



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:52 PM UTC

PDB ID : 2X74 / pdb_00002x74
Title : Human foamy virus integrase - catalytic core.
Authors : Rety, S.; Delelis, O.; Rezabkova, L.; Dubanchet, B.; Legrand, P.; Silhan, J.;
Lewit-Bentley, A.
Deposited on : 2010-02-23
Resolution : 2.34 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:

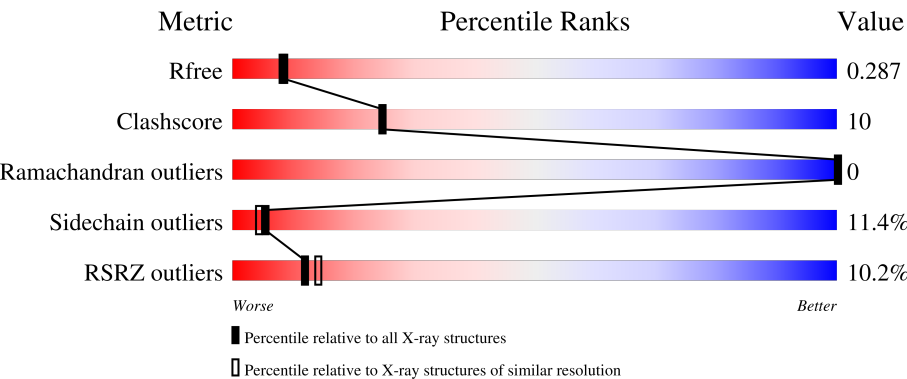
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	200	5% 66% 22% 6% 6%
1	B	200	4% 66% 22% 5% 7%
1	C	200	11% 66% 20% • 11%
1	D	200	16% 65% 20% • 12%
1	E	200	10% 70% 20% • 7%

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Mol	Chain	Length	Quality of chain
1	F	200	9% 70% 19% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9069 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 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	Se	0	2	0
			1514	982	249	279	4			
1	B	186	Total	C	N	O	Se	0	4	0
			1512	978	250	280	4			
1	C	178	Total	C	N	O	Se	0	3	0
			1443	933	242	264	4			
1	D	177	Total	C	N	O	Se	0	2	0
			1429	925	237	263	4			
1	E	186	Total	C	N	O	Se	0	6	0
			1524	986	253	281	4			
1	F	180	Total	C	N	O	Se	0	3	0
			1459	946	238	271	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	MSE	ILE	engineered mutation	UNP P14350
A	180	ARG	LYS	conflict	UNP P14350
A	227	MSE	ILE	engineered mutation	UNP P14350
A	253	MSE	LEU	engineered mutation	UNP P14350
B	127	MSE	ILE	engineered mutation	UNP P14350
B	180	ARG	LYS	conflict	UNP P14350
B	227	MSE	ILE	engineered mutation	UNP P14350
B	253	MSE	LEU	engineered mutation	UNP P14350
C	127	MSE	ILE	engineered mutation	UNP P14350
C	180	ARG	LYS	conflict	UNP P14350
C	227	MSE	ILE	engineered mutation	UNP P14350
C	253	MSE	LEU	engineered mutation	UNP P14350
D	127	MSE	ILE	engineered mutation	UNP P14350
D	180	ARG	LYS	conflict	UNP P14350
D	227	MSE	ILE	engineered mutation	UNP P14350
D	253	MSE	LEU	engineered mutation	UNP P14350
E	127	MSE	ILE	engineered mutation	UNP P14350

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Chain	Residue	Modelled	Actual	Comment	Reference
E	180	ARG	LYS	conflict	UNP P14350
E	227	MSE	ILE	engineered mutation	UNP P14350
E	253	MSE	LEU	engineered mutation	UNP P14350
F	127	MSE	ILE	engineered mutation	UNP P14350
F	180	ARG	LYS	conflict	UNP P14350
F	227	MSE	ILE	engineered mutation	UNP P14350
F	253	MSE	LEU	engineered mutation	UNP P14350

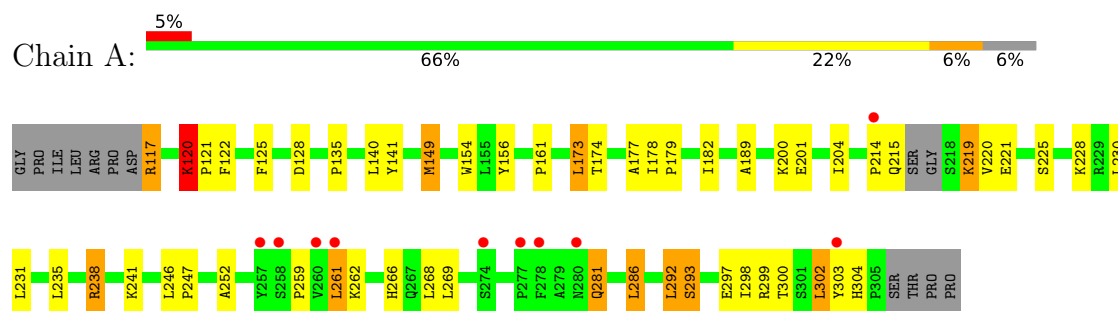
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	55	Total O 55 55	0	0
2	B	54	Total O 54 54	0	0
2	C	19	Total O 19 19	0	0
2	D	6	Total O 6 6	0	0
2	E	35	Total O 35 35	0	0
2	F	19	Total O 19 19	0	0

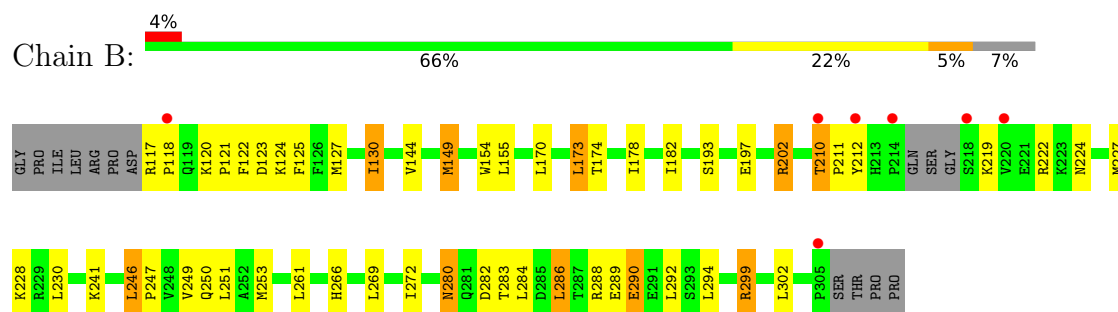
3 Residue-property plots

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.

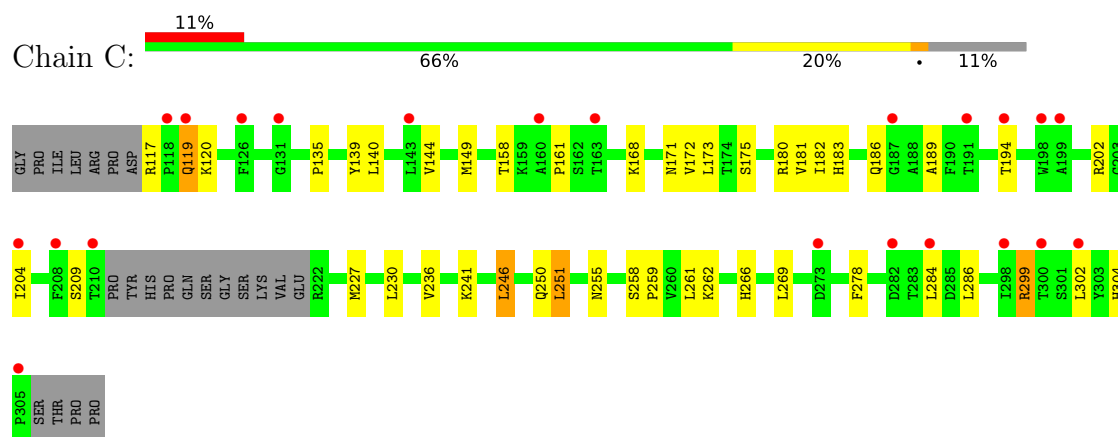
• Molecule 1: INTEGRASE



• Molecule 1: INTEGRASE

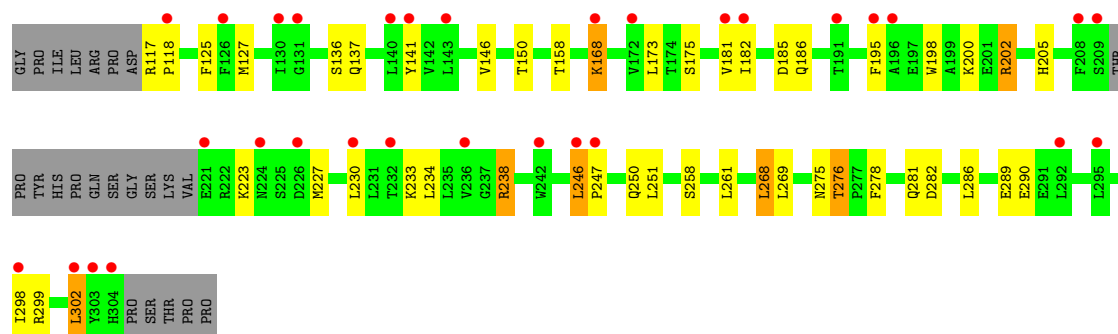


• Molecule 1: INTEGRASE

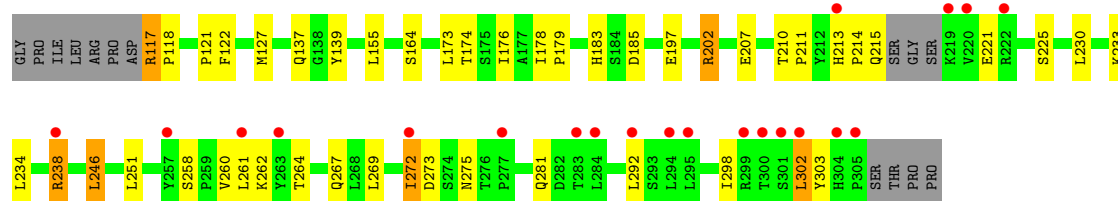


• Molecule 1: INTEGRASE

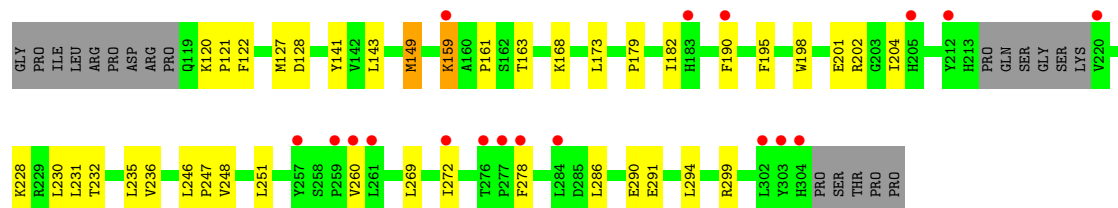




• Molecule 1: INTEGRASE



• Molecule 1: INTEGRASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.18Å 89.11Å 177.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.58 – 2.34 34.58 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.58-2.34) 98.9 (34.58-2.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.233 , 0.294 0.230 , 0.287	Depositor DCC
R_{free} test set	2843 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9069	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	0.66	0/1564	0.91	5/2126 (0.2%)
1	B	0.69	0/1571	0.92	1/2134 (0.0%)
1	C	0.57	0/1493	0.87	0/2027
1	D	0.53	0/1474	0.86	4/1999 (0.2%)
1	E	0.64	0/1594	0.87	4/2167 (0.2%)
1	F	0.60	2/1510 (0.1%)	0.86	0/2050
All	All	0.62	2/9206 (0.0%)	0.88	14/12503 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	149	MSE	SE-CE	-5.35	1.79	1.95
1	F	149	MSE	CG-SE	-5.05	1.80	1.95

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	ILE	N-CA-C	6.45	117.19	110.62
1	A	120	LYS	N-CA-C	6.04	113.66	108.22
1	E	238[A]	ARG	CA-C-N	5.91	127.23	119.84
1	E	238[A]	ARG	C-N-CA	5.91	127.23	119.84
1	E	238[B]	ARG	CA-C-N	5.91	127.23	119.84
1	E	238[B]	ARG	C-N-CA	5.91	127.23	119.84
1	A	219	LYS	N-CA-C	-5.50	106.24	113.12
1	A	238	ARG	CA-C-N	5.36	124.81	119.24
1	A	238	ARG	C-N-CA	5.36	124.81	119.24
1	D	258	SER	CA-C-N	5.06	124.50	119.24
1	D	258	SER	C-N-CA	5.06	124.50	119.24
1	D	238	ARG	CA-C-N	5.04	124.82	119.28
1	D	238	ARG	C-N-CA	5.04	124.82	119.28
1	A	149	MSE	N-CA-C	5.01	116.43	110.97

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	1514	0	1510	37	0
1	B	1512	0	1510	48	0
1	C	1443	0	1452	26	0
1	D	1429	0	1433	23	0
1	E	1524	0	1516	25	0
1	F	1459	0	1456	21	0
2	A	55	0	0	2	0
2	B	54	0	0	3	0
2	C	19	0	0	1	0
2	D	6	0	0	2	0
2	E	35	0	0	1	0
2	F	19	0	0	0	0
All	All	9069	0	8877	174	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 10.

All (174) 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:B:202[A]:ARG:HG2	1:B:202[A]:ARG:HH11	1.18	1.05
1:B:299:ARG:HG2	1:B:299:ARG:HH11	1.23	1.04
1:D:127:MSE:HE2	1:D:182:ILE:HG21	1.42	0.99
1:B:202[A]:ARG:HH11	1:B:202[A]:ARG:CG	1.76	0.98
1:C:299:ARG:HH11	1:C:299:ARG:HG2	1.28	0.96
1:F:127:MSE:HE3	1:F:143:LEU:HD11	1.52	0.89
1:A:117:ARG:CG	1:A:117:ARG:HH11	1.88	0.85
1:A:117:ARG:HH11	1:A:117:ARG:HG2	1.39	0.85
1:D:198:TRP:O	1:D:202:ARG:HD3	1.76	0.85
1:F:299:ARG:HH11	1:F:299:ARG:HG2	1.43	0.82
1:E:210:THR:HB	1:E:211:PRO:HD2	1.64	0.80
1:B:202[A]:ARG:HG2	1:B:202[A]:ARG:NH1	1.90	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:GLN:HA	1:E:221:GLU:HG3	1.64	0.79
1:C:299:ARG:HH11	1:C:299:ARG:CG	1.97	0.78
1:B:193:SER:O	1:B:197[B]:GLU:HG3	1.86	0.76
1:A:215:GLN:HG3	1:A:220:VAL:HG12	1.68	0.75
1:B:127:MSE:HE3	1:B:182:ILE:HG21	1.67	0.75
1:B:127:MSE:HE3	1:B:182:ILE:CG2	2.17	0.74
1:B:210:THR:HG22	1:B:212:TYR:H	1.55	0.72
1:B:299:ARG:HH11	1:B:299:ARG:CG	2.00	0.71
1:C:183:HIS:CE1	1:C:209:SER:HB3	2.27	0.70
1:C:262:LYS:HE2	2:C:2013:HOH:O	1.92	0.69
1:B:155:LEU:H	1:B:250:GLN:NE2	1.91	0.69
1:B:121:PRO:HD3	1:B:149:MSE:HE2	1.73	0.69
1:C:161:PRO:O	1:C:189:ALA:HB2	1.93	0.68
1:A:117:ARG:HG2	1:A:117:ARG:NH1	2.09	0.68
1:B:280:ASN:C	1:B:280:ASN:HD22	2.01	0.68
1:E:202[B]:ARG:HH22	1:F:247:PRO:HB2	1.58	0.68
1:C:180[B]:ARG:HG3	1:C:181:VAL:HG23	1.77	0.66
1:E:185[A]:ASP:OD2	2:E:2020:HOH:O	2.14	0.66
1:D:246:LEU:HB3	1:D:247:PRO:HD3	1.77	0.66
1:A:122:PHE:O	1:A:179:PRO:HA	1.96	0.66
1:B:117:ARG:N	1:B:118:PRO:CD	2.59	0.66
1:E:139:TYR:OH	1:F:168:LYS:HD3	1.96	0.66
1:E:214:PRO:O	1:E:215:GLN:HB2	1.97	0.64
1:D:127:MSE:HE1	1:D:195:PHE:HZ	1.64	0.62
1:B:117:ARG:N	1:B:118:PRO:HD3	2.15	0.61
1:C:139:TYR:OH	1:D:168[B]:LYS:HD3	2.01	0.61
1:D:127:MSE:CE	1:D:182:ILE:HG21	2.25	0.61
1:B:219:LYS:HA	1:B:222:ARG:HB3	1.83	0.60
1:A:247:PRO:HB2	1:B:202[B]:ARG:HH22	1.67	0.60
1:C:180[A]:ARG:HG3	1:C:181:VAL:HG23	1.83	0.59
1:E:258:SER:HB3	1:E:261:LEU:HB2	1.84	0.59
1:D:117:ARG:N	1:D:118:PRO:CD	2.66	0.58
1:F:128:ASP:HB3	1:F:228:LYS:HE2	1.85	0.58
1:B:299:ARG:HG2	1:B:299:ARG:NH1	2.04	0.58
1:D:117:ARG:N	1:D:118:PRO:HD3	2.18	0.57
1:A:117:ARG:CG	1:A:117:ARG:NH1	2.58	0.57
1:A:125:PHE:CE2	1:A:173:LEU:HD13	2.40	0.57
1:E:302:LEU:HD12	1:E:303:TYR:CE2	2.39	0.57
1:A:215:GLN:HG3	1:A:220:VAL:CG1	2.34	0.56
1:B:210:THR:HG23	1:B:211:PRO:HD2	1.86	0.56
1:F:121:PRO:O	1:F:122:PHE:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PRO:HA	1:B:123:ASP:OD2	2.06	0.55
1:E:122:PHE:O	1:E:179:PRO:HA	2.07	0.55
1:E:221:GLU:O	1:E:225:SER:HB2	2.07	0.55
1:D:181:VAL:HG22	1:D:205:HIS:HB3	1.89	0.54
1:A:214:PRO:O	1:A:215:GLN:HB2	2.08	0.54
1:B:289[B]:GLU:HG2	1:B:290:GLU:N	2.22	0.54
1:E:298:ILE:HG23	1:E:302:LEU:HD23	1.88	0.54
1:B:118:PRO:HG3	1:B:124:LYS:HB3	1.90	0.53
1:B:280:ASN:HD22	1:B:282:ASP:H	1.54	0.53
1:B:280:ASN:ND2	1:B:282:ASP:H	2.06	0.53
1:A:259:PRO:O	1:A:262:LYS:HE3	2.08	0.53
1:A:261:LEU:HG	1:A:268:LEU:HD11	1.90	0.53
1:A:293:SER:O	1:A:297:GLU:HG3	2.09	0.53
1:E:210:THR:HB	1:E:211:PRO:CD	2.38	0.53
1:A:261:LEU:HG	1:A:268:LEU:CD1	2.39	0.52
1:F:127:MSE:CE	1:F:190:PHE:CE1	2.92	0.52
1:B:127:MSE:HE3	1:B:182:ILE:HG23	1.92	0.52
1:C:120:LYS:C	1:C:149:MSE:HG3	2.35	0.52
1:D:127:MSE:HE1	1:D:195:PHE:CZ	2.45	0.52
1:F:163:THR:HG23	1:F:195:PHE:HB2	1.90	0.52
1:B:130:ILE:HD11	1:B:228:LYS:HB3	1.92	0.51
1:C:172:VAL:O	1:C:175:SER:HB2	2.10	0.51
1:D:125:PHE:CE2	1:D:173:LEU:HD11	2.45	0.51
1:B:299:ARG:CG	1:B:299:ARG:NH1	2.67	0.51
1:C:182:ILE:HD12	1:C:204:ILE:HG21	1.92	0.51
1:C:266:HIS:HD2	2:D:2004:HOH:O	1.93	0.51
1:A:174:THR:HB	1:A:178:ILE:HD13	1.93	0.50
1:C:251:LEU:HD22	1:C:255:ASN:ND2	2.27	0.50
1:D:141:TYR:HB2	1:D:158:THR:HG23	1.92	0.50
1:E:174:THR:HB	1:E:178:ILE:HD13	1.93	0.50
1:D:276:THR:HG23	1:D:278:PHE:O	2.11	0.49
1:C:183:HIS:HE1	1:C:209:SER:HB3	1.74	0.49
1:B:224:ASN:HB3	1:B:228:LYS:HE3	1.95	0.49
1:B:127:MSE:HE1	1:B:170:LEU:HD11	1.95	0.49
1:C:175:SER:HB3	1:D:250:GLN:CD	2.39	0.48
1:E:234:LEU:HA	1:E:238[B]:ARG:HH21	1.77	0.48
1:F:299:ARG:HG2	1:F:299:ARG:NH1	2.18	0.48
1:E:183:HIS:HD2	1:E:207:GLU:OE2	1.97	0.48
1:F:231:LEU:O	1:F:235:LEU:HG	2.13	0.48
1:C:144:VAL:HG11	1:C:227:MSE:HE1	1.95	0.47
1:C:299:ARG:HG2	1:C:299:ARG:NH1	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:MSE:HE1	1:F:190:PHE:CE1	2.50	0.47
1:A:298:ILE:O	1:A:302:LEU:HB2	2.15	0.47
1:B:283:THR:O	1:B:286:LEU:HB2	2.15	0.47
1:A:220:VAL:HG13	1:A:221:GLU:N	2.30	0.46
1:C:299:ARG:CG	1:C:299:ARG:NH1	2.66	0.46
1:A:128:ASP:OD2	1:A:228:LYS:HE3	2.14	0.46
1:A:182:ILE:HD12	1:A:204:ILE:HG21	1.97	0.46
1:E:302:LEU:HD12	1:E:303:TYR:CD2	2.51	0.46
1:C:251:LEU:HD13	1:C:284:LEU:HD13	1.97	0.46
1:F:141:TYR:CE1	1:F:161:PRO:HD3	2.51	0.46
1:E:272:ILE:HD12	1:E:272:ILE:H	1.81	0.46
1:C:266:HIS:CD2	2:D:2004:HOH:O	2.68	0.46
1:D:281:GLN:O	1:D:299:ARG:NH2	2.49	0.46
1:B:210:THR:HG23	1:B:211:PRO:CD	2.46	0.45
1:E:121:PRO:O	1:E:122:PHE:HB2	2.16	0.45
1:C:119:GLN:O	1:C:149:MSE:HE3	2.17	0.45
1:A:161:PRO:O	1:A:189:ALA:HB2	2.16	0.45
1:A:135:PRO:HG3	1:A:140:LEU:HD21	1.98	0.45
1:A:266:HIS:HD2	2:B:2018:HOH:O	1.99	0.45
1:B:251:LEU:CD1	1:B:284:LEU:HD13	2.47	0.45
1:D:146:VAL:HG21	1:D:227:MSE:HE1	1.99	0.45
1:B:174:THR:HB	1:B:178:ILE:HD13	1.99	0.44
1:A:141:TYR:CE1	1:A:161:PRO:HD3	2.52	0.44
1:A:281:GLN:H	1:A:281:GLN:CD	2.25	0.44
1:D:150:THR:HG22	1:D:268:LEU:HB3	1.99	0.44
1:A:215:GLN:HE21	1:A:219:LYS:H	1.64	0.44
1:B:121:PRO:O	1:B:122:PHE:HB2	2.18	0.44
1:A:154:TRP:HB3	1:A:156:TYR:CE2	2.53	0.43
1:F:198:TRP:CD1	1:F:202:ARG:NH1	2.86	0.43
1:A:214:PRO:O	1:A:215:GLN:CB	2.65	0.43
1:F:272:ILE:H	1:F:272:ILE:HD12	1.82	0.43
1:A:300:THR:O	1:A:304:HIS:HD2	2.00	0.43
1:B:127:MSE:HA	1:B:144:VAL:O	2.18	0.43
1:B:154:TRP:CE2	1:B:173:LEU:HD21	2.54	0.43
1:C:246:LEU:HD23	1:C:246:LEU:HA	1.92	0.43
1:E:264:THR:OG1	1:E:267:GLN:HG3	2.19	0.43
1:E:214:PRO:O	1:E:215:GLN:CB	2.66	0.43
1:D:298:ILE:O	1:D:302:LEU:HB2	2.18	0.43
1:B:202[A]:ARG:HH11	1:B:202[A]:ARG:HG3	1.76	0.43
1:D:230:LEU:O	1:D:234:LEU:HG	2.18	0.43
1:F:182:ILE:HD12	1:F:204:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LEU:HD22	1:C:255:ASN:HD22	1.84	0.42
1:A:286:LEU:HB3	1:A:292:LEU:HD13	2.01	0.42
1:A:302:LEU:HD13	1:A:303:TYR:CE2	2.55	0.42
1:D:125:PHE:CE2	1:D:173:LEU:CD1	3.02	0.42
1:F:232:THR:O	1:F:236:VAL:HG23	2.19	0.42
1:B:249:VAL:O	1:B:253:MSE:HG3	2.20	0.42
1:A:122:PHE:CD2	1:A:125:PHE:HZ	2.38	0.42
1:B:210:THR:CG2	1:B:212:TYR:H	2.27	0.42
1:E:127:MSE:HE3	1:E:127:MSE:HB2	1.98	0.42
1:B:127:MSE:HE1	1:B:170:LEU:CD1	2.50	0.42
1:B:266:HIS:HE1	2:B:2039:HOH:O	2.02	0.42
1:B:125:PHE:CE2	1:B:173:LEU:HD13	2.55	0.42
1:B:130:ILE:HD11	1:B:228:LYS:CG	2.50	0.42
1:D:141:TYR:HB2	1:D:158:THR:CG2	2.50	0.42
1:A:120:LYS:HA	1:A:149:MSE:HE2	2.01	0.41
1:C:250:GLN:CD	1:D:175:SER:HB3	2.45	0.41
1:E:155:LEU:HB3	1:E:246:LEU:HD11	2.02	0.41
1:A:241:LYS:HB2	2:A:2042:HOH:O	2.20	0.41
1:C:135:PRO:HA	1:C:140:LEU:HD23	2.02	0.41
1:F:248:VAL:HG21	1:F:291:GLU:HG2	2.02	0.41
1:A:252:ALA:HB3	1:A:298:ILE:HD13	2.03	0.41
1:E:117:ARG:HA	1:E:118:PRO:HD3	1.93	0.41
1:E:298:ILE:O	1:E:302:LEU:HB2	2.21	0.41
1:A:200:LYS:HB3	1:A:200:LYS:HE2	1.91	0.41
1:B:227:MSE:SE	1:B:227:MSE:C	3.14	0.41
1:E:233:LYS:C	1:E:233:LYS:HD3	2.46	0.41
1:F:122:PHE:O	1:F:179:PRO:HA	2.20	0.41
1:F:299:ARG:NH1	1:F:299:ARG:CG	2.83	0.41
1:F:127:MSE:HE2	1:F:190:PHE:CE1	2.56	0.41
1:A:120:LYS:HB2	1:A:121:PRO:HD2	2.01	0.40
1:B:120:LYS:HA	1:B:149:MSE:HE2	2.03	0.40
1:B:246:LEU:HB3	1:B:247:PRO:HD3	2.03	0.40
1:B:289[B]:GLU:OE1	2:B:2052:HOH:O	2.22	0.40
1:C:258:SER:HA	1:C:259:PRO:HD3	1.94	0.40
1:B:280:ASN:C	1:B:280:ASN:ND2	2.72	0.40
1:A:174:THR:HA	1:A:177:ALA:O	2.20	0.40
2:A:2022:HOH:O	1:B:266:HIS:HD2	2.04	0.40

There are no symmetry-related clashes.

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	185/200 (92%)	182 (98%)	3 (2%)	0	100	100
1	B	186/200 (93%)	180 (97%)	6 (3%)	0	100	100
1	C	177/200 (88%)	172 (97%)	5 (3%)	0	100	100
1	D	175/200 (88%)	169 (97%)	6 (3%)	0	100	100
1	E	188/200 (94%)	181 (96%)	7 (4%)	0	100	100
1	F	179/200 (90%)	171 (96%)	8 (4%)	0	100	100
All	All	1090/1200 (91%)	1055 (97%)	35 (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	172/177 (97%)	154 (90%)	18 (10%)	6	5
1	B	173/177 (98%)	154 (89%)	19 (11%)	6	5
1	C	164/177 (93%)	143 (87%)	21 (13%)	4	3
1	D	162/177 (92%)	138 (85%)	24 (15%)	3	2
1	E	174/177 (98%)	152 (87%)	22 (13%)	4	3
1	F	166/177 (94%)	151 (91%)	15 (9%)	9	9
All	All	1011/1062 (95%)	892 (88%)	119 (12%)	5	4

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	120	LYS
1	A	173	LEU
1	A	201	GLU
1	A	225	SER
1	A	230	LEU
1	A	231	LEU
1	A	235	LEU
1	A	238	ARG
1	A	246	LEU
1	A	261	LEU
1	A	269	LEU
1	A	281	GLN
1	A	286	LEU
1	A	292	LEU
1	A	293	SER
1	A	299	ARG
1	A	302	LEU
1	B	130	ILE
1	B	149	MSE
1	B	173	LEU
1	B	202[A]	ARG
1	B	202[B]	ARG
1	B	210	THR
1	B	230	LEU
1	B	241	LYS
1	B	246	LEU
1	B	261	LEU
1	B	269	LEU
1	B	280	ASN
1	B	286	LEU
1	B	288	ARG
1	B	290	GLU
1	B	292	LEU
1	B	294	LEU
1	B	299	ARG
1	B	302	LEU
1	C	117	ARG
1	C	119	GLN
1	C	158	THR
1	C	168	LYS
1	C	171	ASN

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Mol	Chain	Res	Type
1	C	173	LEU
1	C	186	GLN
1	C	194	THR
1	C	202	ARG
1	C	230	LEU
1	C	236	VAL
1	C	241	LYS
1	C	246	LEU
1	C	251	LEU
1	C	261	LEU
1	C	269	LEU
1	C	278	PHE
1	C	286	LEU
1	C	299	ARG
1	C	302	LEU
1	C	304	HIS
1	D	136	SER
1	D	137	GLN
1	D	168[A]	LYS
1	D	168[B]	LYS
1	D	185	ASP
1	D	186	GLN
1	D	200	LYS
1	D	202	ARG
1	D	223	LYS
1	D	233	LYS
1	D	238	ARG
1	D	246	LEU
1	D	251	LEU
1	D	261	LEU
1	D	268	LEU
1	D	269	LEU
1	D	275[A]	ASN
1	D	275[B]	ASN
1	D	276	THR
1	D	282	ASP
1	D	286	LEU
1	D	289	GLU
1	D	290	GLU
1	D	302	LEU
1	E	117	ARG
1	E	137	GLN

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Mol	Chain	Res	Type
1	E	164	SER
1	E	173	LEU
1	E	176	ILE
1	E	197[A]	GLU
1	E	197[B]	GLU
1	E	202[A]	ARG
1	E	202[B]	ARG
1	E	213	HIS
1	E	230	LEU
1	E	246	LEU
1	E	251	LEU
1	E	260	VAL
1	E	262	LYS
1	E	269	LEU
1	E	272	ILE
1	E	273	ASP
1	E	275	ASN
1	E	281	GLN
1	E	292	LEU
1	E	302	LEU
1	F	120	LYS
1	F	149	MSE
1	F	159[A]	LYS
1	F	159[B]	LYS
1	F	173	LEU
1	F	201	GLU
1	F	230	LEU
1	F	246	LEU
1	F	251	LEU
1	F	260	VAL
1	F	269	LEU
1	F	278	PHE
1	F	286	LEU
1	F	290	GLU
1	F	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	215	GLN
1	A	281	GLN

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Mol	Chain	Res	Type
1	A	296	GLN
1	A	304	HIS
1	B	224	ASN
1	B	250	GLN
1	B	255	ASN
1	B	266	HIS
1	B	275	ASN
1	B	280	ASN
1	B	281	GLN
1	B	296	GLN
1	C	186	GLN
1	C	205	HIS
1	C	224	ASN
1	C	255	ASN
1	C	275	ASN
1	D	137	GLN
1	D	186	GLN
1	D	205	HIS
1	D	224	ASN
1	D	255	ASN
1	E	183	HIS
1	E	213	HIS
1	E	275	ASN
1	E	280	ASN
1	E	281	GLN
1	F	296	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

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	183/200 (91%)	0.23	10 (5%)	30 36	20, 42, 73, 86	2 (1%)
1	B	182/200 (91%)	0.26	7 (3%)	44 50	22, 43, 75, 90	4 (2%)
1	C	174/200 (87%)	0.98	22 (12%)	8 9	36, 60, 88, 98	3 (1%)
1	D	173/200 (86%)	1.23	31 (17%)	3 4	42, 79, 100, 100	2 (1%)
1	E	182/200 (91%)	0.58	21 (11%)	9 11	23, 51, 100, 100	8 (4%)
1	F	176/200 (88%)	0.77	18 (10%)	12 14	35, 57, 90, 100	4 (2%)
All	All	1070/1200 (89%)	0.67	109 (10%)	12 14	20, 54, 94, 100	23 (2%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	PRO	5.4
1	F	220	VAL	4.8
1	E	219	LYS	3.9
1	E	220	VAL	3.8
1	E	284	LEU	3.6
1	C	191	THR	3.4
1	F	260	VAL	3.4
1	A	260	VAL	3.3
1	E	257[A]	TYR	3.3
1	C	210	THR	3.2
1	D	168[A]	LYS	3.2
1	F	257	TYR	3.2
1	B	214	PRO	3.1
1	D	209	SER	3.1
1	F	261	LEU	3.1
1	F	272	ILE	3.0
1	D	246	LEU	3.0
1	D	298	ILE	3.0
1	D	208	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	196	ALA	3.0
1	D	230	LEU	3.0
1	C	199	ALA	2.9
1	F	277	PRO	2.8
1	D	304	HIS	2.8
1	A	278	PHE	2.8
1	F	259	PRO	2.8
1	E	222	ARG	2.8
1	F	183	HIS	2.7
1	E	300	THR	2.7
1	B	218	SER	2.7
1	C	126	PHE	2.7
1	D	224	ASN	2.7
1	E	304	HIS	2.7
1	B	220	VAL	2.7
1	F	276	THR	2.7
1	E	305	PRO	2.7
1	B	305	PRO	2.6
1	E	263	TYR	2.6
1	A	277	PRO	2.6
1	A	214	PRO	2.6
1	D	292	LEU	2.6
1	F	284	LEU	2.6
1	D	242	TRP	2.6
1	B	118	PRO	2.6
1	D	118	PRO	2.6
1	D	181	VAL	2.5
1	C	204	ILE	2.5
1	C	300	THR	2.5
1	F	278	PHE	2.5
1	B	210	THR	2.5
1	C	198	TRP	2.5
1	D	141	TYR	2.5
1	F	205	HIS	2.5
1	C	131	GLY	2.5
1	E	277	PRO	2.5
1	C	194	THR	2.4
1	D	221	GLU	2.4
1	E	302	LEU	2.4
1	E	272	ILE	2.4
1	F	212	TYR	2.4
1	C	208	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	273[A]	ASP	2.3
1	D	130	ILE	2.3
1	F	304	HIS	2.3
1	A	261	LEU	2.3
1	E	294	LEU	2.3
1	C	305	PRO	2.3
1	D	236	VAL	2.3
1	D	302	LEU	2.3
1	E	292	LEU	2.3
1	F	159[A]	LYS	2.3
1	D	131	GLY	2.3
1	F	303	TYR	2.3
1	E	261	LEU	2.2
1	C	187	GLY	2.2
1	E	301	SER	2.2
1	D	195	PHE	2.2
1	D	226	ASP	2.2
1	E	238[A]	ARG	2.2
1	C	160	ALA	2.2
1	D	232	THR	2.2
1	C	284	LEU	2.2
1	D	191	THR	2.2
1	A	257[A]	TYR	2.2
1	C	298	ILE	2.2
1	F	302	LEU	2.2
1	C	119	GLN	2.2
1	B	212	TYR	2.1
1	C	302	LEU	2.1
1	C	143	LEU	2.1
1	D	182	ILE	2.1
1	E	295	LEU	2.1
1	D	247	PRO	2.1
1	E	283	THR	2.1
1	D	140	LEU	2.1
1	D	143	LEU	2.1
1	D	295	LEU	2.1
1	D	126	PHE	2.1
1	F	190	PHE	2.1
1	A	258	SER	2.0
1	A	280	ASN	2.0
1	A	303	TYR	2.0
1	D	303	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	172	VAL	2.0
1	A	274	SER	2.0
1	C	163	THR	2.0
1	E	213	HIS	2.0
1	C	282	ASP	2.0
1	E	299	ARG	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.