



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X6N  
Title : Human foamy virus integrase - catalytic core. Manganese-bound structure.  
Authors : Rety, S.; Delelis, O.; Rezabkova, L.; Dubanchet, B.; Silhan, J.; Lewit-Bentley, A.  
Deposited on : 2010-02-18  
Resolution : 2.06 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

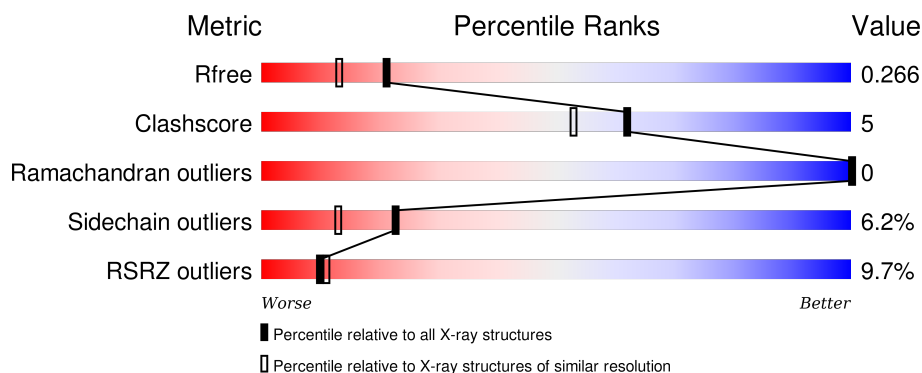
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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))
$R_{free}$	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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>7%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	200	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>9%</div> </div> </div>
1	C	200	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>10%</div> </div> </div>
1	D	200	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>11%</div> </div> </div>
1	E	200	<div> <div>16%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	200	<div><div></div><div>12%</div><div>75%</div><div>14%</div><div>•</div><div>10%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9059 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	188	Total	C	N	O	S	0	2	0
			1515	983	247	281	4			
1	B	183	Total	C	N	O	S	0	4	0
			1488	963	242	279	4			
1	C	180	Total	C	N	O	S	0	1	0
			1438	933	234	267	4			
1	D	178	Total	C	N	O	S	0	0	0
			1426	925	233	264	4			
1	E	179	Total	C	N	O	S	0	0	0
			1432	929	234	265	4			
1	F	180	Total	C	N	O	S	0	0	0
			1440	936	234	266	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	MET	ILE	ENGINEERED MUTATION	UNP P14350
A	180	ARG	LYS	CONFLICT	UNP P14350
A	227	MET	ILE	ENGINEERED MUTATION	UNP P14350
A	253	MET	LEU	ENGINEERED MUTATION	UNP P14350
B	127	MET	ILE	ENGINEERED MUTATION	UNP P14350
B	180	ARG	LYS	CONFLICT	UNP P14350
B	227	MET	ILE	ENGINEERED MUTATION	UNP P14350
B	253	MET	LEU	ENGINEERED MUTATION	UNP P14350
C	127	MET	ILE	ENGINEERED MUTATION	UNP P14350
C	180	ARG	LYS	CONFLICT	UNP P14350
C	227	MET	ILE	ENGINEERED MUTATION	UNP P14350
C	253	MET	LEU	ENGINEERED MUTATION	UNP P14350
D	127	MET	ILE	ENGINEERED MUTATION	UNP P14350
D	180	ARG	LYS	CONFLICT	UNP P14350
D	227	MET	ILE	ENGINEERED MUTATION	UNP P14350
D	253	MET	LEU	ENGINEERED MUTATION	UNP P14350
E	127	MET	ILE	ENGINEERED MUTATION	UNP P14350

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Chain	Residue	Modelled	Actual	Comment	Reference
E	180	ARG	LYS	CONFLICT	UNP P14350
E	227	MET	ILE	ENGINEERED MUTATION	UNP P14350
E	253	MET	LEU	ENGINEERED MUTATION	UNP P14350
F	127	MET	ILE	ENGINEERED MUTATION	UNP P14350
F	180	ARG	LYS	CONFLICT	UNP P14350
F	227	MET	ILE	ENGINEERED MUTATION	UNP P14350
F	253	MET	LEU	ENGINEERED MUTATION	UNP P14350

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

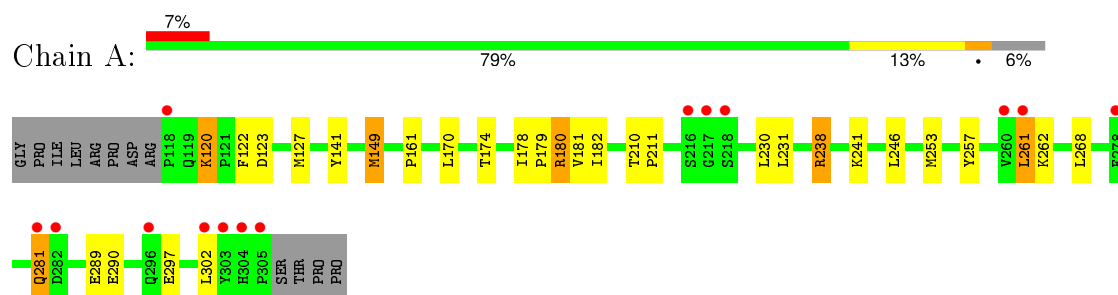
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	B	75	Total O 75 75	0	0
3	C	47	Total O 47 47	0	0
3	D	22	Total O 22 22	0	0
3	E	52	Total O 52 52	0	0
3	F	36	Total O 36 36	0	0

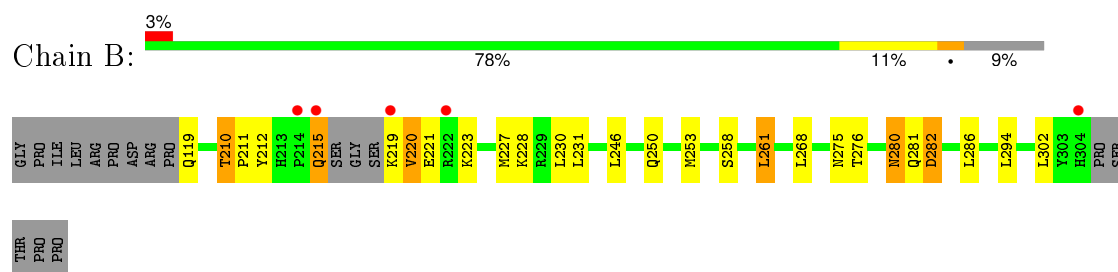
### 3 Residue-property plots [i](#)

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.

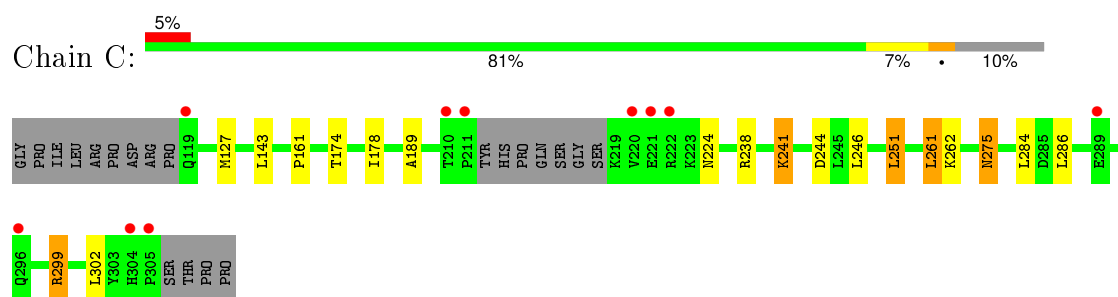
#### • Molecule 1: INTEGRASE



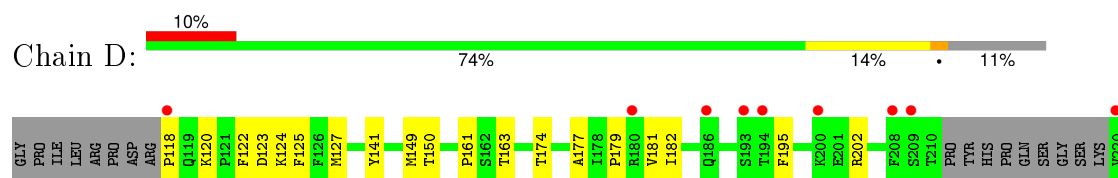
#### • Molecule 1: INTEGRASE

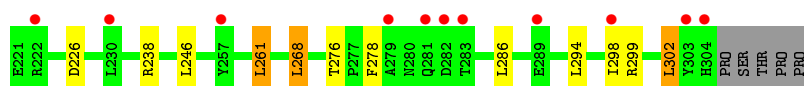


#### • Molecule 1: INTEGRASE

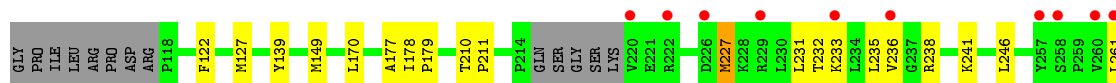
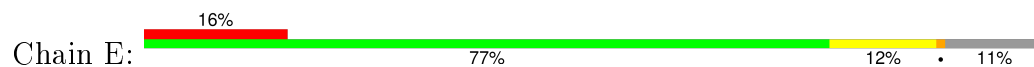


#### • Molecule 1: INTEGRASE

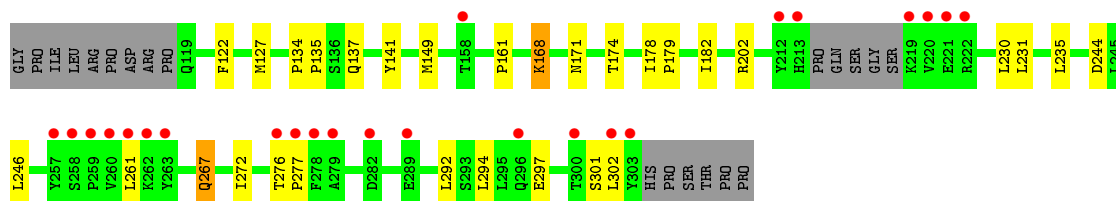
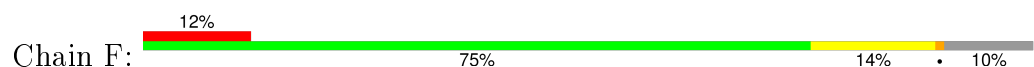




• Molecule 1: INTEGRASE



• Molecule 1: INTEGRASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.77Å 89.23Å 177.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.62 – 2.06 44.27 – 2.06	Depositor EDS
% Data completeness (in resolution range)	93.5 (44.62-2.06) 93.5 (44.27-2.06)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.226 , 0.270 0.224 , 0.266	Depositor DCC
$R_{free}$ test set	4193 reflections (5.62%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.6	EDS
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 78830 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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](#)

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

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	0.42	0/1569	0.57	0/2140
1	B	0.45	0/1548	0.58	0/2109
1	C	0.40	0/1481	0.54	0/2020
1	D	0.35	0/1464	0.53	0/1994
1	E	0.40	0/1472	0.52	0/2007
1	F	0.40	0/1479	0.54	0/2016
All	All	0.40	0/9013	0.55	0/12286

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 [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	1515	0	1509	20	0
1	B	1488	0	1477	16	0
1	C	1438	0	1432	12	0
1	D	1426	0	1430	18	0
1	E	1432	0	1433	15	0
1	F	1440	0	1436	16	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	82	0	0	0	0
3	B	75	0	0	3	0
3	C	47	0	0	0	0
3	D	22	0	0	0	0
3	E	52	0	0	0	0
3	F	36	0	0	2	0
All	All	9059	0	8717	95	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 5.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ARG:HH11	1:C:299:ARG:HG2	1.23	1.01
1:C:127:MET:HE2	1:C:143:LEU:HD11	1.61	0.80
1:E:210:THR:HB	1:E:211:PRO:HD2	1.65	0.78
1:B:210:THR:HG22	1:B:212:TYR:H	1.51	0.73
1:E:127:MET:HE1	1:E:170:LEU:HD11	1.73	0.70
1:C:299:ARG:HH11	1:C:299:ARG:CG	2.04	0.70
1:A:120:LYS:HA	1:A:149:MET:HE2	1.73	0.70
1:D:122:PHE:O	1:D:179:PRO:HA	1.93	0.68
1:C:299:ARG:NH1	1:C:299:ARG:HG2	2.04	0.66
1:E:296:GLN:O	1:E:300:THR:HG23	1.95	0.66
1:A:123:ASP:O	1:A:180:ARG:HG2	1.97	0.65
1:E:238:ARG:HG2	1:E:241:LYS:HE2	1.79	0.64
1:A:180:ARG:HG3	1:A:181:VAL:HG23	1.83	0.61
1:A:174:THR:HB	1:A:178:ILE:HD13	1.81	0.60
1:E:210:THR:HB	1:E:211:PRO:CD	2.31	0.60
1:B:210:THR:HG23	1:B:211:PRO:HD2	1.83	0.60
3:B:2038:HOH:O	1:D:118:PRO:HG3	2.03	0.59
1:A:261:LEU:HG	1:A:268:LEU:HD11	1.84	0.58
1:A:257[A]:TYR:HE2	1:A:281:GLN:HE22	1.52	0.57
1:A:241:LYS:HD2	1:A:290:GLU:OE1	2.06	0.56
1:C:261:LEU:O	1:C:262:LYS:HB2	2.06	0.55
1:E:275:ASN:HD22	1:E:275:ASN:N	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LEU:HG	1:B:268:LEU:HD11	1.89	0.54
1:A:231:LEU:HD11	1:A:253:MET:SD	2.48	0.54
1:B:250:GLN:HA	1:B:253:MET:HE2	1.89	0.54
1:A:122:PHE:O	1:A:179:PRO:HA	2.07	0.54
1:A:127:MET:CE	1:A:182:ILE:HG21	2.37	0.54
1:B:219:LYS:O	1:B:223:LYS:HB2	2.07	0.54
1:F:174:THR:HB	1:F:178:ILE:HD13	1.89	0.54
1:F:127:MET:HE3	1:F:182:ILE:CG2	2.39	0.53
1:B:261:LEU:HG	1:B:268:LEU:CD1	2.39	0.52
1:D:120:LYS:HA	1:D:149:MET:HE2	1.92	0.52
1:B:215:GLN:HB3	1:B:221:GLU:HB2	1.92	0.51
1:B:119:GLN:HB2	3:B:2002:HOH:O	2.11	0.51
1:E:122:PHE:O	1:E:179:PRO:HA	2.10	0.51
1:B:280:ASN:HD22	1:B:282:ASP:H	1.58	0.51
1:D:298:ILE:O	1:D:302:LEU:HB2	2.11	0.51
1:F:127:MET:CE	1:F:182:ILE:HG21	2.41	0.51
1:D:127:MET:CE	1:D:182:ILE:HG21	2.41	0.50
1:F:297:GLU:O	1:F:301:SER:HB3	2.11	0.50
1:B:215:GLN:HB2	1:B:220:VAL:HG23	1.93	0.50
1:E:275:ASN:H	1:E:275:ASN:HD22	1.60	0.50
1:A:127:MET:CE	1:A:170:LEU:HD11	2.42	0.49
1:B:210:THR:HG22	1:B:212:TYR:N	2.24	0.49
1:D:150:THR:HG22	1:D:268:LEU:HB3	1.93	0.49
1:D:124:LYS:HA	1:D:181:VAL:O	2.13	0.49
1:D:120:LYS:HA	1:D:149:MET:CE	2.43	0.49
1:D:120:LYS:CA	1:D:149:MET:HE2	2.42	0.49
1:A:261:LEU:HG	1:A:268:LEU:CD1	2.43	0.48
1:B:276:THR:OG1	1:B:281:GLN:NE2	2.46	0.48
1:B:211:PRO:HD3	1:D:261:LEU:HD11	1.95	0.48
1:D:127:MET:HE1	1:D:182:ILE:HG21	1.95	0.47
1:A:210:THR:HB	1:A:211:PRO:HD2	1.96	0.47
1:F:272:ILE:H	1:F:272:ILE:HD12	1.78	0.47
1:A:141:TYR:CE1	1:A:161:PRO:HD3	2.50	0.46
1:E:122:PHE:CD2	1:E:177:ALA:HB3	2.50	0.46
1:F:171:ASN:CB	3:F:2014:HOH:O	2.64	0.46
1:E:232:THR:O	1:E:236:VAL:HG23	2.16	0.45
1:F:171:ASN:HB2	3:F:2014:HOH:O	2.17	0.45
1:C:251:LEU:HD13	1:C:284:LEU:HD13	1.99	0.45
1:A:127:MET:HE3	1:A:182:ILE:HG21	1.98	0.45
1:C:174:THR:HB	1:C:178:ILE:HD13	1.98	0.45
1:F:141:TYR:CE1	1:F:161:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:NH2	1:A:297:GLU:OE1	2.37	0.45
1:E:227:MET:CE	1:E:231:LEU:HD22	2.47	0.44
1:D:122:PHE:CD2	1:D:177:ALA:HB3	2.52	0.44
1:C:241:LYS:HE2	1:C:244:ASP:OD1	2.18	0.44
1:F:122:PHE:O	1:F:179:PRO:HA	2.18	0.44
1:F:127:MET:HE3	1:F:182:ILE:HG21	1.98	0.43
1:F:267:GLN:HB3	1:F:267:GLN:HE21	1.62	0.43
1:A:127:MET:HE1	1:A:170:LEU:HD21	2.00	0.43
1:F:137:GLN:NE2	1:F:244:ASP:OD2	2.51	0.43
1:D:174:THR:HG22	1:D:179:PRO:HD3	2.00	0.42
3:B:2040:HOH:O	1:D:118:PRO:HB3	2.20	0.42
1:C:299:ARG:NH1	1:C:299:ARG:CG	2.70	0.42
1:D:141:TYR:CE1	1:D:161:PRO:HD3	2.54	0.42
1:C:275:ASN:HD22	1:C:275:ASN:HA	1.60	0.42
1:E:231:LEU:O	1:E:235:LEU:HG	2.19	0.42
1:E:127:MET:CE	1:E:170:LEU:HD11	2.45	0.42
1:B:280:ASN:C	1:B:280:ASN:HD22	2.22	0.41
1:A:127:MET:HE2	1:A:182:ILE:CG2	2.50	0.41
1:D:276:THR:C	1:D:278:PHE:H	2.24	0.41
1:F:276:THR:HA	1:F:277:PRO:HD3	1.94	0.41
1:A:257[B]:TYR:OH	1:A:262:LYS:HA	2.20	0.41
1:E:139:TYR:OH	1:F:168:LYS:HE3	2.21	0.41
1:B:227:MET:HG3	1:B:228:LYS:N	2.36	0.41
1:F:231:LEU:O	1:F:235:LEU:HG	2.21	0.41
1:F:134:PRO:HA	1:F:135:PRO:HD3	1.87	0.41
1:A:127:MET:HE2	1:A:182:ILE:HG21	2.02	0.40
1:C:224:ASN:HA	1:C:224:ASN:HD22	1.66	0.40
1:D:163:THR:HG23	1:D:195:PHE:HB2	2.03	0.40
1:C:161:PRO:O	1:C:189:ALA:HB2	2.21	0.40
1:D:122:PHE:CD2	1:D:125:PHE:HZ	2.38	0.40
1:E:178:ILE:HA	1:E:179:PRO:HD2	1.99	0.40
1:B:258:SER:HB3	1:B:261:LEU:HB2	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	188/200 (94%)	183 (97%)	5 (3%)	0	100	100
1	B	183/200 (92%)	179 (98%)	4 (2%)	0	100	100
1	C	177/200 (88%)	175 (99%)	2 (1%)	0	100	100
1	D	174/200 (87%)	172 (99%)	2 (1%)	0	100	100
1	E	175/200 (88%)	168 (96%)	7 (4%)	0	100	100
1	F	176/200 (88%)	169 (96%)	7 (4%)	0	100	100
All	All	1073/1200 (89%)	1046 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/181 (95%)	162 (94%)	10 (6%)	25	14
1	B	170/181 (94%)	157 (92%)	13 (8%)	16	7
1	C	162/181 (90%)	153 (94%)	9 (6%)	26	16
1	D	161/181 (89%)	150 (93%)	11 (7%)	20	11
1	E	162/181 (90%)	154 (95%)	8 (5%)	31	21
1	F	161/181 (89%)	151 (94%)	10 (6%)	23	13
All	All	988/1086 (91%)	927 (94%)	61 (6%)	23	13

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LYS
1	A	149	MET
1	A	180	ARG

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Mol	Chain	Res	Type
1	A	230	LEU
1	A	238	ARG
1	A	246	LEU
1	A	261	LEU
1	A	281	GLN
1	A	289	GLU
1	A	302	LEU
1	B	210	THR
1	B	215	GLN
1	B	220	VAL
1	B	230	LEU
1	B	231	LEU
1	B	246	LEU
1	B	261	LEU
1	B	275	ASN
1	B	280	ASN
1	B	282	ASP
1	B	286	LEU
1	B	294	LEU
1	B	302	LEU
1	C	238	ARG
1	C	241	LYS
1	C	246	LEU
1	C	251	LEU
1	C	261	LEU
1	C	275	ASN
1	C	286	LEU
1	C	299	ARG
1	C	302	LEU
1	D	123	ASP
1	D	202	ARG
1	D	226	ASP
1	D	238	ARG
1	D	246	LEU
1	D	261	LEU
1	D	268	LEU
1	D	286	LEU
1	D	294	LEU
1	D	299	ARG
1	D	302	LEU
1	E	149	MET
1	E	227	MET

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Mol	Chain	Res	Type
1	E	233	LYS
1	E	246	LEU
1	E	261	LEU
1	E	275	ASN
1	E	289	GLU
1	E	290	GLU
1	F	149	MET
1	F	168	LYS
1	F	202	ARG
1	F	230	LEU
1	F	246	LEU
1	F	261	LEU
1	F	267	GLN
1	F	292	LEU
1	F	294	LEU
1	F	302	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	183	HIS
1	A	186	GLN
1	A	213	HIS
1	A	281	GLN
1	A	296	GLN
1	A	304	HIS
1	B	119	GLN
1	B	224	ASN
1	B	275	ASN
1	B	280	ASN
1	B	281	GLN
1	C	224	ASN
1	C	275	ASN
1	C	281	GLN
1	D	119	GLN
1	E	137	GLN
1	E	275	ASN
1	F	183	HIS
1	F	266	HIS

### 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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	188/200 (94%)	0.49	14 (7%) 17 19	17, 31, 62, 69	1 (0%)
1	B	183/200 (91%)	0.21	5 (2%) 58 63	18, 34, 57, 80	0
1	C	180/200 (90%)	0.21	10 (5%) 28 31	27, 41, 67, 78	0
1	D	178/200 (89%)	0.63	20 (11%) 7 7	30, 58, 83, 89	1 (0%)
1	E	179/200 (89%)	0.76	32 (17%) 2 2	21, 42, 87, 91	1 (0%)
1	F	180/200 (90%)	0.63	24 (13%) 4 4	24, 44, 79, 86	1 (0%)
All	All	1088/1200 (90%)	0.49	105 (9%) 10 11	17, 41, 80, 91	4 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	260	VAL	8.9
1	A	305	PRO	7.4
1	F	259	PRO	6.5
1	A	216	SER	5.8
1	B	214	PRO	5.6
1	E	289	GLU	5.3
1	E	292	LEU	5.2
1	D	304	HIS	5.2
1	E	296	GLN	5.0
1	F	303	TYR	5.0
1	F	258	SER	4.9
1	F	222	ARG	4.8
1	E	273	ASP	4.8
1	E	261	LEU	4.8
1	E	222	ARG	4.7
1	B	219	LYS	4.5
1	E	281	GLN	4.4
1	F	263	TYR	4.4
1	C	222	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	279	ALA	4.3
1	E	257	TYR	4.2
1	E	260	VAL	4.1
1	F	257	TYR	4.0
1	F	213	HIS	4.0
1	D	303	TYR	4.0
1	E	220	VAL	3.9
1	E	298	ILE	3.9
1	C	211	PRO	3.9
1	D	209	SER	3.8
1	E	300	THR	3.8
1	D	222	ARG	3.8
1	E	282	ASP	3.8
1	A	303	TYR	3.7
1	E	258	SER	3.7
1	A	260	VAL	3.7
1	D	279	ALA	3.6
1	E	284	LEU	3.6
1	D	281	GLN	3.6
1	E	294	LEU	3.6
1	A	304	HIS	3.6
1	F	221	GLU	3.5
1	E	295	LEU	3.3
1	B	215	GLN	3.2
1	F	302	LEU	3.2
1	A	281	GLN	3.1
1	A	278	PHE	3.1
1	E	229	ARG	3.1
1	E	286	LEU	3.1
1	D	289	GLU	3.0
1	F	220	VAL	3.0
1	C	220	VAL	3.0
1	C	305	PRO	3.0
1	E	299	ARG	3.0
1	D	220	VAL	3.0
1	F	261	LEU	2.9
1	F	278	PHE	2.9
1	D	194	THR	2.9
1	F	300	THR	2.9
1	F	262	LYS	2.8
1	E	293	SER	2.8
1	E	278	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	289	GLU	2.7
1	E	283	THR	2.7
1	F	289	GLU	2.7
1	D	282	ASP	2.6
1	B	304	HIS	2.6
1	F	212	TYR	2.6
1	C	119	GLN	2.6
1	D	283	THR	2.6
1	D	186	GLN	2.5
1	D	180	ARG	2.5
1	A	282	ASP	2.5
1	F	296	GLN	2.5
1	E	226	ASP	2.4
1	E	277	PRO	2.4
1	E	233	LYS	2.4
1	E	287	THR	2.4
1	C	210	THR	2.4
1	E	276	THR	2.4
1	D	208	PHE	2.4
1	A	218	SER	2.4
1	E	236	VAL	2.4
1	D	200	LYS	2.4
1	F	282	ASP	2.4
1	F	276	THR	2.3
1	A	302	LEU	2.3
1	D	230	LEU	2.3
1	C	221	GLU	2.3
1	A	118	PRO	2.3
1	D	118	PRO	2.3
1	B	222	ARG	2.3
1	F	219	LYS	2.2
1	F	279	ALA	2.2
1	A	296	GLN	2.2
1	C	304	HIS	2.1
1	D	298	ILE	2.1
1	A	261	LEU	2.1
1	C	296	GLN	2.1
1	A	217	GLY	2.1
1	F	158	THR	2.1
1	F	277	PRO	2.1
1	E	288	ARG	2.0
1	E	280	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	257	TYR	2.0
1	D	193	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	C	1197	1/1	0.94	0.05	-	60,60,60,60	0
2	MN	D	1196	1/1	0.87	0.06	-	85,85,85,85	0
2	MN	B	1196	1/1	0.99	0.10	-	55,55,55,55	0
2	MN	F	1195	1/1	0.99	0.05	-	41,41,41,41	0
2	MN	A	1197	1/1	1.00	0.04	-	31,31,31,31	0
2	MN	E	1193	1/1	1.00	0.04	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.