



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:48 AM UTC

PDB ID : 2ITG / pdb_00002itg
Title : CATALYTIC DOMAIN OF HIV-1 INTEGRASE: ORDERED ACTIVE SITE
IN THE F185H CONSTRUCT
Authors : Bujacz, G.; Alexandratos, J.; Wlodawer, A.; Zhou-Liu, Q.; Clement-Mella, C.
Deposited on : 1996-09-13
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

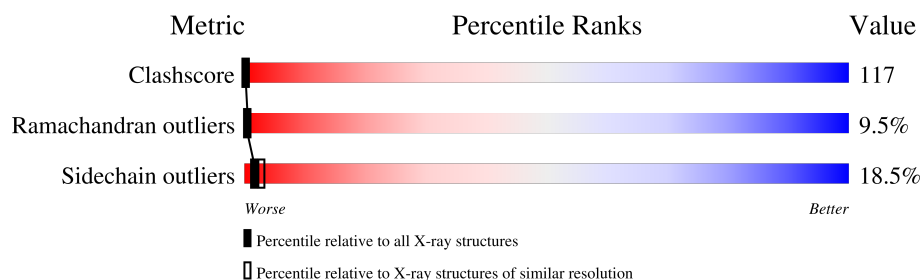
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

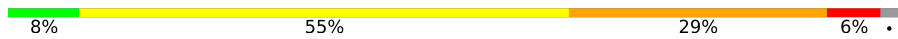
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	163	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1291 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 HUMAN IMMUNODEFICIENCY VIRUS-1 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1233	783	216	229	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	HIS	PHE	engineered mutation	UNP P12497

- Molecule 2 is water.

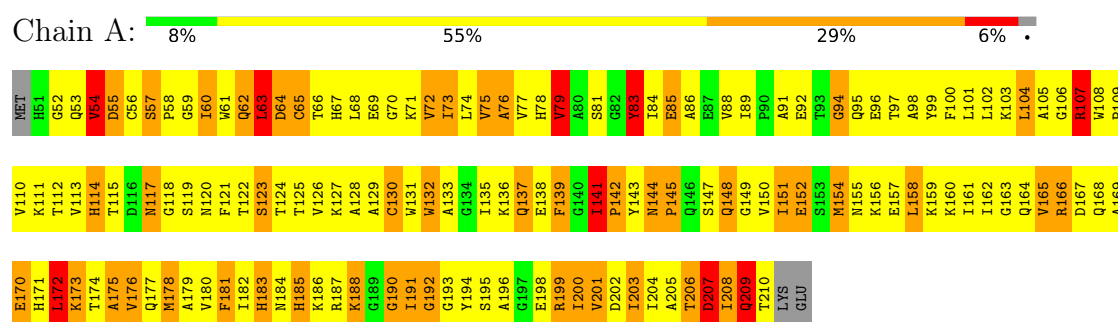
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS-1 INTEGRASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.40 Å 72.40 Å 65.56 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	79.8 (10.00-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1291	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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	0.78	0/1260	1.97	48/1709 (2.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	CYS	CA-CB-SG	10.39	138.31	114.40
1	A	152	GLU	N-CA-C	8.86	121.77	109.18
1	A	130	CYS	N-CA-C	-8.77	101.69	112.38
1	A	155	ASN	CA-CB-CG	8.71	121.31	112.60
1	A	107	ARG	CA-C-O	-8.39	111.57	120.55
1	A	144	ASN	N-CA-C	8.18	115.58	108.22
1	A	178	MET	N-CA-C	-7.98	102.52	111.14
1	A	72	VAL	CB-CA-C	-7.82	103.52	111.80
1	A	181	PHE	CA-CB-CG	-7.16	106.64	113.80
1	A	75	VAL	N-CA-C	7.14	118.15	107.51
1	A	76	ALA	CA-C-O	-7.13	112.65	120.43
1	A	209	GLN	N-CA-C	7.07	120.11	110.35
1	A	107	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	A	73	ILE	CA-C-O	-6.86	114.52	122.13
1	A	107	ARG	CD-NE-CZ	-6.82	114.86	124.40
1	A	64	ASP	N-CA-C	6.80	120.57	107.44
1	A	141	ILE	CB-CA-C	-6.72	99.13	111.36
1	A	72	VAL	N-CA-C	6.65	116.81	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	LEU	CB-CA-C	6.50	120.84	110.19
1	A	147	SER	CA-C-O	-6.34	114.34	121.25
1	A	60	ILE	N-CA-C	6.27	116.90	107.75
1	A	154	MET	N-CA-C	-6.08	105.83	113.18
1	A	207	ASP	CB-CA-C	-6.03	103.78	111.86
1	A	165	VAL	N-CA-C	5.98	118.57	111.09
1	A	114	HIS	CA-CB-CG	-5.92	107.89	113.80
1	A	176	VAL	CA-C-N	5.90	128.67	120.29
1	A	176	VAL	C-N-CA	5.90	128.67	120.29
1	A	62	GLN	CA-C-N	-5.80	114.92	123.05
1	A	62	GLN	C-N-CA	-5.80	114.92	123.05
1	A	64	ASP	CB-CA-C	-5.71	103.13	111.23
1	A	141	ILE	N-CA-CB	5.64	119.10	111.21
1	A	85	GLU	CA-C-O	-5.61	114.55	121.11
1	A	208	ILE	CA-C-N	5.54	132.29	121.66
1	A	208	ILE	C-N-CA	5.54	132.29	121.66
1	A	54	VAL	N-CA-C	5.33	120.43	109.34
1	A	175	ALA	CA-C-O	-5.29	114.89	120.55
1	A	63	LEU	N-CA-CB	-5.28	102.26	110.55
1	A	94	GLY	N-CA-C	-5.22	106.33	113.27
1	A	137	GLN	CA-C-O	-5.22	115.47	121.47
1	A	199	ARG	CD-NE-CZ	5.19	131.66	124.40
1	A	57	SER	CA-C-N	5.18	125.47	119.47
1	A	57	SER	C-N-CA	5.18	125.47	119.47
1	A	186	LYS	N-CA-C	5.15	116.57	109.15
1	A	96	GLU	CA-C-O	-5.14	115.39	120.90
1	A	172	LEU	N-CA-C	-5.12	105.39	110.97
1	A	151	ILE	N-CA-C	5.10	115.05	108.82
1	A	152	GLU	CA-C-O	5.10	127.41	121.49
1	A	83	TYR	CA-C-O	-5.08	114.97	120.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain

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	1233	0	1226	287	0
2	A	58	0	0	10	0
All	All	1291	0	1226	287	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 117.

All (287) 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:196:ALA:HA	1:A:199:ARG:NH2	1.58	1.18
1:A:168:GLN:HG2	1:A:178:MET:HE1	1.27	1.11
1:A:57:SER:HB2	1:A:60:ILE:HD11	1.31	1.09
1:A:111:LYS:NZ	1:A:210:THR:HB	1.67	1.08
1:A:160:LYS:HZ1	1:A:161:ILE:HG12	0.96	1.08
1:A:160:LYS:NZ	1:A:161:ILE:HG12	1.69	1.07
1:A:73:ILE:HD13	1:A:176:VAL:CG2	1.85	1.06
1:A:170:GLU:HB2	1:A:171:HIS:CD2	1.91	1.06
1:A:172:LEU:HD12	1:A:176:VAL:HG23	1.37	1.05
1:A:203:ILE:HG22	1:A:208:ILE:HD13	1.06	1.05
1:A:58:PRO:HB3	1:A:208:ILE:CD1	1.88	1.04
1:A:112:THR:HG22	1:A:136:LYS:HB2	1.38	1.03
1:A:111:LYS:HZ3	1:A:210:THR:HB	1.21	1.03
1:A:58:PRO:HB3	1:A:208:ILE:HD12	1.01	1.00
1:A:209:GLN:HG3	1:A:210:THR:N	1.76	1.00
1:A:58:PRO:CB	1:A:208:ILE:HD12	1.92	0.99
1:A:209:GLN:HG3	1:A:210:THR:H	1.28	0.99
1:A:77:VAL:HG22	1:A:84:ILE:HG22	1.45	0.99
1:A:99:TYR:CD2	1:A:103:LYS:HD2	1.97	0.98
1:A:203:ILE:HG22	1:A:208:ILE:CD1	1.95	0.97
1:A:203:ILE:CG2	1:A:208:ILE:HG21	1.94	0.97
1:A:73:ILE:HD13	1:A:176:VAL:HG21	1.47	0.96
1:A:196:ALA:HA	1:A:199:ARG:HH21	1.19	0.95
1:A:203:ILE:CG2	1:A:208:ILE:HD13	1.97	0.94
1:A:57:SER:HB2	1:A:60:ILE:CD1	2.00	0.92
1:A:141:ILE:H	1:A:142:PRO:CD	1.82	0.92
1:A:204:ILE:HA	1:A:208:ILE:HD11	1.53	0.90
1:A:99:TYR:CE2	1:A:103:LYS:HD2	2.06	0.89
1:A:112:THR:HG22	1:A:136:LYS:CB	2.00	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HG23	1:A:208:ILE:HG21	1.52	0.89
1:A:170:GLU:HB2	1:A:171:HIS:HD2	1.38	0.88
1:A:204:ILE:HA	1:A:208:ILE:CD1	2.03	0.88
1:A:77:VAL:HG22	1:A:84:ILE:CG2	2.03	0.88
1:A:117:ASN:C	1:A:117:ASN:HD22	1.82	0.87
1:A:139:PHE:CD2	2:A:311:HOH:O	2.29	0.86
1:A:192:GLY:O	1:A:194:TYR:N	2.09	0.85
1:A:73:ILE:HD13	1:A:176:VAL:HG22	1.56	0.84
1:A:58:PRO:CG	1:A:208:ILE:HB	2.07	0.82
1:A:76:ALA:HB2	1:A:100:PHE:CE2	2.15	0.81
1:A:194:TYR:HA	1:A:198:GLU:OE1	1.80	0.81
1:A:188:LYS:HE3	1:A:188:LYS:HA	1.61	0.81
1:A:160:LYS:HZ1	1:A:161:ILE:CG1	1.90	0.79
1:A:141:ILE:H	1:A:142:PRO:HD3	1.47	0.79
1:A:76:ALA:HB2	1:A:100:PHE:HE2	1.47	0.79
1:A:168:GLN:HB2	2:A:318:HOH:O	1.83	0.79
1:A:95:GLN:HA	1:A:125:THR:HG21	1.66	0.77
1:A:204:ILE:HA	1:A:208:ILE:CG1	2.15	0.77
1:A:172:LEU:CD1	1:A:176:VAL:HG23	2.16	0.76
1:A:174:THR:O	1:A:178:MET:HG3	1.86	0.76
1:A:187:ARG:HG3	1:A:195:SER:HB3	1.68	0.76
1:A:191:ILE:HG22	1:A:191:ILE:O	1.84	0.76
1:A:73:ILE:CD1	1:A:176:VAL:CG2	2.64	0.75
1:A:66:THR:HG22	1:A:67:HIS:H	1.48	0.75
1:A:192:GLY:C	1:A:194:TYR:HD1	1.96	0.74
1:A:158:LEU:O	1:A:162:ILE:HG13	1.88	0.74
1:A:151:ILE:CG2	1:A:152:GLU:H	2.01	0.73
1:A:151:ILE:HG22	1:A:152:GLU:N	2.03	0.73
1:A:172:LEU:HD12	1:A:176:VAL:CG2	2.16	0.73
1:A:123:SER:O	1:A:127:LYS:N	2.14	0.73
1:A:203:ILE:HG22	1:A:208:ILE:HG21	1.70	0.73
1:A:166:ARG:O	1:A:169:ALA:N	2.22	0.73
1:A:111:LYS:HZ2	1:A:210:THR:HB	1.54	0.72
1:A:181:PHE:CD1	1:A:181:PHE:C	2.68	0.71
1:A:151:ILE:CG2	1:A:152:GLU:N	2.54	0.71
1:A:132:TRP:CD2	1:A:132:TRP:O	2.44	0.70
1:A:168:GLN:CG	1:A:178:MET:HE1	2.16	0.70
1:A:74:LEU:O	1:A:86:ALA:HA	1.91	0.70
1:A:192:GLY:O	1:A:194:TYR:HD1	1.73	0.70
1:A:77:VAL:CG2	1:A:84:ILE:HG22	2.21	0.70
1:A:204:ILE:HA	1:A:208:ILE:HG12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLY:HA3	2:A:302:HOH:O	1.93	0.69
1:A:203:ILE:O	1:A:208:ILE:HG23	1.93	0.69
1:A:166:ARG:O	1:A:167:ASP:C	2.33	0.69
1:A:149:GLY:O	1:A:150:VAL:HG13	1.93	0.68
1:A:204:ILE:CA	1:A:208:ILE:HD11	2.24	0.67
1:A:63:LEU:HD13	1:A:101:LEU:HD21	1.76	0.67
1:A:204:ILE:CA	1:A:208:ILE:CD1	2.71	0.67
1:A:132:TRP:O	1:A:132:TRP:CE3	2.48	0.67
1:A:141:ILE:HD12	1:A:142:PRO:N	2.08	0.67
1:A:112:THR:CG2	1:A:136:LYS:HB2	2.22	0.66
1:A:124:THR:O	1:A:128:ALA:N	2.14	0.66
1:A:191:ILE:O	1:A:191:ILE:CG2	2.44	0.66
1:A:114:HIS:CG	1:A:115:THR:H	2.14	0.65
1:A:202:ASP:O	1:A:203:ILE:C	2.38	0.65
1:A:77:VAL:HG13	1:A:84:ILE:HG22	1.76	0.65
1:A:73:ILE:CD1	1:A:176:VAL:HG22	2.27	0.65
1:A:187:ARG:HG2	1:A:194:TYR:C	2.21	0.65
1:A:57:SER:O	1:A:60:ILE:HG13	1.96	0.65
1:A:73:ILE:CD1	1:A:176:VAL:HG21	2.24	0.65
1:A:176:VAL:O	1:A:180:VAL:HG23	1.97	0.64
1:A:58:PRO:HG3	1:A:208:ILE:HB	1.77	0.64
1:A:113:VAL:O	1:A:137:GLN:HA	1.98	0.64
1:A:203:ILE:O	1:A:204:ILE:C	2.41	0.64
1:A:183:HIS:C	1:A:183:HIS:CD2	2.75	0.63
1:A:180:VAL:O	1:A:181:PHE:C	2.38	0.63
1:A:128:ALA:O	1:A:131:TRP:HB3	1.98	0.63
1:A:73:ILE:HD11	1:A:172:LEU:HD11	1.80	0.63
1:A:63:LEU:CD1	1:A:101:LEU:HD21	2.29	0.63
1:A:156:LYS:O	1:A:157:GLU:C	2.41	0.63
1:A:81:SER:OG	1:A:200:ILE:HB	1.98	0.62
1:A:200:ILE:HG13	1:A:204:ILE:HD11	1.80	0.62
1:A:131:TRP:C	1:A:133:ALA:H	2.07	0.62
1:A:173:LYS:O	1:A:177:GLN:HG2	2.00	0.62
1:A:141:ILE:N	1:A:142:PRO:CD	2.56	0.62
1:A:154:MET:HG2	1:A:183:HIS:HE1	1.64	0.62
1:A:89:ILE:HD12	1:A:91:ALA:O	2.00	0.62
1:A:83:TYR:CB	1:A:200:ILE:HG21	2.29	0.61
1:A:138:GLU:HG3	1:A:139:PHE:N	2.16	0.61
1:A:204:ILE:CA	1:A:208:ILE:HG12	2.30	0.61
1:A:171:HIS:HB3	2:A:331:HOH:O	2.00	0.61
1:A:110:VAL:HG12	1:A:110:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG12	1:A:77:VAL:HG23	1.83	0.60
1:A:98:ALA:O	1:A:99:TYR:C	2.43	0.60
1:A:66:THR:HG22	1:A:67:HIS:N	2.16	0.60
1:A:204:ILE:O	1:A:207:ASP:N	2.32	0.60
1:A:83:TYR:CG	1:A:200:ILE:HG21	2.37	0.60
1:A:196:ALA:CA	1:A:199:ARG:NH2	2.51	0.60
1:A:69:GLU:O	1:A:71:LYS:N	2.33	0.60
1:A:83:TYR:CD1	1:A:83:TYR:C	2.80	0.59
1:A:107:ARG:CZ	1:A:107:ARG:CB	2.80	0.59
1:A:169:ALA:CB	1:A:175:ALA:HB2	2.31	0.59
1:A:205:ALA:C	1:A:207:ASP:H	2.10	0.59
1:A:54:VAL:HG21	1:A:203:ILE:HG12	1.82	0.59
1:A:118:GLY:O	1:A:119:SER:C	2.44	0.59
1:A:83:TYR:HB2	1:A:200:ILE:CG2	2.32	0.59
1:A:161:ILE:HA	1:A:164:GLN:HG3	1.83	0.59
1:A:178:MET:O	1:A:181:PHE:HB3	2.03	0.58
1:A:160:LYS:NZ	1:A:161:ILE:CG1	2.58	0.58
1:A:114:HIS:CE1	1:A:115:THR:O	2.57	0.58
1:A:117:ASN:C	1:A:117:ASN:ND2	2.52	0.58
1:A:60:ILE:O	1:A:79:VAL:HG23	2.04	0.58
1:A:52:GLY:O	1:A:54:VAL:HG22	2.04	0.58
1:A:129:ALA:C	1:A:131:TRP:N	2.59	0.58
1:A:138:GLU:HG3	1:A:139:PHE:H	1.68	0.58
1:A:181:PHE:HD1	1:A:182:ILE:N	2.02	0.57
1:A:151:ILE:C	1:A:152:GLU:HG3	2.29	0.57
1:A:162:ILE:O	1:A:163:GLY:C	2.48	0.57
1:A:209:GLN:CG	1:A:210:THR:H	2.10	0.56
1:A:158:LEU:O	1:A:158:LEU:HD23	2.05	0.56
1:A:83:TYR:CD2	1:A:200:ILE:HG21	2.41	0.56
1:A:131:TRP:C	1:A:133:ALA:N	2.62	0.55
1:A:200:ILE:CG1	1:A:204:ILE:HD11	2.36	0.55
1:A:141:ILE:HD12	1:A:141:ILE:C	2.31	0.55
1:A:138:GLU:CG	1:A:139:PHE:N	2.69	0.55
1:A:199:ARG:O	1:A:200:ILE:C	2.50	0.55
1:A:69:GLU:C	1:A:71:LYS:H	2.14	0.55
1:A:83:TYR:HB2	1:A:200:ILE:HG21	1.87	0.55
1:A:118:GLY:C	1:A:120:ASN:N	2.62	0.54
1:A:119:SER:O	1:A:122:THR:OG1	2.23	0.54
1:A:181:PHE:CD1	1:A:182:ILE:N	2.75	0.54
1:A:138:GLU:O	1:A:139:PHE:HB2	2.06	0.54
1:A:144:ASN:O	1:A:145:PRO:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:HIS:HA	2:A:331:HOH:O	2.06	0.54
1:A:114:HIS:CG	1:A:115:THR:N	2.73	0.54
1:A:194:TYR:HB3	1:A:198:GLU:HB2	1.90	0.54
1:A:195:SER:OG	1:A:198:GLU:HG3	2.08	0.54
1:A:107:ARG:NH1	1:A:107:ARG:HB3	2.21	0.54
1:A:202:ASP:O	1:A:205:ALA:HB3	2.08	0.54
1:A:202:ASP:HA	1:A:205:ALA:HB3	1.90	0.54
1:A:172:LEU:O	1:A:175:ALA:N	2.40	0.53
1:A:195:SER:O	1:A:196:ALA:C	2.52	0.53
1:A:202:ASP:O	1:A:203:ILE:O	2.25	0.53
1:A:151:ILE:HG23	1:A:152:GLU:H	1.73	0.53
1:A:61:TRP:CD1	1:A:110:VAL:HG22	2.44	0.53
1:A:204:ILE:N	1:A:208:ILE:HD13	2.24	0.52
1:A:78:HIS:O	1:A:79:VAL:C	2.51	0.52
1:A:170:GLU:C	1:A:171:HIS:CD2	2.87	0.52
1:A:81:SER:O	1:A:199:ARG:NH2	2.43	0.52
1:A:195:SER:H	1:A:198:GLU:HB2	1.75	0.52
1:A:205:ALA:O	1:A:207:ASP:N	2.42	0.52
1:A:129:ALA:C	1:A:131:TRP:H	2.16	0.52
1:A:173:LYS:O	1:A:174:THR:C	2.52	0.52
1:A:99:TYR:CD2	1:A:103:LYS:CD	2.84	0.52
1:A:118:GLY:O	1:A:120:ASN:N	2.43	0.52
1:A:200:ILE:O	1:A:201:VAL:C	2.52	0.51
1:A:58:PRO:HG2	1:A:208:ILE:HB	1.89	0.51
1:A:101:LEU:O	1:A:102:LEU:C	2.53	0.51
1:A:201:VAL:O	1:A:205:ALA:N	2.33	0.51
1:A:92:GLU:CG	1:A:92:GLU:O	2.59	0.51
1:A:69:GLU:OE2	1:A:166:ARG:NE	2.43	0.50
1:A:65:CYS:SG	1:A:120:ASN:ND2	2.84	0.50
1:A:158:LEU:C	1:A:158:LEU:CD2	2.85	0.50
1:A:67:HIS:CE1	1:A:72:VAL:HG22	2.47	0.50
1:A:141:ILE:H	1:A:142:PRO:HD2	1.69	0.50
1:A:204:ILE:O	1:A:205:ALA:C	2.55	0.50
1:A:123:SER:OG	1:A:126:VAL:HG23	2.11	0.50
1:A:131:TRP:O	1:A:133:ALA:N	2.45	0.49
1:A:156:LYS:O	1:A:159:LYS:N	2.46	0.49
1:A:55:ASP:OD1	1:A:55:ASP:C	2.56	0.49
1:A:158:LEU:CD2	1:A:162:ILE:HD11	2.42	0.49
1:A:148:GLN:HG2	2:A:327:HOH:O	2.12	0.49
1:A:165:VAL:O	1:A:166:ARG:C	2.53	0.49
1:A:204:ILE:N	1:A:208:ILE:CD1	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD22	1:A:121:PHE:CZ	2.48	0.49
1:A:112:THR:HA	1:A:136:LYS:O	2.12	0.49
1:A:190:GLY:O	1:A:191:ILE:C	2.56	0.49
1:A:196:ALA:O	1:A:200:ILE:HG22	2.13	0.49
1:A:63:LEU:HD22	1:A:121:PHE:CE1	2.47	0.49
1:A:62:GLN:HG3	1:A:64:ASP:OD1	2.13	0.48
1:A:183:HIS:C	1:A:185:HIS:N	2.68	0.48
1:A:183:HIS:CD2	1:A:184:ASN:N	2.80	0.48
1:A:88:VAL:HG12	1:A:88:VAL:O	2.13	0.48
1:A:176:VAL:O	1:A:179:ALA:HB3	2.13	0.48
1:A:107:ARG:HD2	1:A:108:TRP:NE1	2.28	0.48
1:A:112:THR:CA	1:A:136:LYS:O	2.62	0.48
1:A:172:LEU:CD1	1:A:176:VAL:CG2	2.86	0.48
1:A:144:ASN:CB	1:A:145:PRO:HD2	2.44	0.47
1:A:111:LYS:CD	1:A:210:THR:OG1	2.62	0.47
1:A:141:ILE:O	1:A:142:PRO:C	2.55	0.47
1:A:192:GLY:C	1:A:194:TYR:CD1	2.85	0.47
1:A:200:ILE:O	1:A:204:ILE:HG13	2.15	0.47
1:A:172:LEU:O	1:A:173:LYS:C	2.56	0.47
1:A:160:LYS:C	1:A:160:LYS:HD2	2.40	0.47
1:A:55:ASP:OD1	1:A:56:CYS:N	2.48	0.47
1:A:154:MET:C	1:A:156:LYS:N	2.72	0.47
1:A:165:VAL:O	1:A:168:GLN:N	2.48	0.47
1:A:101:LEU:O	1:A:105:ALA:N	2.38	0.47
1:A:161:ILE:O	1:A:165:VAL:HG22	2.14	0.47
1:A:83:TYR:CB	1:A:200:ILE:CG2	2.93	0.46
1:A:178:MET:O	1:A:179:ALA:C	2.57	0.46
1:A:68:LEU:O	1:A:69:GLU:C	2.58	0.46
1:A:202:ASP:CA	1:A:205:ALA:HB3	2.45	0.46
1:A:108:TRP:HB3	1:A:109:PRO:HD2	1.97	0.46
1:A:107:ARG:CZ	1:A:107:ARG:HB2	2.46	0.46
1:A:77:VAL:CG1	1:A:84:ILE:HG22	2.43	0.46
1:A:181:PHE:O	1:A:185:HIS:HB2	2.16	0.46
1:A:194:TYR:CA	1:A:198:GLU:OE1	2.58	0.46
1:A:165:VAL:O	1:A:168:GLN:HB3	2.17	0.45
1:A:66:THR:O	1:A:72:VAL:HG13	2.16	0.45
1:A:184:ASN:O	1:A:195:SER:HB2	2.16	0.45
1:A:171:HIS:CA	2:A:331:HOH:O	2.65	0.45
1:A:58:PRO:HB3	1:A:208:ILE:CG1	2.45	0.45
1:A:130:CYS:HB3	1:A:135:ILE:HB	1.98	0.45
1:A:132:TRP:O	1:A:132:TRP:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:HG12	1:A:135:ILE:HG12	1.99	0.44
1:A:199:ARG:HE	1:A:199:ARG:HB2	1.20	0.44
1:A:161:ILE:CA	1:A:164:GLN:HG3	2.47	0.44
1:A:205:ALA:C	1:A:207:ASP:N	2.70	0.44
1:A:111:LYS:HD3	1:A:210:THR:OG1	2.16	0.44
1:A:114:HIS:ND1	1:A:115:THR:N	2.65	0.44
1:A:77:VAL:HG13	1:A:84:ILE:CG2	2.45	0.44
1:A:171:HIS:CB	2:A:331:HOH:O	2.62	0.44
1:A:61:TRP:HB2	1:A:113:VAL:HG12	2.00	0.44
1:A:99:TYR:O	1:A:103:LYS:HD3	2.18	0.44
1:A:117:ASN:HD22	1:A:118:GLY:N	2.12	0.44
1:A:144:ASN:O	1:A:145:PRO:C	2.61	0.44
1:A:172:LEU:HA	1:A:172:LEU:HD13	1.75	0.44
1:A:183:HIS:O	1:A:184:ASN:C	2.59	0.44
1:A:83:TYR:OH	1:A:85:GLU:OE2	2.34	0.43
1:A:94:GLY:O	1:A:95:GLN:C	2.60	0.43
1:A:170:GLU:C	1:A:171:HIS:CG	2.96	0.43
1:A:187:ARG:O	1:A:188:LYS:HE3	2.18	0.43
1:A:192:GLY:O	1:A:194:TYR:CD1	2.63	0.43
1:A:69:GLU:O	1:A:71:LYS:HG3	2.17	0.43
1:A:169:ALA:HB3	1:A:175:ALA:HB2	1.99	0.43
1:A:204:ILE:HG13	1:A:204:ILE:H	1.48	0.43
1:A:92:GLU:O	1:A:92:GLU:HG2	2.18	0.43
1:A:180:VAL:O	1:A:183:HIS:N	2.52	0.42
1:A:173:LYS:C	1:A:175:ALA:N	2.75	0.42
1:A:159:LYS:HB2	1:A:159:LYS:HE3	1.82	0.42
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.72	0.42
1:A:54:VAL:HG12	1:A:55:ASP:H	1.84	0.42
1:A:104:LEU:CD2	1:A:110:VAL:HG21	2.50	0.42
1:A:66:THR:HG21	1:A:159:LYS:HE2	2.02	0.42
1:A:76:ALA:HB2	1:A:100:PHE:CZ	2.53	0.42
1:A:173:LYS:O	1:A:175:ALA:N	2.53	0.41
1:A:59:GLY:HA2	2:A:301:HOH:O	2.20	0.41
1:A:161:ILE:O	1:A:161:ILE:HG22	2.20	0.41
1:A:61:TRP:CD1	1:A:61:TRP:N	2.88	0.41
1:A:104:LEU:HD23	1:A:110:VAL:HG21	2.02	0.41
1:A:110:VAL:O	1:A:110:VAL:CG1	2.68	0.41
1:A:139:PHE:CE2	2:A:311:HOH:O	2.62	0.41
1:A:160:LYS:O	1:A:164:GLN:HG3	2.20	0.41
1:A:60:ILE:HG22	1:A:79:VAL:HG21	2.03	0.41
1:A:158:LEU:HD23	1:A:158:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:O	1:A:174:THR:HG22	2.21	0.41
1:A:160:LYS:HE3	1:A:161:ILE:HG13	2.02	0.41
1:A:63:LEU:CD1	1:A:101:LEU:CD2	2.98	0.40
1:A:107:ARG:HD2	1:A:107:ARG:HH11	1.50	0.40
1:A:112:THR:CB	1:A:136:LYS:O	2.69	0.40
1:A:177:GLN:OE1	1:A:177:GLN:HA	2.21	0.40
1:A:98:ALA:O	1:A:100:PHE:N	2.54	0.40
1:A:100:PHE:O	1:A:101:LEU:C	2.63	0.40
1:A:194:TYR:HB3	1:A:198:GLU:CB	2.50	0.40
1:A:157:GLU:O	1:A:160:LYS:HB3	2.20	0.40
1:A:203:ILE:C	1:A:208:ILE:HG23	2.47	0.40
1:A:118:GLY:O	1:A:121:PHE:N	2.52	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	158/163 (97%)	107 (68%)	36 (23%)	15 (10%)	0 0

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ILE
1	A	173	LYS
1	A	193	GLY
1	A	203	ILE
1	A	70	GLY
1	A	79	VAL
1	A	145	PRO
1	A	206	THR
1	A	132	TRP

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Mol	Chain	Res	Type
1	A	192	GLY
1	A	139	PHE
1	A	143	TYR
1	A	142	PRO
1	A	201	VAL
1	A	190	GLY

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	130/133 (98%)	106 (82%)	24 (18%)	1 3

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	54	VAL
1	A	55	ASP
1	A	63	LEU
1	A	65	CYS
1	A	79	VAL
1	A	83	TYR
1	A	97	THR
1	A	104	LEU
1	A	117	ASN
1	A	123	SER
1	A	148	GLN
1	A	158	LEU
1	A	166	ARG
1	A	170	GLU
1	A	172	LEU
1	A	183	HIS
1	A	185	HIS
1	A	188	LYS
1	A	191	ILE

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Mol	Chain	Res	Type
1	A	200	ILE
1	A	206	THR
1	A	207	ASP
1	A	209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	67	HIS
1	A	117	ASN
1	A	120	ASN
1	A	137	GLN
1	A	148	GLN
1	A	164	GLN
1	A	183	HIS
1	A	209	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.