



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X74  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

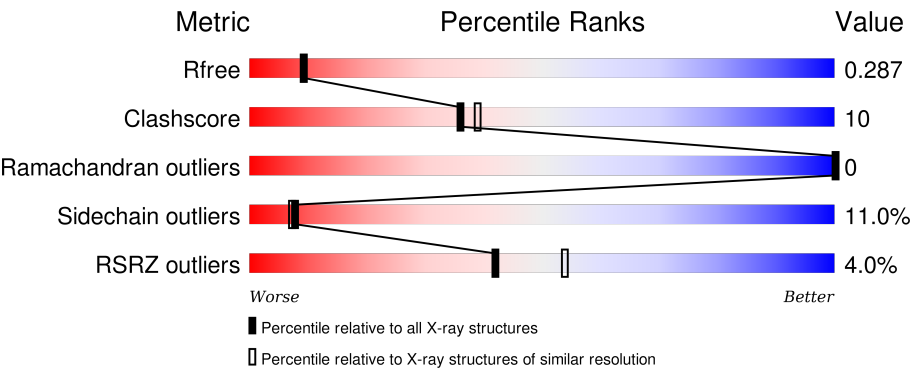
# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>2%</div><div><div></div><div>66%</div><div>24%</div><div>•</div><div>7%</div></div></div>
1	B	200	<div><div>2%</div><div><div></div><div>66%</div><div>23%</div><div>5%</div><div>7%</div></div></div>
1	C	200	<div><div>3%</div><div><div></div><div>68%</div><div>19%</div><div>•</div><div>11%</div></div></div>
1	D	200	<div><div>6%</div><div><div></div><div>66%</div><div>20%</div><div>•</div><div>12%</div></div></div>
1	E	200	<div><div>5%</div><div><div></div><div>72%</div><div>19%</div><div>•</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	200	<div> <div>5%</div> <div>71%</div> <div>19%</div> <div>10%</div> </div>

## 2 Entry composition [i](#)

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

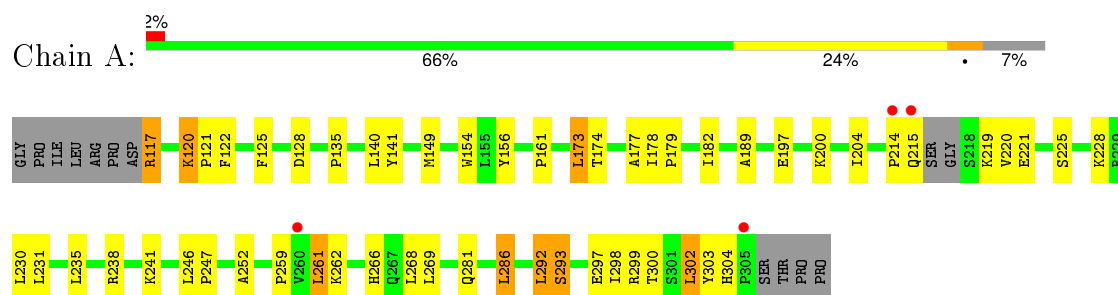
- Molecule 2 is water.

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

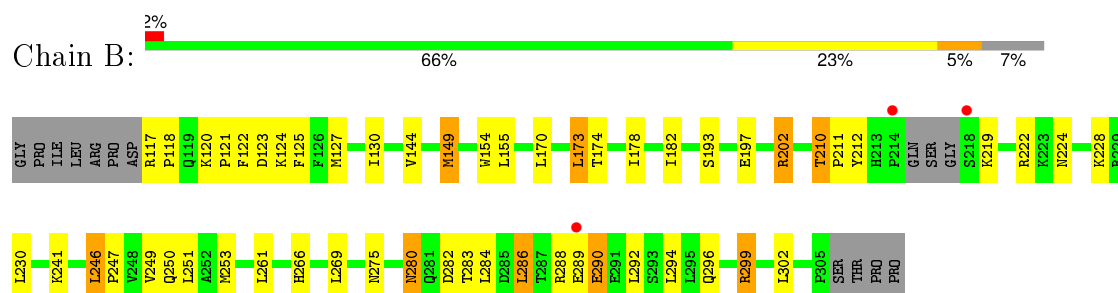
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

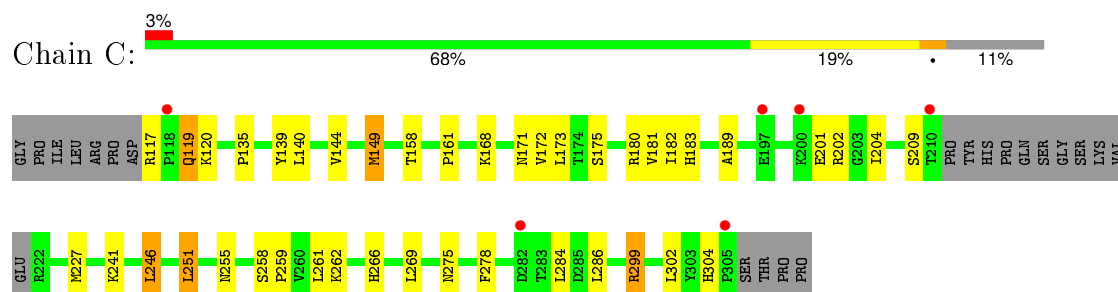
#### • Molecule 1: INTEGRASE



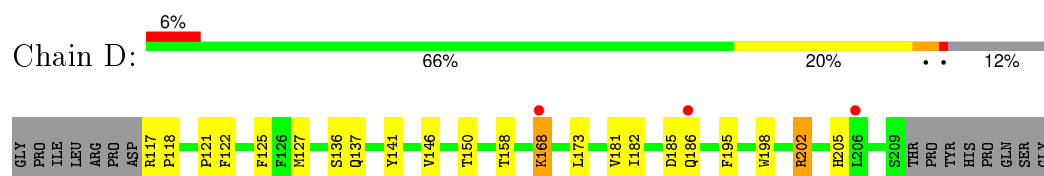
#### • Molecule 1: INTEGRASE

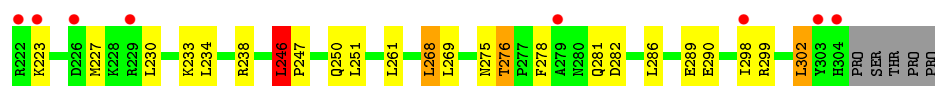


#### • Molecule 1: INTEGRASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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) 98.8 (34.58-2.34)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	2831 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57426 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.54	0/1564	0.65	0/2126
1	B	0.58	0/1571	0.68	0/2134
1	C	0.45	0/1493	0.61	0/2027
1	D	0.42	0/1474	0.59	1/1999 (0.1%)
1	E	0.51	0/1594	0.60	0/2167
1	F	0.49	0/1510	0.61	0/2050
All	All	0.50	0/9206	0.63	1/12503 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	36	0
1	B	1512	0	1510	47	0
1	C	1443	0	1452	25	0
1	D	1429	0	1433	23	0
1	E	1524	0	1516	24	0
1	F	1459	0	1456	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	171	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 (171) 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:HH11	1:B:202[A]:ARG:HG2	1.18	1.05
1:B:299:ARG:HH11	1:B:299:ARG:HG2	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:HH11	1:A:117:ARG:CG	1.88	0.85
1:A:117:ARG:HG2	1:A:117:ARG:HH11	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:NH1	1:B:202[A]:ARG:HG2	1.90	0.79
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:E:202[B]:ARG:HH22	1:F:247:PRO:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:280:ASN:C	1:B:280:ASN:HD22	2.01	0.63
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:NH1	1:A:117:ARG:CG	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
1:B:118:PRO:HA	1:B:123:ASP:OD2	2.06	0.55
1:E:221:GLU:O	1:E:225:SER:HB2	2.07	0.55
1:E:122:PHE:O	1:E:179:PRO:HA	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:F:127:MSE:CE	1:F:190:PHE:CE1	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HG	1:A:268:LEU:CD1	2.39	0.52
1:B:127:MSE:HE3	1:B:182:ILE:HG23	1.92	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:D:125:PHE:CE2	1:D:173:LEU:HD11	2.45	0.51
1:C:172:VAL:O	1:C:175:SER:HB2	2.10	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:E:174:THR:HB	1:E:178:ILE:HD13	1.93	0.50
1:D:141:TYR:HB2	1:D:158:THR:HG23	1.92	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:F:299:ARG:NH1	1:F:299:ARG:HG2	2.18	0.48
1:E:234:LEU:HA	1:E:238[B]:ARG:HH21	1.77	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:120:LYS:C	1:C:149:MSE:HG3	2.35	0.47
1:C:299:ARG:NH1	1:C:299:ARG:HG2	2.09	0.47
1:C:144:VAL:HG11	1:C:227:MSE:HE1	1.95	0.47
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:C:299:ARG:NH1	1:C:299:ARG:CG	2.66	0.46
1:A:220:VAL:HG13	1:A:221:GLU:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:214:PRO:O	1:A:215:GLN:CB	2.65	0.44
1:C:175:SER:HB3	1:D:250:GLN:CD	2.39	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:F:272:ILE:H	1:F:272:ILE:HD12	1.82	0.43
1:B:127:MSE:HA	1:B:144:VAL:O	2.18	0.43
1:E:264:THR:OG1	1:E:267:GLN:HG3	2.19	0.43
1:A:300:THR:O	1:A:304:HIS:HD2	2.00	0.43
1:B:154:TRP:CE2	1:B:173:LEU:HD21	2.54	0.43
1:C:246:LEU:HA	1:C:246:LEU:HD23	1.92	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
1:C:251:LEU:HD22	1:C:255:ASN:HD22	1.84	0.42
1:A:302:LEU:HD13	1:A:303:TYR:CE2	2.55	0.42
1:A:286:LEU:HB3	1:A:292:LEU:HD13	2.01	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:HB2	1:E:127:MSE:HE3	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: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:B:125:PHE:CE2	1:B:173:LEU:HD13	2.55	0.42
1:A:120:LYS:HA	1:A:149:MSE:HE2	2.01	0.41
1:E:155:LEU:HB3	1:E:246:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LYS:HB2	2:A:2042:HOH:O	2.20	0.41
1:B:280:ASN:C	1:B:280:ASN:ND2	2.72	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:E:298:ILE:O	1:E:302:LEU:HB2	2.21	0.41
1:A:252:ALA:HB3	1:A:298:ILE:HD13	2.03	0.41
1:D:121:PRO:O	1:D:122:PHE:HB2	2.21	0.41
1:E:117:ARG:HA	1:E:118:PRO:HD3	1.93	0.41
1:F:299:ARG:NH1	1:F:299:ARG:CG	2.83	0.41
1:F:122:PHE:O	1:F:179:PRO:HA	2.20	0.41
1:A:200:LYS:HE2	1:A:200:LYS:HB3	1.91	0.41
1:F:127:MSE:HE2	1:F:190:PHE:CE1	2.56	0.41
1:B:120:LYS:HA	1:B:149:MSE:HE2	2.03	0.40
1:A:120:LYS:HB2	1:A:121:PRO:HD2	2.01	0.40
1:B:289[B]:GLU:OE1	2:B:2052:HOH:O	2.22	0.40
1:B:246:LEU:HB3	1:B:247:PRO:HD3	2.03	0.40
1:C:258:SER:HA	1:C:259:PRO:HD3	1.94	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 [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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	8	8
1	B	173/177 (98%)	153 (88%)	20 (12%)	7	6
1	C	164/177 (93%)	144 (88%)	20 (12%)	6	5
1	D	162/177 (92%)	139 (86%)	23 (14%)	4	3
1	E	174/177 (98%)	154 (88%)	20 (12%)	7	6
1	F	166/177 (94%)	152 (92%)	14 (8%)	14	14
All	All	1011/1062 (95%)	896 (89%)	115 (11%)	8	6

All (115) 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	197	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

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Mol	Chain	Res	Type
1	A	286	LEU
1	A	292	LEU
1	A	293	SER
1	A	299	ARG
1	A	302	LEU
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	275	ASN
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	296	GLN
1	B	299	ARG
1	B	302	LEU
1	C	117	ARG
1	C	119	GLN
1	C	149	MSE
1	C	158	THR
1	C	168	LYS
1	C	171	ASN
1	C	173	LEU
1	C	201	GLU
1	C	202	ARG
1	C	241	LYS
1	C	246	LEU
1	C	251	LEU
1	C	261	LEU
1	C	269	LEU
1	C	275	ASN
1	C	278	PHE
1	C	286	LEU

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Mol	Chain	Res	Type
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	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
1	E	164	SER
1	E	173	LEU
1	E	180	ARG
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	225	SER
1	E	230	LEU
1	E	246	LEU
1	E	262	LYS
1	E	269	LEU
1	E	272	ILE

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Mol	Chain	Res	Type
1	E	273	ASP
1	E	275	ASN
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	229	ARG
1	F	230	LEU
1	F	246	LEU
1	F	269	LEU
1	F	278	PHE
1	F	286	LEU
1	F	288	ARG
1	F	290	GLU
1	F	294	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	266	HIS
1	A	296	GLN
1	A	304	HIS
1	B	137	GLN
1	B	250	GLN
1	B	266	HIS
1	B	275	ASN
1	B	280	ASN
1	C	186	GLN
1	C	224	ASN
1	C	275	ASN
1	D	137	GLN
1	D	186	GLN
1	D	224	ASN
1	E	183	HIS
1	E	213	HIS
1	E	280	ASN
1	E	281	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	183/200 (91%)	0.06	4 (2%) 65 76	24, 42, 73, 86	0
1	B	182/200 (91%)	0.03	3 (1%) 74 83	22, 44, 75, 90	0
1	C	174/200 (87%)	0.30	6 (3%) 49 60	39, 60, 88, 98	0
1	D	173/200 (86%)	0.55	12 (6%) 20 30	47, 79, 100, 100	0
1	E	182/200 (91%)	0.28	9 (4%) 33 46	27, 51, 100, 100	3 (1%)
1	F	176/200 (88%)	0.27	9 (5%) 32 45	35, 57, 90, 100	1 (0%)
All	All	1070/1200 (89%)	0.25	43 (4%) 42 54	22, 54, 94, 100	4 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	VAL	7.1
1	C	210	THR	5.7
1	C	118	PRO	4.1
1	B	218	SER	3.5
1	D	304	HIS	3.4
1	E	302	LEU	3.4
1	A	260	VAL	3.3
1	A	215	GLN	3.3
1	D	226	ASP	3.0
1	D	206	LEU	2.9
1	E	263	TYR	2.8
1	E	304	HIS	2.7
1	B	214	PRO	2.7
1	A	305	PRO	2.7
1	D	303	TYR	2.7
1	D	221	GLU	2.6
1	D	223	LYS	2.6
1	D	222	ARG	2.5
1	D	298	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	186	GLN	2.5
1	C	282	ASP	2.4
1	E	117	ARG	2.4
1	E	273	ASP	2.4
1	F	213	HIS	2.3
1	C	200	LYS	2.3
1	D	168[A]	LYS	2.3
1	F	276	THR	2.3
1	F	277	PRO	2.2
1	C	197	GLU	2.2
1	E	262	LYS	2.2
1	F	222	ARG	2.2
1	E	261	LEU	2.2
1	E	286	LEU	2.2
1	A	214	PRO	2.1
1	C	305	PRO	2.1
1	F	122	PHE	2.1
1	D	279	ALA	2.1
1	D	229	ARG	2.1
1	F	212	TYR	2.1
1	F	190	PHE	2.0
1	F	278	PHE	2.0
1	F	302	LEU	2.0
1	B	289[A]	GLU	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 carbohydrates 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.