	2 (1%)	0	100	100
1	E	191/232 (82%)	189 (99%)	1 (0%)	1 (0%)	29	68
1	F	200/232 (86%)	197 (98%)	3 (2%)	0	100	100
1	G	200/232 (86%)	196 (98%)	4 (2%)	0	100	100
1	H	189/232 (82%)	187 (99%)	2 (1%)	0	100	100
1	I	200/232 (86%)	198 (99%)	2 (1%)	0	100	100
1	J	194/232 (84%)	192 (99%)	2 (1%)	0	100	100
1	K	187/232 (81%)	185 (99%)	1 (0%)	1 (0%)	29	68
1	L	189/232 (82%)	186 (98%)	3 (2%)	0	100	100
All	All	2344/2784 (84%)	2315 (99%)	26 (1%)	3 (0%)	51	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	148	PRO
1	E	148	PRO
1	K	148	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	173/193 (90%)	172 (99%)	1 (1%)	86	95
1	B	173/193 (90%)	173 (100%)	0	100	100
1	C	169/193 (88%)	169 (100%)	0	100	100
1	D	167/193 (86%)	167 (100%)	0	100	100
1	E	168/193 (87%)	168 (100%)	0	100	100
1	F	171/193 (89%)	171 (100%)	0	100	100
1	G	171/193 (89%)	171 (100%)	0	100	100
1	H	167/193 (86%)	167 (100%)	0	100	100
1	I	169/193 (88%)	169 (100%)	0	100	100
1	J	169/193 (88%)	169 (100%)	0	100	100
1	K	164/193 (85%)	162 (99%)	2 (1%)	71	90
1	L	165/193 (86%)	165 (100%)	0	100	100
All	All	2026/2316 (88%)	2023 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LYS
1	K	199[A]	CYS
1	K	199[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	63	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	207/232 (89%)	-0.40	1 (0%)	91	75	39, 77, 125, 149	0
1	B	210/232 (90%)	-0.31	0	100	100	39, 72, 143, 193	0
1	C	202/232 (87%)	-0.30	0	100	100	36, 83, 147, 203	0
1	D	198/232 (85%)	-0.25	0	100	100	48, 85, 150, 186	1 (0%)
1	E	198/232 (85%)	-0.27	0	100	100	44, 87, 157, 196	1 (0%)
1	F	206/232 (88%)	-0.28	0	100	100	53, 94, 150, 208	0
1	G	205/232 (88%)	-0.27	1 (0%)	91	75	41, 87, 145, 184	0
1	H	196/232 (84%)	-0.25	1 (0%)	91	75	54, 97, 163, 194	1 (0%)
1	I	205/232 (88%)	-0.03	8 (3%)	39	15	57, 98, 153, 199	1 (0%)
1	J	201/232 (86%)	-0.23	5 (2%)	57	29	52, 94, 165, 212	0
1	K	194/232 (83%)	-0.19	4 (2%)	63	34	66, 103, 160, 222	0
1	L	197/232 (84%)	-0.25	2 (1%)	82	59	59, 104, 171, 223	0
All	All	2419/2784 (86%)	-0.25	22 (0%)	84	63	36, 92, 156, 223	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	209	GLY	5.3
1	J	210	ALA	4.3
1	J	208	PRO	4.1
1	I	199[A]	CYS	3.5
1	L	7	GLN	3.3
1	K	5	ASN	3.3
1	L	201	GLN	3.0
1	K	6	ALA	2.8
1	I	10	MET	2.7
1	J	207	GLY	2.7
1	I	216	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	193	GLN	2.6
1	A	181	GLU	2.5
1	J	214	GLU	2.4
1	I	203	LEU	2.4
1	I	163	ARG	2.4
1	I	28	GLU	2.3
1	I	201	GLN	2.3
1	I	145	MET	2.2
1	H	28	GLU	2.2
1	K	11	ILE	2.2
1	K	2	ILE	2.1

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.