



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:10 PM UTC

PDB ID : 3H4E / pdb_00003h4e
Title : X-ray Structure of Hexameric HIV-1 CA
Authors : Pornillos, O.
Deposited on : 2009-04-19
Resolution : 2.70 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

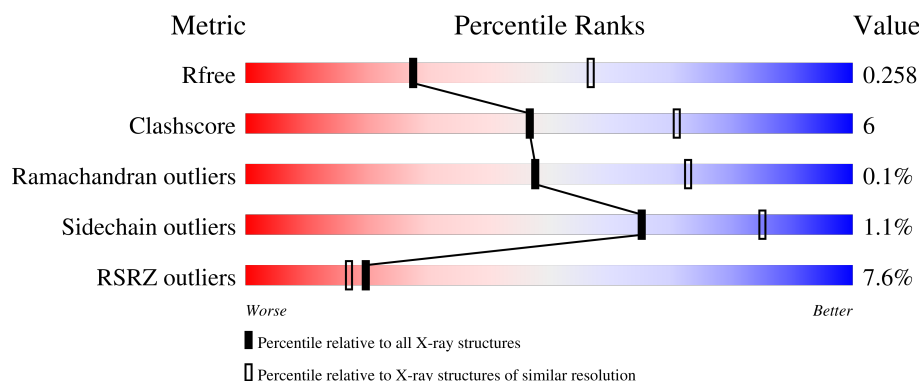
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	 7% 82% 12% • 6%
1	B	231	 6% 71% 16% • 12%
1	C	231	 8% 81% 11% 8%
1	D	231	 9% 73% 13% 13%
1	E	231	 6% 79% 10% 10%

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Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19082 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
			1632	1028	284	306	14			
1	B	204	Total	C	N	O	S	0	0	0
			1564	986	271	293	14			
1	C	212	Total	C	N	O	S	0	0	0
			1618	1015	283	306	14			
1	D	200	Total	C	N	O	S	0	0	0
			1522	955	266	287	14			
1	E	207	Total	C	N	O	S	0	0	0
			1574	991	273	297	13			
1	F	219	Total	C	N	O	S	0	0	0
			1661	1044	290	313	14			
1	G	218	Total	C	N	O	S	0	0	0
			1652	1037	288	313	14			
1	H	208	Total	C	N	O	S	0	0	0
			1587	999	278	296	14			
1	I	211	Total	C	N	O	S	0	0	0
			1588	1005	273	296	14			
1	J	214	Total	C	N	O	S	0	0	0
			1630	1022	286	308	14			
1	K	198	Total	C	N	O	S	0	0	0
			1509	950	262	283	14			
1	L	205	Total	C	N	O	S	0	0	0
			1545	973	265	294	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP P12497
A	45	CYS	GLU	engineered mutation	UNP P12497
A	184	ALA	TRP	engineered mutation	UNP P12497
A	185	ALA	MET	engineered mutation	UNP P12497
B	14	CYS	ALA	engineered mutation	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	GLU	engineered mutation	UNP P12497
B	184	ALA	TRP	engineered mutation	UNP P12497
B	185	ALA	MET	engineered mutation	UNP P12497
C	14	CYS	ALA	engineered mutation	UNP P12497
C	45	CYS	GLU	engineered mutation	UNP P12497
C	184	ALA	TRP	engineered mutation	UNP P12497
C	185	ALA	MET	engineered mutation	UNP P12497
D	14	CYS	ALA	engineered mutation	UNP P12497
D	45	CYS	GLU	engineered mutation	UNP P12497
D	184	ALA	TRP	engineered mutation	UNP P12497
D	185	ALA	MET	engineered mutation	UNP P12497
E	14	CYS	ALA	engineered mutation	UNP P12497
E	45	CYS	GLU	engineered mutation	UNP P12497
E	184	ALA	TRP	engineered mutation	UNP P12497
E	185	ALA	MET	engineered mutation	UNP P12497
F	14	CYS	ALA	engineered mutation	UNP P12497
F	45	CYS	GLU	engineered mutation	UNP P12497
F	184	ALA	TRP	engineered mutation	UNP P12497
F	185	ALA	MET	engineered mutation	UNP P12497
G	14	CYS	ALA	engineered mutation	UNP P12497
G	45	CYS	GLU	engineered mutation	UNP P12497
G	184	ALA	TRP	engineered mutation	UNP P12497
G	185	ALA	MET	engineered mutation	UNP P12497
H	14	CYS	ALA	engineered mutation	UNP P12497
H	45	CYS	GLU	engineered mutation	UNP P12497
H	184	ALA	TRP	engineered mutation	UNP P12497
H	185	ALA	MET	engineered mutation	UNP P12497
I	14	CYS	ALA	engineered mutation	UNP P12497
I	45	CYS	GLU	engineered mutation	UNP P12497
I	184	ALA	TRP	engineered mutation	UNP P12497
I	185	ALA	MET	engineered mutation	UNP P12497
J	14	CYS	ALA	engineered mutation	UNP P12497
J	45	CYS	GLU	engineered mutation	UNP P12497
J	184	ALA	TRP	engineered mutation	UNP P12497
J	185	ALA	MET	engineered mutation	UNP P12497
K	14	CYS	ALA	engineered mutation	UNP P12497
K	45	CYS	GLU	engineered mutation	UNP P12497
K	184	ALA	TRP	engineered mutation	UNP P12497
K	185	ALA	MET	engineered mutation	UNP P12497
L	14	CYS	ALA	engineered mutation	UNP P12497
L	45	CYS	GLU	engineered mutation	UNP P12497
L	184	ALA	TRP	engineered mutation	UNP P12497

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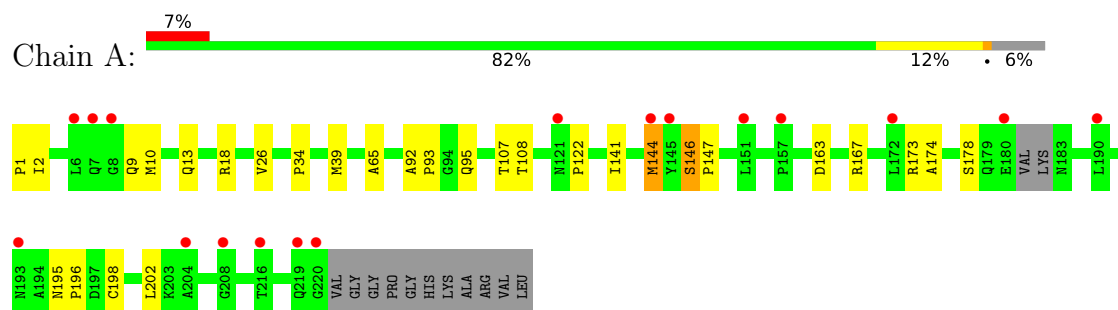
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Chain	Residue	Modelled	Actual	Comment	Reference
L	185	ALA	MET	engineered mutation	UNP P12497

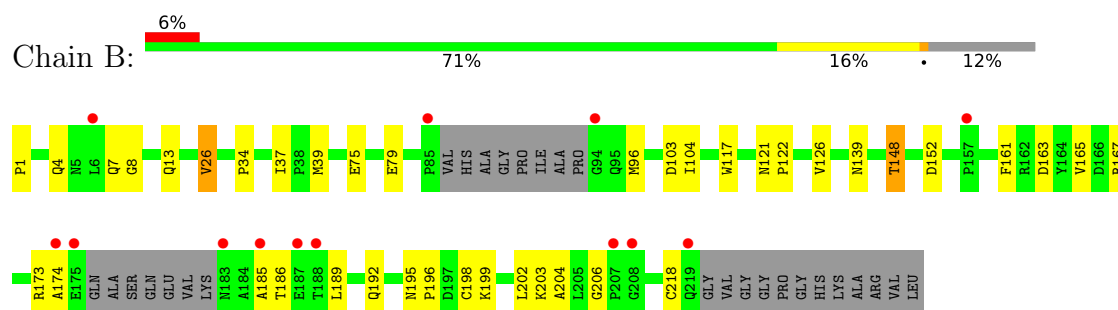
3 Residue-property plots [i](#)

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.

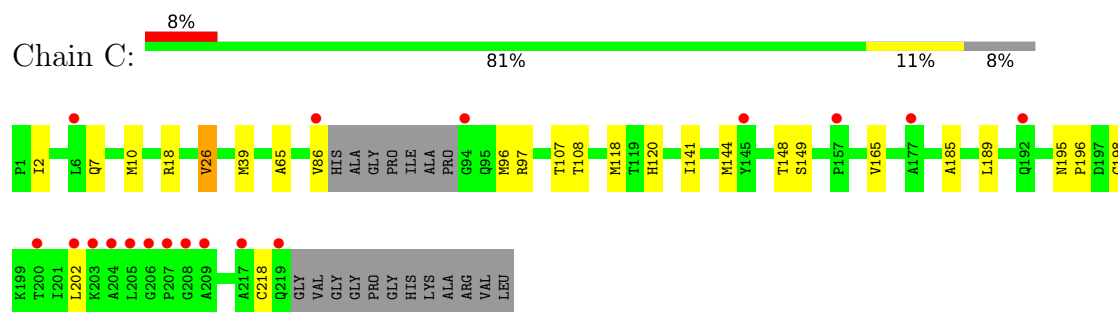
• Molecule 1: Capsid protein p24



• Molecule 1: Capsid protein p24

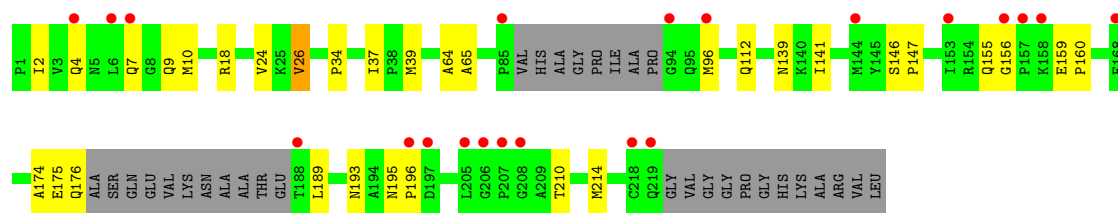


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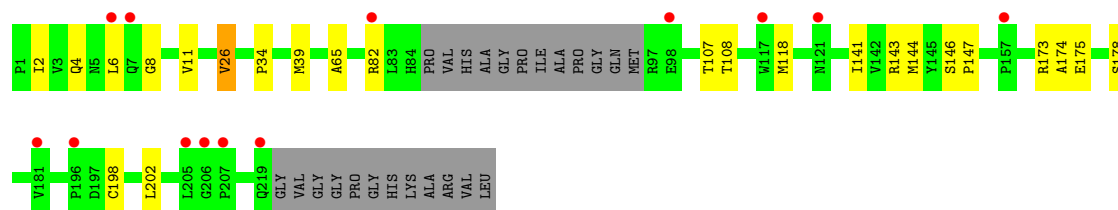
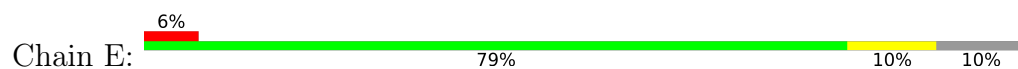


• Molecule 1: Capsid protein p24

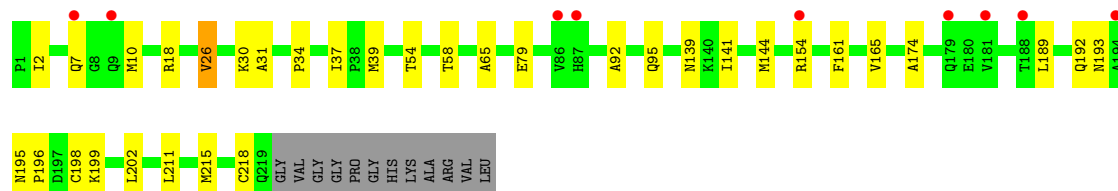
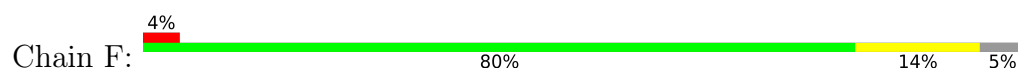




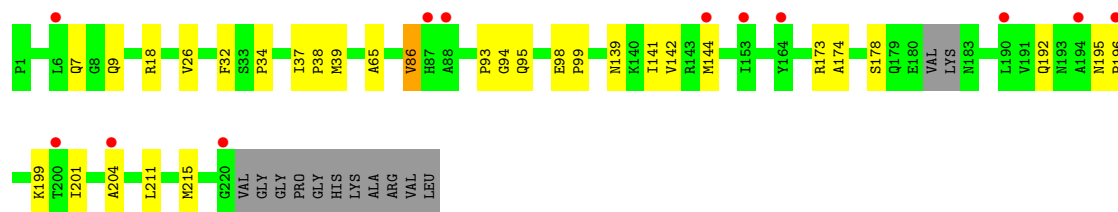
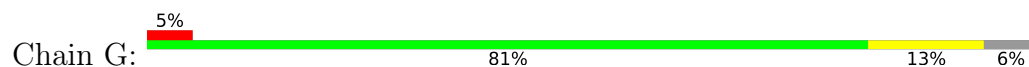
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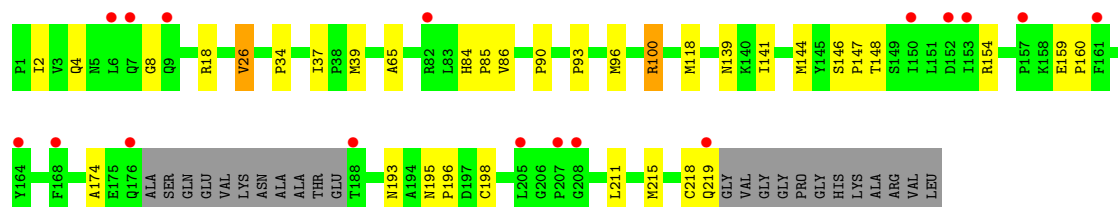
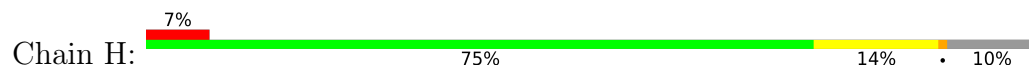
• Molecule 1: Capsid protein p24



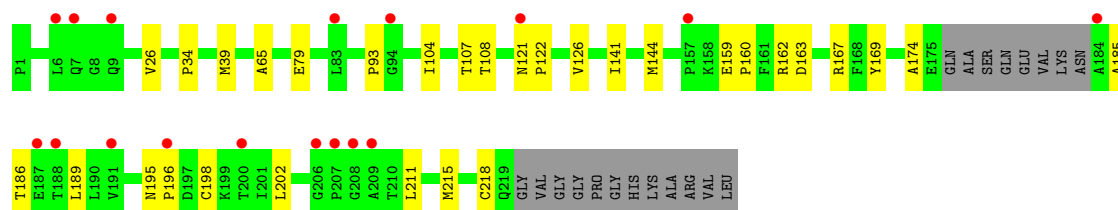
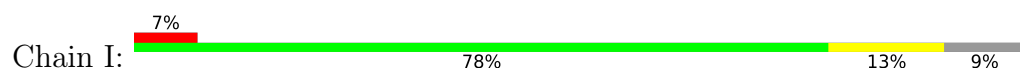
• Molecule 1: Capsid protein p24



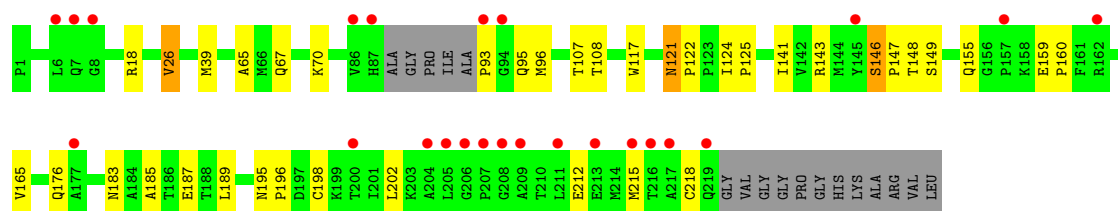
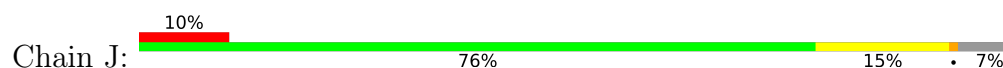
• Molecule 1: Capsid protein p24



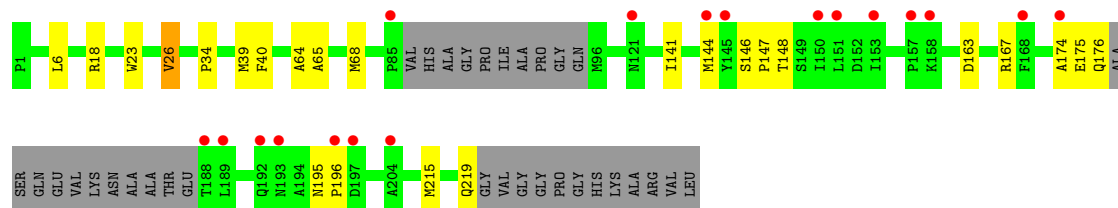
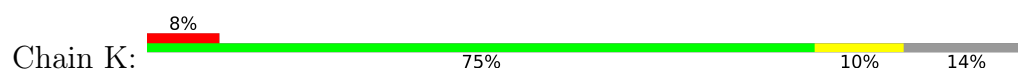
● Molecule 1: Capsid protein p24



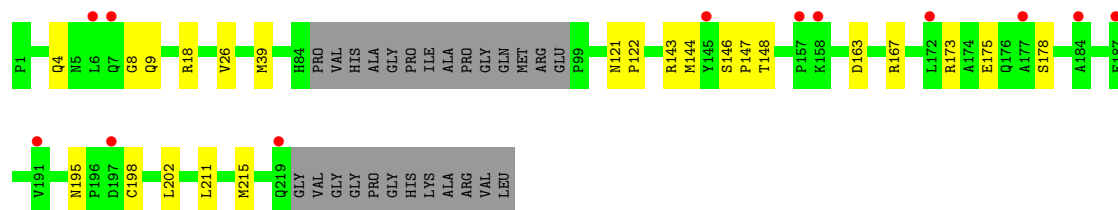
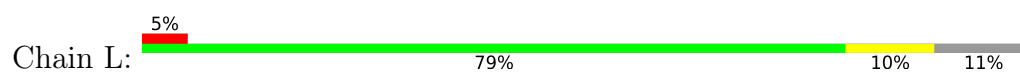
● Molecule 1: Capsid protein p24



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● Molecule 1: Capsid protein p24



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.06Å 136.66Å 208.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.74 – 2.70 34.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (34.74-2.70) 95.8 (34.74-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.238 , 0.263 (Not available) , 0.258	Depositor DCC
R_{free} test set	2565 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19082	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

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	0.47	0/1668	0.81	2/2273 (0.1%)
1	B	0.46	0/1596	0.78	0/2168
1	C	0.46	0/1651	0.78	0/2246
1	D	0.47	0/1554	0.79	0/2112
1	E	0.48	0/1606	0.76	0/2185
1	F	0.46	0/1697	0.77	0/2310
1	G	0.44	0/1687	0.80	0/2297
1	H	0.44	0/1623	0.76	0/2210
1	I	0.47	0/1624	0.80	0/2213
1	J	0.46	0/1664	0.81	2/2263 (0.1%)
1	K	0.46	0/1541	0.75	0/2096
1	L	0.46	0/1577	0.75	0/2148
All	All	0.46	0/19488	0.78	4/26521 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	146	SER	CA-C-N	8.81	128.52	119.19
1	J	146	SER	C-N-CA	8.81	128.52	119.19
1	A	146	SER	CA-C-N	7.28	128.53	120.45
1	A	146	SER	C-N-CA	7.28	128.53	120.45

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	1632	0	1575	20	0
1	B	1564	0	1533	27	0
1	C	1618	0	1573	18	0
1	D	1522	0	1455	19	0
1	E	1574	0	1532	14	1
1	F	1661	0	1612	23	0
1	G	1652	0	1604	20	0
1	H	1587	0	1546	22	0
1	I	1588	0	1544	21	0
1	J	1630	0	1583	26	1
1	K	1509	0	1452	18	0
1	L	1545	0	1483	14	0
All	All	19082	0	18492	213	1

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 6.

All (213) 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:J:212:GLU:HG3	1:K:144:MET:SD	2.10	0.91
1:H:4:GLN:NE2	1:H:8:GLY:HA2	1.89	0.88
1:C:96:MET:HE2	1:H:93:PRO:HA	1.59	0.85
1:B:199:LYS:O	1:B:203:LYS:HG3	1.76	0.84
1:H:154:ARG:HG2	1:H:193:ASN:HB3	1.68	0.75
1:D:96:MET:HE2	1:G:93:PRO:HA	1.72	0.72
1:G:18:ARG:NH2	1:H:18:ARG:HH11	1.88	0.70
1:G:18:ARG:HH22	1:H:18:ARG:HH11	1.42	0.68
1:L:4:GLN:HE21	1:L:8:GLY:HA2	1.58	0.67
1:C:185:ALA:O	1:C:189:LEU:HB2	1.94	0.67
1:C:2:ILE:HG22	1:C:10:MET:HE3	1.74	0.67
1:B:4:GLN:NE2	1:B:8:GLY:HA2	2.10	0.66
1:G:192:GLN:O	1:G:199:LYS:HE2	1.96	0.66
1:B:4:GLN:HE21	1:B:8:GLY:HA2	1.62	0.65
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.79	0.64
1:B:96:MET:HE2	1:I:93:PRO:HA	1.78	0.64
1:K:175:GLU:O	1:K:176:GLN:HG2	1.97	0.64
1:H:86:VAL:HG21	1:H:100:ARG:HG2	1.80	0.63
1:D:175:GLU:O	1:D:176:GLN:HG2	1.98	0.63
1:E:6:LEU:HD13	1:F:7:GLN:NE2	2.13	0.62
1:I:34:PRO:HG3	1:I:174:ALA:HA	1.83	0.61
1:E:6:LEU:HD22	1:F:7:GLN:HE21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:ILE:HG22	1:F:10:MET:HE3	1.83	0.59
1:K:18:ARG:NH2	1:L:18:ARG:HG2	2.18	0.59
1:A:93:PRO:HB3	1:J:96:MET:HE2	1.84	0.59
1:J:185:ALA:O	1:J:189:LEU:HB2	2.02	0.59
1:H:154:ARG:HG2	1:H:193:ASN:CB	2.33	0.58
1:A:18:ARG:HG3	1:F:18:ARG:NH1	2.18	0.58
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.86	0.58
1:G:34:PRO:HG3	1:G:174:ALA:HA	1.85	0.58
1:B:7:GLN:HE22	1:C:7:GLN:HE21	1.52	0.56
1:B:148:THR:HG22	1:B:152:ASP:HB2	1.87	0.56
1:L:173:ARG:HA	1:L:178:SER:O	2.06	0.55
1:J:18:ARG:CZ	1:K:18:ARG:HD3	2.36	0.55
1:E:4:GLN:NE2	1:E:8:GLY:HA2	2.23	0.54
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.90	0.54
1:C:202:LEU:HD21	1:C:218:CYS:SG	2.47	0.54
1:I:162:ARG:HG3	1:I:215:MET:HE1	1.90	0.54
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.90	0.54
1:A:2:ILE:HG22	1:A:10:MET:HE3	1.90	0.54
1:A:34:PRO:HG3	1:A:174:ALA:HA	1.90	0.53
1:J:65:ALA:HB1	1:J:141:ILE:HD13	1.89	0.53
1:H:37:ILE:HD13	1:H:139:ASN:OD1	2.09	0.53
1:J:165:VAL:HG12	1:K:64:ALA:HB2	1.89	0.53
1:J:215:MET:HB2	1:K:144:MET:HE1	1.90	0.53
1:J:183:ASN:O	1:J:187:GLU:HG3	2.09	0.52
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.92	0.52
1:C:198:CYS:O	1:C:202:LEU:HG	2.10	0.52
1:G:94:GLY:O	1:G:95:GLN:HG2	2.09	0.51
1:A:198:CYS:O	1:A:202:LEU:HG	2.11	0.51
1:C:97:ARG:HB2	1:H:90:PRO:HB2	1.92	0.51
1:B:7:GLN:HA	1:B:7:GLN:NE2	2.26	0.51
1:A:122:PRO:HG3	1:I:122:PRO:HB3	1.91	0.51
1:B:198:CYS:HB3	1:B:218:CYS:SG	2.51	0.51
1:E:198:CYS:O	1:E:202:LEU:HG	2.11	0.51
1:J:202:LEU:HD21	1:J:218:CYS:SG	2.51	0.50
1:H:34:PRO:HG3	1:H:174:ALA:HA	1.94	0.50
1:I:198:CYS:O	1:I:202:LEU:HG	2.11	0.50
1:J:107:THR:HG22	1:J:108:THR:HG23	1.93	0.50
1:E:143:ARG:HG2	1:E:175:GLU:O	2.11	0.50
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.92	0.50
1:B:198:CYS:O	1:B:202:LEU:HG	2.13	0.49
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:VAL:HG21	1:E:39:MET:HG2	1.95	0.49
1:J:198:CYS:SG	1:J:218:CYS:HB3	2.52	0.49
1:J:198:CYS:O	1:J:202:LEU:HG	2.12	0.49
1:I:185:ALA:O	1:I:189:LEU:HB2	2.13	0.49
1:B:75:GLU:O	1:B:79:GLU:HG3	2.13	0.49
1:I:163:ASP:O	1:I:167:ARG:HG3	2.13	0.49
1:B:148:THR:CG2	1:B:152:ASP:HB2	2.43	0.49
1:F:92:ALA:HB3	1:F:95:GLN:HG3	1.96	0.48
1:J:93:PRO:HD2	1:J:95:GLN:HE21	1.78	0.48
1:B:103:ASP:HB3	1:B:117:TRP:CH2	2.49	0.48
1:A:93:PRO:CB	1:J:96:MET:HE2	2.43	0.48
1:A:146:SER:HA	1:A:147:PRO:HD3	1.62	0.48
1:K:34:PRO:HG3	1:K:174:ALA:HA	1.95	0.48
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.95	0.48
1:A:195:ASN:HB2	1:A:196:PRO:CD	2.43	0.48
1:F:65:ALA:HB1	1:F:141:ILE:HD13	1.96	0.47
1:G:32:PHE:O	1:G:142:VAL:HG22	2.14	0.47
1:A:107:THR:HG22	1:A:108:THR:HG23	1.97	0.47
1:G:195:ASN:HB2	1:G:196:PRO:CD	2.44	0.47
1:A:144:MET:HE2	1:A:144:MET:HB3	1.60	0.47
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.95	0.47
1:G:173:ARG:HA	1:G:178:SER:O	2.14	0.47
1:A:122:PRO:HG3	1:I:122:PRO:HG3	1.97	0.47
1:E:34:PRO:HG3	1:E:174:ALA:HA	1.96	0.47
1:F:192:GLN:HA	1:F:199:LYS:HE3	1.97	0.46
1:I:107:THR:HG22	1:I:108:THR:HG23	1.97	0.46
1:B:104:ILE:HG12	1:B:126:VAL:HG12	1.96	0.46
1:D:34:PRO:HG3	1:D:174:ALA:HA	1.96	0.46
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.97	0.46
1:J:146:SER:HA	1:J:147:PRO:HD3	1.58	0.46
1:H:144:MET:HE2	1:H:144:MET:HB3	1.59	0.46
1:C:2:ILE:HD12	1:C:118:MET:HE2	1.97	0.46
1:I:79:GLU:HA	1:I:79:GLU:OE1	2.15	0.46
1:G:201:ILE:O	1:G:204:ALA:HB3	2.16	0.46
1:F:211:LEU:O	1:F:215:MET:HG3	2.16	0.46
1:D:195:ASN:HB2	1:D:196:PRO:CD	2.46	0.45
1:H:2:ILE:HD12	1:H:118:MET:HE2	1.97	0.45
1:J:195:ASN:HB2	1:J:196:PRO:CD	2.46	0.45
1:H:26:VAL:HG21	1:H:39:MET:HG2	1.97	0.45
1:L:215:MET:HE2	1:L:215:MET:HB3	1.89	0.45
1:J:212:GLU:HB2	1:K:68:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:23:TRP:CZ3	1:K:40:PHE:HB2	2.52	0.45
1:B:26:VAL:HG21	1:B:39:MET:HG2	1.99	0.45
1:B:34:PRO:HG3	1:B:174:ALA:HA	1.99	0.45
1:G:86:VAL:HG13	1:G:98:GLU:HB2	1.98	0.45
1:B:185:ALA:O	1:B:189:LEU:HB2	2.16	0.45
1:G:144:MET:HE2	1:G:144:MET:HB3	1.65	0.45
1:K:18:ARG:HH21	1:L:18:ARG:HG2	1.79	0.45
1:E:2:ILE:HD12	1:E:118:MET:HE2	1.99	0.45
1:H:96:MET:HE2	1:H:96:MET:HB3	1.86	0.45
1:D:9:GLN:HE22	1:G:9:GLN:HE21	1.63	0.44
1:F:189:LEU:HD11	1:F:193:ASN:ND2	2.31	0.44
1:J:143:ARG:HD3	1:J:176:GLN:OE1	2.16	0.44
1:A:92:ALA:O	1:A:95:GLN:HB2	2.17	0.44
1:C:148:THR:HG22	1:C:149:SER:O	2.17	0.44
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.97	0.44
1:B:161:PHE:O	1:B:165:VAL:HG23	2.16	0.44
1:D:159:GLU:HA	1:D:160:PRO:HD3	1.90	0.44
1:F:154:ARG:HG3	1:F:193:ASN:HB3	1.99	0.44
1:G:211:LEU:O	1:G:215:MET:HG3	2.17	0.44
1:K:146:SER:HA	1:K:147:PRO:HD3	1.85	0.44
1:F:198:CYS:O	1:F:202:LEU:HG	2.17	0.44
1:J:26:VAL:HG21	1:J:39:MET:HG2	2.00	0.44
1:E:173:ARG:HA	1:E:178:SER:O	2.18	0.44
1:F:79:GLU:OE1	1:F:79:GLU:HA	2.18	0.44
1:K:6:LEU:HD23	1:K:6:LEU:HA	1.75	0.44
1:F:144:MET:HB3	1:F:144:MET:HE2	1.60	0.44
1:D:7:GLN:HB3	1:G:7:GLN:NE2	2.32	0.43
1:F:34:PRO:HG3	1:F:174:ALA:HA	2.00	0.43
1:K:163:ASP:O	1:K:167:ARG:HG3	2.18	0.43
1:B:204:ALA:C	1:B:206:GLY:H	2.27	0.43
1:A:1:PRO:HD2	1:A:13:GLN:O	2.18	0.43
1:A:9:GLN:OE1	1:A:9:GLN:HA	2.18	0.43
1:L:211:LEU:O	1:L:215:MET:HG3	2.19	0.43
1:C:26:VAL:HG21	1:C:39:MET:HG2	2.00	0.43
1:F:37:ILE:HD13	1:F:139:ASN:OD1	2.19	0.43
1:F:195:ASN:C	1:F:195:ASN:OD1	2.61	0.43
1:H:146:SER:HA	1:H:147:PRO:HD3	1.75	0.43
1:L:26:VAL:HG21	1:L:39:MET:HG2	2.01	0.43
1:B:34:PRO:HB2	1:B:173:ARG:HD3	2.01	0.42
1:C:144:MET:HB3	1:C:144:MET:HE2	1.64	0.42
1:D:189:LEU:HD11	1:D:193:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:ASN:HA	1:J:122:PRO:HA	1.93	0.42
1:J:215:MET:HE2	1:J:215:MET:HB3	1.94	0.42
1:C:86:VAL:O	1:C:86:VAL:HG23	2.19	0.42
1:C:107:THR:HG22	1:C:108:THR:HG23	1.99	0.42
1:H:198:CYS:SG	1:H:218:CYS:HB3	2.60	0.42
1:I:121:ASN:HA	1:I:122:PRO:HA	1.83	0.42
1:K:195:ASN:HB2	1:K:196:PRO:CD	2.48	0.42
1:D:210:THR:O	1:D:214:MET:HG3	2.19	0.42
1:C:65:ALA:HB1	1:C:141:ILE:HD13	2.01	0.42
1:G:65:ALA:HB1	1:G:141:ILE:HD13	2.02	0.42
1:J:124:ILE:HA	1:J:125:PRO:HD3	1.91	0.42
1:K:215:MET:O	1:K:219:GLN:HG3	2.20	0.42
1:C:96:MET:HE1	1:C:120:HIS:CD2	2.55	0.42
1:D:155:GLN:HG2	1:D:156:GLY:O	2.20	0.42
1:E:107:THR:HG22	1:E:108:THR:HG23	2.01	0.42
1:F:202:LEU:HD21	1:F:218:CYS:SG	2.59	0.42
1:G:37:ILE:HD13	1:G:139:ASN:OD1	2.18	0.42
1:A:173:ARG:HA	1:A:178:SER:O	2.20	0.42
1:C:195:ASN:HB2	1:C:196:PRO:CD	2.50	0.42
1:L:195:ASN:OD1	1:L:195:ASN:C	2.63	0.42
1:B:1:PRO:HD2	1:B:13:GLN:O	2.19	0.42
1:E:144:MET:HE2	1:E:144:MET:HB3	1.61	0.42
1:J:148:THR:HG22	1:J:149:SER:O	2.19	0.42
1:F:54:THR:O	1:F:58:THR:HG23	2.18	0.42
1:I:211:LEU:O	1:I:215:MET:HG3	2.19	0.42
1:L:163:ASP:O	1:L:167:ARG:HG3	2.20	0.42
1:A:93:PRO:HG3	1:J:117:TRP:CE2	2.55	0.42
1:D:4:GLN:HE21	1:E:11:VAL:HG11	1.84	0.42
1:G:98:GLU:HA	1:G:99:PRO:HD3	1.83	0.42
1:B:117:TRP:CE2	1:I:93:PRO:HG2	2.55	0.41
1:F:195:ASN:HB2	1:F:196:PRO:CD	2.50	0.41
1:H:159:GLU:HA	1:H:160:PRO:HD3	1.92	0.41
1:I:144:MET:HB3	1:I:144:MET:HE2	1.64	0.41
1:L:143:ARG:HG2	1:L:175:GLU:O	2.19	0.41
1:B:204:ALA:C	1:B:206:GLY:N	2.76	0.41
1:E:146:SER:HA	1:E:147:PRO:HD3	1.87	0.41
1:F:161:PHE:O	1:F:165:VAL:HG23	2.20	0.41
1:B:37:ILE:HD13	1:B:139:ASN:OD1	2.20	0.41
1:F:215:MET:HE2	1:F:215:MET:HB3	1.90	0.41
1:G:37:ILE:HB	1:G:38:PRO:HD3	2.03	0.41
1:H:84:HIS:O	1:H:85:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:195:ASN:HB2	1:I:196:PRO:CD	2.50	0.41
1:L:144:MET:HE2	1:L:144:MET:HB3	1.65	0.41
1:A:65:ALA:HB1	1:A:141:ILE:HD13	2.02	0.41
1:C:18:ARG:HH21	1:D:18:ARG:HH21	1.69	0.41
1:D:146:SER:HA	1:D:147:PRO:HD3	1.82	0.41
1:H:195:ASN:HB2	1:H:196:PRO:CD	2.50	0.41
1:B:192:GLN:HA	1:B:199:LYS:HE3	2.02	0.41
1:H:211:LEU:O	1:H:215:MET:HG3	2.21	0.41
1:L:198:CYS:O	1:L:202:LEU:HG	2.21	0.41
1:F:30:LYS:O	1:F:31:ALA:C	2.64	0.41
1:I:26:VAL:HG21	1:I:39:MET:HG2	2.01	0.41
1:B:195:ASN:HB2	1:B:196:PRO:CD	2.51	0.41
1:C:165:VAL:HG12	1:D:64:ALA:HB2	2.02	0.41
1:H:198:CYS:HB3	1:H:218:CYS:SG	2.61	0.41
1:I:104:ILE:HG12	1:I:126:VAL:HG12	2.01	0.41
1:I:198:CYS:SG	1:I:218:CYS:HB3	2.60	0.41
1:A:163:ASP:O	1:A:167:ARG:HG3	2.21	0.41
1:B:121:ASN:HA	1:B:122:PRO:HA	1.92	0.40
1:J:159:GLU:HA	1:J:160:PRO:HD3	1.89	0.40
1:D:37:ILE:HD13	1:D:139:ASN:OD1	2.21	0.40
1:K:175:GLU:C	1:K:176:GLN:CG	2.94	0.40
1:L:121:ASN:HA	1:L:122:PRO:HA	1.90	0.40
1:I:169:TYR:CZ	1:J:67:GLN:HG2	2.56	0.40
1:B:163:ASP:O	1:B:167:ARG:HG3	2.22	0.40
1:D:175:GLU:C	1:D:176:GLN:CG	2.95	0.40
1:I:159:GLU:HA	1:I:160:PRO:HD3	1.96	0.40
1:L:146:SER:HA	1:L:147:PRO:HD3	1.75	0.40

All (1) 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:E:82:ARG:NH1	1:J:155:GLN:O[3_454]	2.16	0.04

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	214/231 (93%)	212 (99%)	2 (1%)	0	100	100
1	B	198/231 (86%)	194 (98%)	3 (2%)	1 (0%)	24	48
1	C	208/231 (90%)	205 (99%)	3 (1%)	0	100	100
1	D	194/231 (84%)	191 (98%)	3 (2%)	0	100	100
1	E	203/231 (88%)	197 (97%)	6 (3%)	0	100	100
1	F	217/231 (94%)	210 (97%)	7 (3%)	0	100	100
1	G	214/231 (93%)	209 (98%)	5 (2%)	0	100	100
1	H	204/231 (88%)	201 (98%)	3 (2%)	0	100	100
1	I	207/231 (90%)	203 (98%)	3 (1%)	1 (0%)	24	48
1	J	210/231 (91%)	206 (98%)	4 (2%)	0	100	100
1	K	192/231 (83%)	190 (99%)	2 (1%)	0	100	100
1	L	201/231 (87%)	197 (98%)	4 (2%)	0	100	100
All	All	2462/2772 (89%)	2415 (98%)	45 (2%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	186	THR
1	B	186	THR

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	168/193 (87%)	167 (99%)	1 (1%)	78	91
1	B	166/193 (86%)	164 (99%)	2 (1%)	63	84
1	C	171/193 (89%)	170 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	158/193 (82%)	155 (98%)	3 (2%)	50	77
1	E	165/193 (86%)	164 (99%)	1 (1%)	78	91
1	F	172/193 (89%)	171 (99%)	1 (1%)	78	91
1	G	173/193 (90%)	172 (99%)	1 (1%)	78	91
1	H	168/193 (87%)	164 (98%)	4 (2%)	43	72
1	I	165/193 (86%)	165 (100%)	0	100	100
1	J	172/193 (89%)	169 (98%)	3 (2%)	53	79
1	K	158/193 (82%)	156 (99%)	2 (1%)	61	83
1	L	160/193 (83%)	158 (99%)	2 (1%)	61	83
All	All	1996/2316 (86%)	1975 (99%)	21 (1%)	65	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	MET
1	B	26	VAL
1	B	148	THR
1	C	26	VAL
1	D	24	VAL
1	D	26	VAL
1	D	112	GLN
1	E	26	VAL
1	F	26	VAL
1	G	86	VAL
1	H	26	VAL
1	H	100	ARG
1	H	148	THR
1	H	219	GLN
1	J	26	VAL
1	J	70	LYS
1	J	121	ASN
1	K	26	VAL
1	K	148	THR
1	L	9	GLN
1	L	148	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	95	GLN
1	A	179	GLN
1	B	7	GLN
1	B	120	HIS
1	C	120	HIS
1	C	179	GLN
1	D	4	GLN
1	D	7	GLN
1	D	13	GLN
1	E	4	GLN
1	E	176	GLN
1	F	7	GLN
1	F	12	HIS
1	F	13	GLN
1	F	67	GLN
1	F	84	HIS
1	G	9	GLN
1	G	219	GLN
1	H	84	HIS
1	I	95	GLN
1	J	67	GLN
1	J	179	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 ⓘ

There are no ligands in this entry.

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	218/231 (94%)	0.38	17 (7%) 19 16	31, 51, 88, 116	0
1	B	204/231 (88%)	0.39	13 (6%) 25 22	31, 53, 84, 116	0
1	C	212/231 (91%)	0.32	18 (8%) 16 14	32, 51, 88, 117	0
1	D	200/231 (86%)	0.44	21 (10%) 11 9	33, 51, 89, 119	0
1	E	207/231 (89%)	0.47	13 (6%) 26 23	33, 52, 85, 113	0
1	F	219/231 (94%)	0.27	9 (4%) 41 37	33, 51, 89, 115	0
1	G	218/231 (94%)	0.39	12 (5%) 30 27	34, 53, 91, 116	0
1	H	208/231 (90%)	0.41	17 (8%) 17 15	35, 53, 89, 119	0
1	I	211/231 (91%)	0.49	17 (8%) 18 15	35, 52, 86, 116	0
1	J	214/231 (92%)	0.38	24 (11%) 10 8	32, 52, 88, 116	0
1	K	198/231 (85%)	0.44	18 (9%) 15 12	33, 52, 88, 116	0
1	L	205/231 (88%)	0.36	12 (5%) 28 25	33, 53, 89, 117	0
All	All	2514/2772 (90%)	0.39	191 (7%) 20 17	31, 52, 89, 119	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	THR	7.0
1	K	188	THR	5.2
1	H	153	ILE	4.8
1	E	98	GLU	4.4
1	H	207	PRO	4.2
1	I	187	GLU	4.2
1	I	206	GLY	4.1
1	C	177	ALA	4.1
1	J	208	GLY	3.9
1	J	93	PRO	3.8
1	D	197	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	220	GLY	3.8
1	J	94	GLY	3.7
1	A	157	PRO	3.7
1	A	180	GLU	3.7
1	B	94	GLY	3.7
1	C	86	VAL	3.7
1	J	219	GLN	3.7
1	K	197	ASP	3.7
1	K	174	ALA	3.7
1	C	206	GLY	3.6
1	J	7	GLN	3.6
1	B	174	ALA	3.5
1	I	196	PRO	3.5
1	D	219	GLN	3.5
1	J	205	LEU	3.5
1	E	157	PRO	3.5
1	H	161	PHE	3.5
1	J	87	HIS	3.5
1	K	150	ILE	3.4
1	D	207	PRO	3.4
1	K	204	ALA	3.4
1	D	6	LEU	3.4
1	B	187	GLU	3.4
1	J	177	ALA	3.4
1	J	145	TYR	3.4
1	B	207	PRO	3.3
1	I	207	PRO	3.3
1	F	194	ALA	3.3
1	K	153	ILE	3.3
1	B	85	PRO	3.2
1	A	121	ASN	3.2
1	I	6	LEU	3.2
1	E	7	GLN	3.2
1	C	205	LEU	3.2
1	D	158	LYS	3.2
1	J	157	PRO	3.2
1	C	157	PRO	3.1
1	H	219	GLN	3.0
1	D	157	PRO	3.0
1	H	157	PRO	3.0
1	E	181	VAL	3.0
1	A	7	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	121	ASN	3.0
1	E	219	GLN	3.0
1	G	88	ALA	3.0
1	D	196	PRO	2.9
1	B	188	THR	2.9
1	I	191	VAL	2.9
1	C	219	GLN	2.9
1	A	193	ASN	2.9
1	K	145	TYR	2.9
1	C	208	GLY	2.9
1	J	204	ALA	2.9
1	C	200	THR	2.9
1	E	6	LEU	2.9
1	I	121	ASN	2.8
1	C	145	TYR	2.8
1	A	8	GLY	2.8
1	B	185	ALA	2.8
1	I	184	ALA	2.8
1	C	207	PRO	2.8
1	E	196	PRO	2.8
1	G	196	PRO	2.8
1	D	208	GLY	2.8
1	D	85	PRO	2.7
1	G	144	MET	2.7
1	G	194	ALA	2.7
1	J	207	PRO	2.7
1	L	7	GLN	2.6
1	H	82	ARG	2.6
1	C	209	ALA	2.6
1	F	181	VAL	2.6
1	I	209	ALA	2.6
1	G	153	ILE	2.6
1	J	206	GLY	2.6
1	J	6	LEU	2.5
1	K	158	LYS	2.5
1	B	208	GLY	2.5
1	K	85	PRO	2.5
1	J	217	ALA	2.5
1	A	216	THR	2.5
1	J	86	VAL	2.5
1	L	191	VAL	2.5
1	H	168	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	6	LEU	2.5
1	H	9	GLN	2.5
1	K	193	ASN	2.4
1	L	145	TYR	2.4
1	K	192	GLN	2.4
1	G	190	LEU	2.4
1	C	94	GLY	2.4
1	K	196	PRO	2.4
1	J	200	THR	2.4
1	K	151	LEU	2.4
1	D	96	MET	2.4
1	A	220	GLY	2.4
1	L	219	GLN	2.4
1	J	211	LEU	2.4
1	D	168	PHE	2.4
1	E	205	LEU	2.3
1	J	215	MET	2.3
1	B	219	GLN	2.3
1	E	82	ARG	2.3
1	F	9	GLN	2.3
1	C	202	LEU	2.3
1	C	217	ALA	2.3
1	I	83	LEU	2.3
1	G	200	THR	2.3
1	I	188	THR	2.3
1	F	7	GLN	2.3
1	I	9	GLN	2.3
1	I	94	GLY	2.3
1	G	6	LEU	2.3
1	H	188	THR	2.3
1	A	144	MET	2.3
1	J	213	GLU	2.3
1	J	8	GLY	2.3
1	A	145	TYR	2.3
1	F	179	GLN	2.3
1	H	208	GLY	2.3
1	H	205	LEU	2.3
1	D	153	ILE	2.2
1	L	187	GLU	2.2
1	K	121	ASN	2.2
1	E	207	PRO	2.2
1	H	152	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	208	GLY	2.2
1	D	144	MET	2.2
1	F	154	ARG	2.2
1	D	4	GLN	2.2
1	D	7	GLN	2.2
1	H	7	GLN	2.2
1	B	6	LEU	2.2
1	D	205	LEU	2.2
1	J	162	ARG	2.2
1	I	157	PRO	2.2
1	D	94	GLY	2.2
1	K	189	LEU	2.2
1	L	184	ALA	2.2
1	L	158	LYS	2.2
1	A	6	LEU	2.2
1	H	150	ILE	2.2
1	C	204	ALA	2.1
1	L	177	ALA	2.1
1	C	192	GLN	2.1
1	C	203	LYS	2.1
1	C	6	LEU	2.1
1	K	144	MET	2.1
1	J	209	ALA	2.1
1	B	175	GLU	2.1
1	F	188	THR	2.1
1	H	176	GLN	2.1
1	A	190	LEU	2.1
1	D	156	GLY	2.1
1	F	86	VAL	2.1
1	G	204	ALA	2.1
1	A	219	GLN	2.1
1	I	7	GLN	2.1
1	L	6	LEU	2.1
1	B	183	ASN	2.1
1	D	206	GLY	2.1
1	E	206	GLY	2.1
1	K	168	PHE	2.1
1	L	197	ASP	2.1
1	A	204	ALA	2.1
1	I	200	THR	2.1
1	B	157	PRO	2.1
1	K	157	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	151	LEU	2.1
1	F	87	HIS	2.1
1	I	208	GLY	2.1
1	H	164	TYR	2.1
1	J	216	THR	2.0
1	A	172	LEU	2.0
1	L	172	LEU	2.0
1	D	218	CYS	2.0
1	G	164	TYR	2.0
1	E	117	TRP	2.0
1	L	157	PRO	2.0
1	G	87	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.