



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:21 AM UTC

PDB ID : 2X6N / pdb_00002x6n
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

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

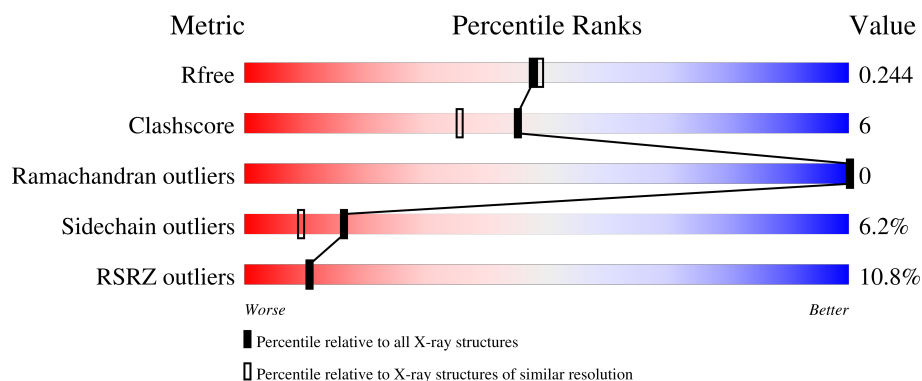
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (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 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	8% 78% 13% • 6%
1	B	200	3% 76% 14% • 8%
1	C	200	7% 80% 8% • 10%
1	D	200	15% 73% 14% • 11%
1	E	200	13% 76% 12% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	200	12% 76% 14% • 10%

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

Continued on next page...

Continued from previous page...

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 (CCD ID: MN) (formula: Mn).

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

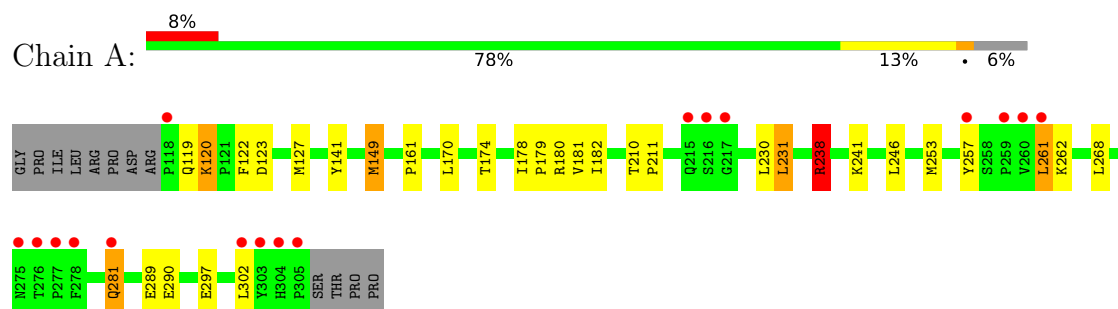
- Molecule 3 is water.

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

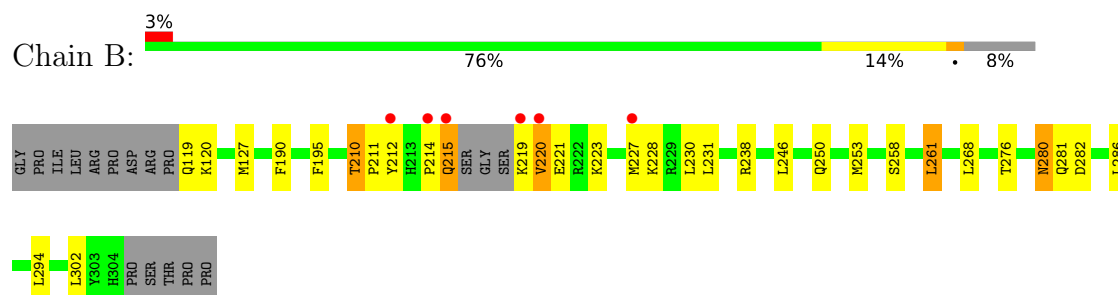
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

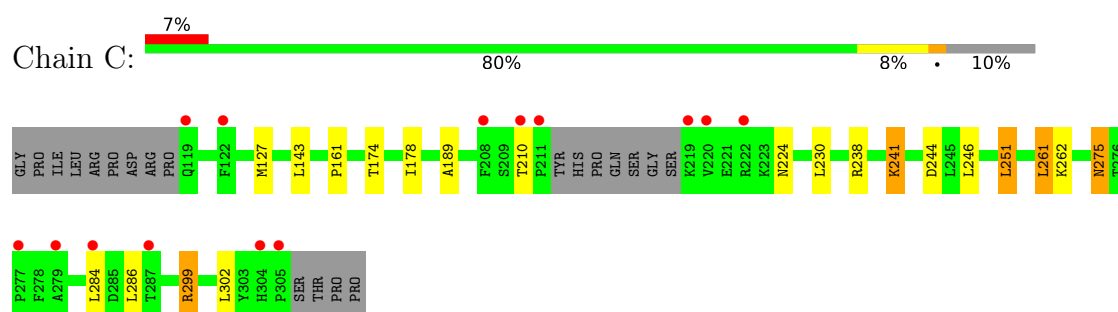
• Molecule 1: INTEGRASE



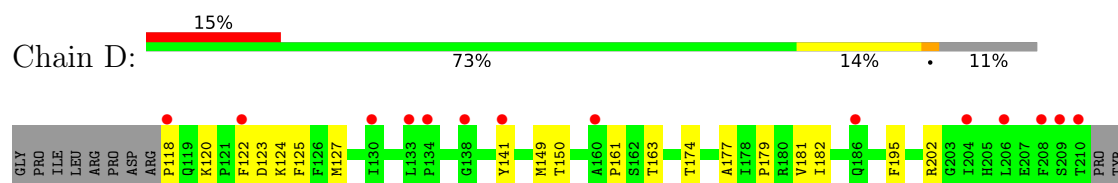
• Molecule 1: INTEGRASE

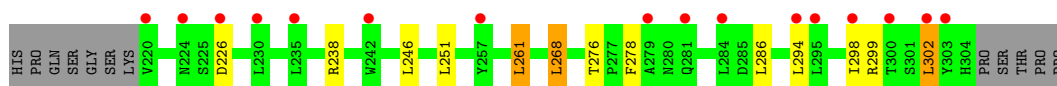


• Molecule 1: INTEGRASE

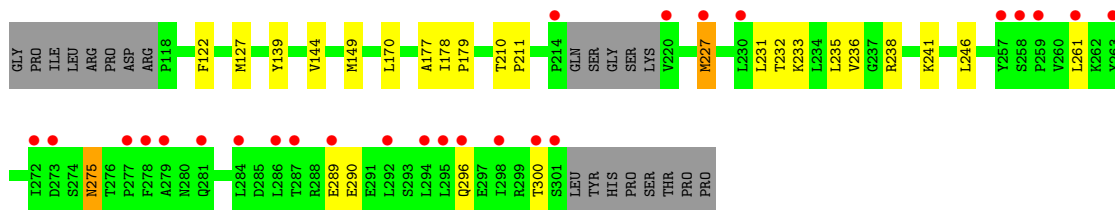
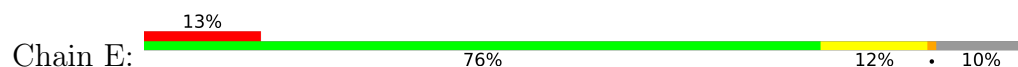


• Molecule 1: INTEGRASE

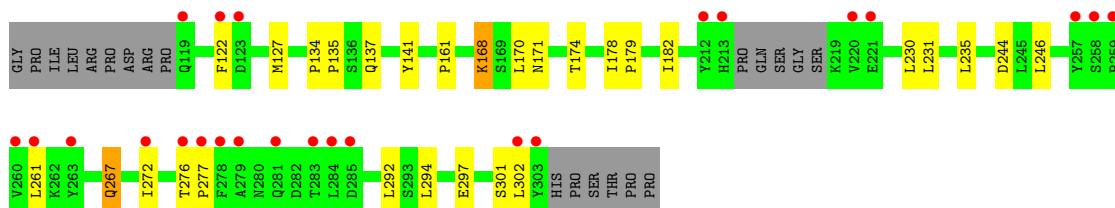
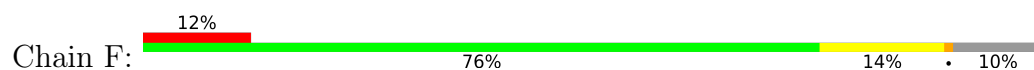




● Molecule 1: INTEGRASE



● 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	84.77Å 89.23Å 177.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.62 – 2.06 44.62 – 2.06	Depositor EDS
% Data completeness (in resolution range)	93.5 (44.62-2.06) 93.8 (44.62-2.06)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.226 , 0.270 (Not available) , 0.244	Depositor DCC
R_{free} test set	4226 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9059	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 ⓘ

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	0.54	0/1569	0.83	2/2140 (0.1%)
1	B	0.55	0/1548	0.80	3/2109 (0.1%)
1	C	0.49	0/1481	0.79	0/2020
1	D	0.45	0/1464	0.77	0/1994
1	E	0.50	0/1472	0.77	0/2007
1	F	0.50	0/1479	0.77	0/2016
All	All	0.51	0/9013	0.79	5/12286 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	CA-C-N	5.74	125.86	119.32
1	A	238	ARG	C-N-CA	5.74	125.86	119.32
1	B	238	ARG	CA-C-N	5.42	124.88	119.24
1	B	238	ARG	C-N-CA	5.42	124.88	119.24
1	B	120	LYS	N-CA-C	5.39	114.50	108.25

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	1515	0	1509	18	0
1	B	1488	0	1477	19	0
1	C	1438	0	1432	12	0
1	D	1426	0	1430	20	0
1	E	1432	0	1433	18	0
1	F	1440	0	1436	18	0
2	A	1	0	0	0	0
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	103	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 6.

All (103) 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:A:127:MET:HE3	1:A:182:ILE:HG21	1.40	1.03
1:C:299:ARG:HH11	1:C:299:ARG:HG2	1.23	1.01
1:A:127:MET:HE1	1:A:170:LEU:HD11	1.49	0.94
1:D:127:MET:HE2	1:D:182:ILE:HG21	1.53	0.90
1:C:127:MET:HE2	1:C:143:LEU:HD11	1.58	0.82
1:E:210:THR:HB	1:E:211:PRO:HD2	1.65	0.78
1:E:144:VAL:HG11	1:E:227:MET:HE1	1.68	0.75
1:A:127:MET:HE3	1:A:182:ILE:CG2	2.17	0.74
1:B:210:THR:HG22	1:B:212:TYR:H	1.51	0.73
1:C:299:ARG:HH11	1:C:299:ARG:CG	2.04	0.70
1:D:122:PHE:O	1:D:179:PRO:HA	1.93	0.68
1:A:120:LYS:HA	1:A:149:MET:HE2	1.76	0.67
1:C:299:ARG:HG2	1:C:299:ARG:NH1	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:D:127:MET:HE2	1:D:182:ILE:CG2	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ARG:HG2	1:E:241:LYS:HE2	1.79	0.64
1:E:127:MET:HE1	1:E:170:LEU:HD11	1.80	0.63
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:B:210:THR:HG23	1:B:211:PRO:HD2	1.83	0.60
1:E:210:THR:HB	1:E:211:PRO:CD	2.31	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:127:MET:HE1	1:A:170:LEU:CD1	2.30	0.57
1:A:257[A]:TYR:HE2	1:A:281:GLN:HE22	1.52	0.57
1:B:250:GLN:HA	1:B:253:MET:HE2	1.87	0.56
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:N	1:E:275:ASN:HD22	2.05	0.55
1:F:127:MET:HE3	1:F:182:ILE:CG2	2.37	0.55
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:A:122:PHE:O	1:A:179:PRO:HA	2.07	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:B:261:LEU:HG	1:B:268:LEU:CD1	2.39	0.52
1:B:119:GLN:HB2	3:B:2002:HOH:O	2.11	0.51
1:B:215:GLN:HB3	1:B:221:GLU:HB2	1.92	0.51
1:B:280:ASN:HD22	1:B:282:ASP:H	1.58	0.51
1:E:122:PHE:O	1:E:179:PRO:HA	2.10	0.51
1:D:127:MET:HE1	1:D:195:PHE:CZ	2.46	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: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:HD22	1:E:275:ASN:H	1.60	0.50
1:B:210:THR:HG22	1:B:212:TYR:N	2.24	0.49
1:D:124:LYS:HA	1:D:181:VAL:O	2.13	0.49
1:D:150:THR:HG22	1:D:268:LEU:HB3	1.93	0.49
1:D:120:LYS:HA	1:D:149:MET:CE	2.43	0.49
1:D:120:LYS:HA	1:D:149:MET:HE2	1.95	0.48
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:E:144:VAL:CG1	1:E:227:MET:HE1	2.40	0.48
1:B:280:ASN:HD22	1:B:280:ASN:C	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:THR:HB	1:A:211:PRO:HD2	1.96	0.47
1:D:120:LYS:CA	1:D:149:MET:HE2	2.44	0.47
1:F:127:MET:HE3	1:F:182:ILE:HG21	1.95	0.47
1:F:272:ILE:H	1:F:272:ILE:HD12	1.78	0.47
1:E:127:MET:CE	1:E:170:LEU:HD11	2.45	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:D:276:THR:C	1:D:278:PHE:H	2.24	0.46
1:E:127:MET:HE3	1:E:127:MET:HB2	1.80	0.46
1:F:171:ASN:CB	3:F:2014:HOH:O	2.64	0.46
1:D:127:MET:HE1	1:D:195:PHE:HZ	1.81	0.45
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:C:174:THR:HB	1:C:178:ILE:HD13	1.98	0.45
1:A:238:ARG:NH2	1:A:297:GLU:OE1	2.37	0.45
1:F:141:TYR:CE1	1:F:161:PRO:HD3	2.52	0.45
1:B:127:MET:HE1	1:B:195:PHE:CZ	2.52	0.44
1:E:227:MET:CE	1:E:231:LEU:HD22	2.47	0.44
1:C:241:LYS:HE2	1:C:244:ASP:OD1	2.18	0.44
1:D:122:PHE:CD2	1:D:177:ALA:HB3	2.52	0.44
1:F:122:PHE:O	1:F:179:PRO:HA	2.18	0.44
1:F:267:GLN:HE21	1:F:267:GLN:HB3	1.62	0.43
1:F:137:GLN:NE2	1:F:244:ASP:OD2	2.51	0.43
1:B:214:PRO:O	1:B:215:GLN:C	2.62	0.43
3:B:2040:HOH:O	1:D:118:PRO:HB3	2.20	0.42
1:D:174:THR:HG22	1:D:179:PRO:HD3	2.00	0.42
1:C:299:ARG:CG	1:C:299:ARG:NH1	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:F:127:MET:HE1	1:F:170:LEU:HD11	2.02	0.42
1:E:231:LEU:O	1:E:235:LEU:HG	2.19	0.42
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:F:127:MET:HE3	1:F:182:ILE:HG23	2.01	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:134:PRO:HA	1:F:135:PRO:HD3	1.87	0.41
1:F:231:LEU:O	1:F:235:LEU:HG	2.21	0.41
1:C:224:ASN:HD22	1:C:224:ASN:HA	1.66	0.40
1:C:161:PRO:O	1:C:189:ALA:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:THR:HG23	1:D:195:PHE:HB2	2.03	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:127:MET:HE3	1:B:190:PHE:CD1	2.56	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 [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	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 [i](#)

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%)	161 (94%)	11 (6%)	16	9
1	B	170/181 (94%)	159 (94%)	11 (6%)	15	8
1	C	162/181 (90%)	151 (93%)	11 (7%)	14	8
1	D	161/181 (89%)	149 (92%)	12 (8%)	12	6
1	E	162/181 (90%)	154 (95%)	8 (5%)	22	15
1	F	161/181 (89%)	153 (95%)	8 (5%)	22	14
All	All	988/1086 (91%)	927 (94%)	61 (6%)	16	9

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

Mol	Chain	Res	Type
1	A	119	GLN
1	A	120	LYS
1	A	149	MET
1	A	230	LEU
1	A	231	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	280	ASN
1	B	286	LEU
1	B	294	LEU
1	B	302	LEU
1	C	210	THR
1	C	230	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	251	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
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	168	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	213	HIS
1	A	255	ASN
1	A	281	GLN
1	A	296	GLN
1	A	304	HIS
1	B	183	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	186	GLN
1	B	224	ASN
1	B	275	ASN
1	B	280	ASN
1	B	281	GLN
1	B	304	HIS
1	C	224	ASN
1	C	255	ASN
1	C	275	ASN
1	C	281	GLN
1	D	119	GLN
1	D	255	ASN
1	E	137	GLN
1	E	183	HIS
1	E	255	ASN
1	E	275	ASN
1	F	183	HIS
1	F	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 ⓘ

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, 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	188/200 (94%)	0.32	17 (9%)	15 15	17, 31, 62, 69	3 (1%)
1	B	183/200 (91%)	0.26	6 (3%)	49 49	18, 33, 57, 80	4 (2%)
1	C	180/200 (90%)	0.63	14 (7%)	19 19	27, 41, 67, 78	1 (0%)
1	D	178/200 (89%)	1.26	30 (16%)	4 4	30, 58, 83, 89	1 (0%)
1	E	179/200 (89%)	0.76	26 (14%)	6 6	21, 42, 87, 91	1 (0%)
1	F	180/200 (90%)	0.82	24 (13%)	7 7	24, 43, 79, 86	1 (0%)
All	All	1088/1200 (90%)	0.67	117 (10%)	11 11	17, 41, 80, 91	11 (1%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	PRO	5.7
1	A	216	SER	5.1
1	C	211	PRO	4.8
1	A	277	PRO	4.8
1	F	277	PRO	4.7
1	F	278	PHE	4.6
1	B	220	VAL	4.6
1	D	303	TYR	4.5
1	F	261	LEU	4.5
1	E	300	THR	4.4
1	D	118	PRO	4.3
1	A	278	PHE	4.3
1	E	261	LEU	4.3
1	C	220	VAL	4.2
1	D	220	VAL	4.2
1	E	220	VAL	4.1
1	F	220	VAL	4.0
1	F	276	THR	3.8
1	E	287	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	258	SER	3.8
1	D	279	ALA	3.8
1	E	273	ASP	3.7
1	F	260	VAL	3.6
1	A	118	PRO	3.6
1	A	305	PRO	3.6
1	F	259	PRO	3.6
1	D	230	LEU	3.5
1	D	302	LEU	3.5
1	B	219	LYS	3.4
1	A	276	THR	3.3
1	F	284	LEU	3.2
1	C	305	PRO	3.2
1	E	292	LEU	3.2
1	D	160	ALA	3.2
1	E	301	SER	3.1
1	D	298	ILE	3.1
1	E	272	ILE	3.1
1	A	281	GLN	3.1
1	E	214	PRO	3.0
1	F	303	TYR	3.0
1	D	208	PHE	3.0
1	E	279	ALA	3.0
1	A	257[A]	TYR	3.0
1	A	302	LEU	2.9
1	E	295	LEU	2.9
1	F	263	TYR	2.9
1	E	284	LEU	2.9
1	E	298	ILE	2.9
1	E	278	PHE	2.9
1	F	119	GLN	2.8
1	F	212	TYR	2.8
1	A	261	LEU	2.8
1	D	130	ILE	2.8
1	F	272	ILE	2.8
1	D	294	LEU	2.7
1	D	295	LEU	2.7
1	E	289	GLU	2.7
1	D	281	GLN	2.7
1	E	277	PRO	2.7
1	B	212	TYR	2.7
1	D	300	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	230	LEU	2.6
1	A	217	GLY	2.6
1	C	279	ALA	2.6
1	E	296	GLN	2.6
1	C	277	PRO	2.6
1	E	263	TYR	2.5
1	F	123	ASP	2.5
1	D	206	LEU	2.5
1	A	303	TYR	2.5
1	D	224	ASN	2.5
1	F	302	LEU	2.5
1	D	242	TRP	2.5
1	D	204	ILE	2.5
1	C	210	THR	2.5
1	F	213	HIS	2.5
1	E	257	TYR	2.4
1	F	257	TYR	2.4
1	D	133	LEU	2.4
1	B	215	GLN	2.4
1	F	281	GLN	2.4
1	C	304	HIS	2.4
1	A	260	VAL	2.4
1	F	283	THR	2.4
1	D	141	TYR	2.3
1	F	279	ALA	2.3
1	C	119	GLN	2.3
1	E	227	MET	2.3
1	E	258	SER	2.3
1	F	285	ASP	2.3
1	C	284	LEU	2.3
1	E	294	LEU	2.3
1	D	122	PHE	2.2
1	C	222	ARG	2.2
1	E	286	LEU	2.2
1	E	259	PRO	2.2
1	D	226	ASP	2.2
1	D	209	SER	2.2
1	C	219	LYS	2.2
1	C	122	PHE	2.1
1	D	235	LEU	2.1
1	F	122	PHE	2.1
1	F	221	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	186	GLN	2.1
1	D	284	LEU	2.1
1	A	275	ASN	2.1
1	C	287	THR	2.1
1	D	138	GLY	2.1
1	C	208	PHE	2.1
1	A	259	PRO	2.0
1	D	257	TYR	2.0
1	B	227	MET	2.0
1	A	215	GLN	2.0
1	E	281	GLN	2.0
1	A	304	HIS	2.0
1	D	134	PRO	2.0
1	D	210	THR	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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	D	1196	1/1	0.91	0.07	85,85,85,85	0
2	MN	C	1197	1/1	0.97	0.15	60,60,60,60	0
2	MN	B	1196	1/1	0.98	0.04	55,55,55,55	0
2	MN	A	1197	1/1	0.99	0.11	31,31,31,31	0
2	MN	E	1193	1/1	1.00	0.07	44,44,44,44	0
2	MN	F	1195	1/1	1.00	0.06	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.