



# Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 04:09 AM EDT

PDB ID : 3HPG / pdb\_00003hpg  
Title : Visna virus integrase (residues 1-219) in complex with LEDGF IBD: examples of open integrase dimer-dimer interfaces  
Authors : Hare, S.; Labeja, A.; Cherepanov, P.  
Deposited on : 2009-06-04  
Resolution : 3.28 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

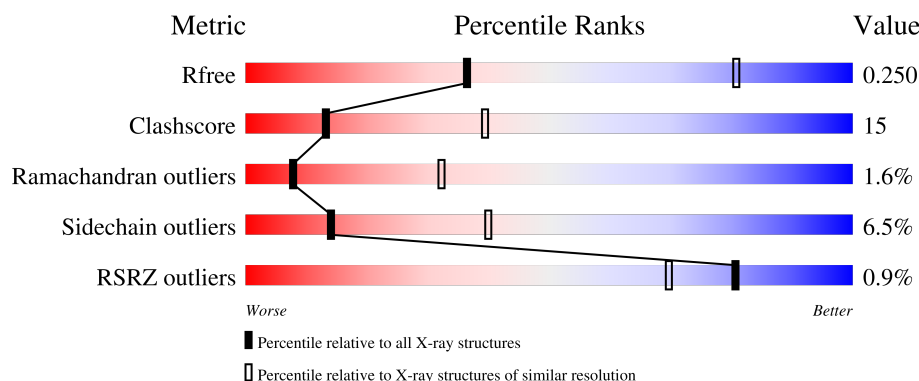
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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))
$R_{free}$	164625	1214 (3.30-3.26)
Clashscore	180529	1265 (3.30-3.26)
Ramachandran outliers	177936	1264 (3.30-3.26)
Sidechain outliers	177891	1263 (3.30-3.26)
RSRZ outliers	164620	1215 (3.30-3.26)

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  $\geq 3$ , 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	219	
1	B	219	
1	C	219	
1	D	219	
1	E	219	

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Mol	Chain	Length	Quality of chain
1	F	219	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>68%20%5%7%</div></div></div>
2	G	95	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>55%21%23%</div></div></div>
2	H	95	<div><div><div></div><div></div><div></div><div></div></div><div>49%21%28%</div></div>
2	I	95	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>54%17%28%</div></div></div>
2	J	95	<div><div><div></div><div></div><div></div><div></div></div><div>56%24%19%</div></div>
2	K	95	<div><div><div></div><div></div><div></div><div></div></div><div>49%20%29%</div></div>
2	L	95	<div><div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>49%14%36%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12792 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	194	Total	C	N	O	S	0	0	0
			1529	973	257	292	7			
1	B	209	Total	C	N	O	S	0	0	0
			1644	1044	280	312	8			
1	C	198	Total	C	N	O	S	0	0	0
			1562	993	265	296	8			
1	D	196	Total	C	N	O	S	0	0	0
			1545	981	262	295	7			
1	E	193	Total	C	N	O	S	0	0	0
			1528	972	259	290	7			
1	F	203	Total	C	N	O	S	0	0	0
			1590	1014	266	303	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P35956
A	2	VAL	-	expression tag	UNP P35956
B	1	MET	-	expression tag	UNP P35956
B	2	VAL	-	expression tag	UNP P35956
C	1	MET	-	expression tag	UNP P35956
C	2	VAL	-	expression tag	UNP P35956
D	1	MET	-	expression tag	UNP P35956
D	2	VAL	-	expression tag	UNP P35956
E	1	MET	-	expression tag	UNP P35956
E	2	VAL	-	expression tag	UNP P35956
F	1	MET	-	expression tag	UNP P35956
F	2	VAL	-	expression tag	UNP P35956

- Molecule 2 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	73	Total	C	N	O	S	0	0	0
			604	377	110	111	6			
2	H	68	Total	C	N	O	S	0	0	0
			553	341	102	104	6			
2	I	68	Total	C	N	O	S	0	0	0
			551	339	102	104	6			
2	J	77	Total	C	N	O	S	0	0	0
			629	392	114	117	6			
2	K	67	Total	C	N	O	S	0	0	0
			551	345	99	101	6			
2	L	61	Total	C	N	O	S	0	0	0
			500	309	94	92	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	436	LEU	-	expression tag	UNP O75475
G	437	GLU	-	expression tag	UNP O75475
G	438	VAL	-	expression tag	UNP O75475
G	439	LEU	-	expression tag	UNP O75475
G	440	PHE	-	expression tag	UNP O75475
G	441	GLN	-	expression tag	UNP O75475
H	436	LEU	-	expression tag	UNP O75475
H	437	GLU	-	expression tag	UNP O75475
H	438	VAL	-	expression tag	UNP O75475
H	439	LEU	-	expression tag	UNP O75475
H	440	PHE	-	expression tag	UNP O75475
H	441	GLN	-	expression tag	UNP O75475
I	436	LEU	-	expression tag	UNP O75475
I	437	GLU	-	expression tag	UNP O75475
I	438	VAL	-	expression tag	UNP O75475
I	439	LEU	-	expression tag	UNP O75475
I	440	PHE	-	expression tag	UNP O75475
I	441	GLN	-	expression tag	UNP O75475
J	436	LEU	-	expression tag	UNP O75475
J	437	GLU	-	expression tag	UNP O75475
J	438	VAL	-	expression tag	UNP O75475
J	439	LEU	-	expression tag	UNP O75475
J	440	PHE	-	expression tag	UNP O75475
J	441	GLN	-	expression tag	UNP O75475
K	436	LEU	-	expression tag	UNP O75475
K	437	GLU	-	expression tag	UNP O75475
K	438	VAL	-	expression tag	UNP O75475
K	439	LEU	-	expression tag	UNP O75475

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Chain	Residue	Modelled	Actual	Comment	Reference
K	440	PHE	-	expression tag	UNP O75475
K	441	GLN	-	expression tag	UNP O75475
L	436	LEU	-	expression tag	UNP O75475
L	437	GLU	-	expression tag	UNP O75475
L	438	VAL	-	expression tag	UNP O75475
L	439	LEU	-	expression tag	UNP O75475
L	440	PHE	-	expression tag	UNP O75475
L	441	GLN	-	expression tag	UNP O75475

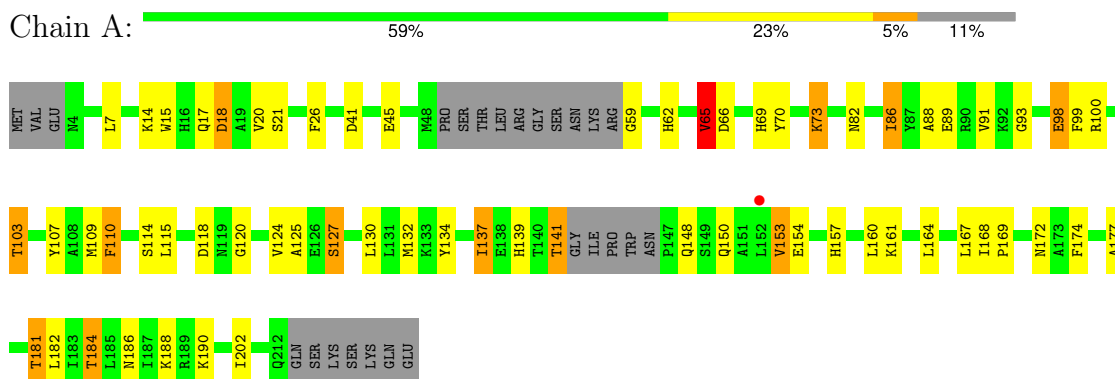
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

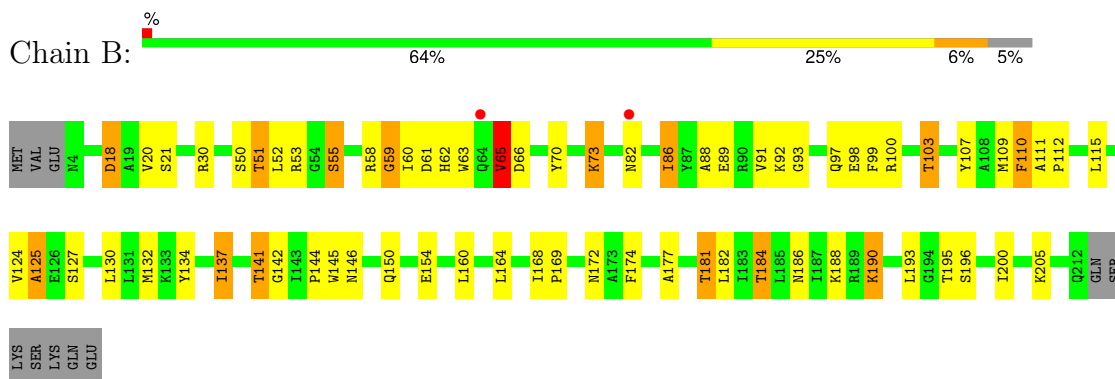
### 3 Residue-property plots [i](#)

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.

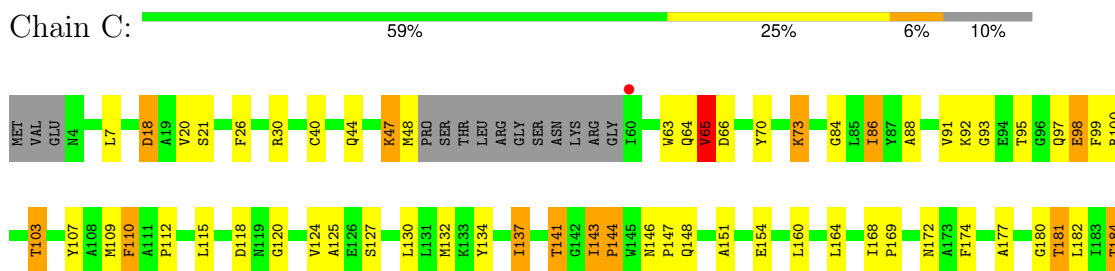
- Molecule 1: Integrase



- Molecule 1: Integrase

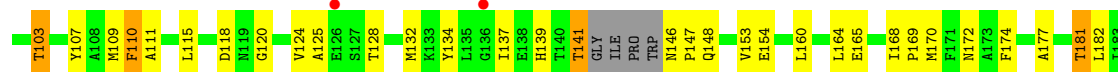
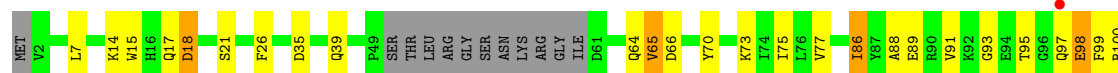


- Molecule 1: Integrase

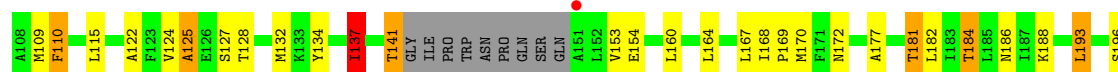
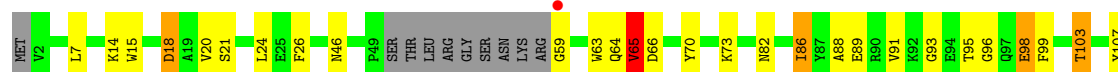




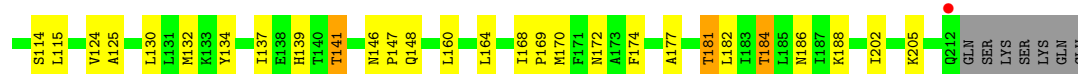
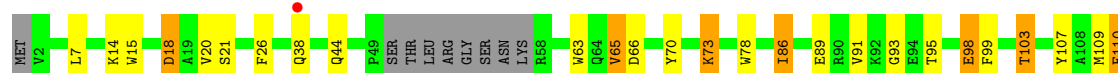
• Molecule 1: Integrase



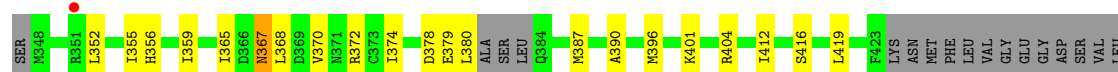
• Molecule 1: Integrase



• Molecule 1: Integrase



• Molecule 2: PC4 and SFRS1-interacting protein

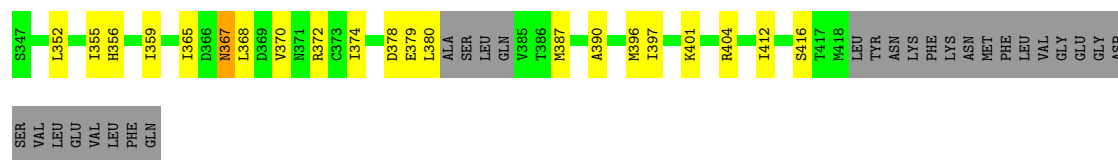




GLU  
VAL  
LEU  
PHE  
GLN

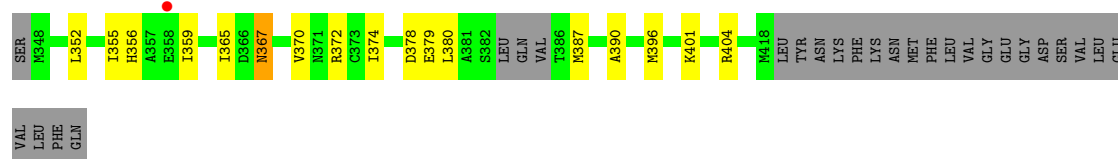
• Molecule 2: PC4 and SFRS1-interacting protein

Chain H: 49% 21% 28%



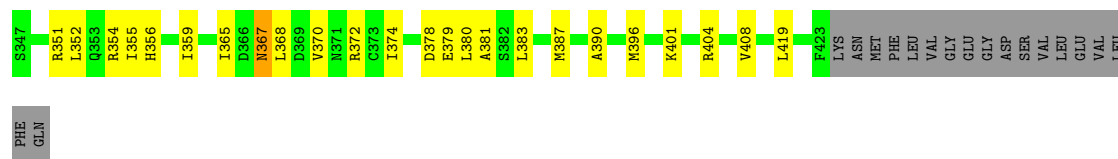
• Molecule 2: PC4 and SFRS1-interacting protein

Chain I: 54% 17% 28%



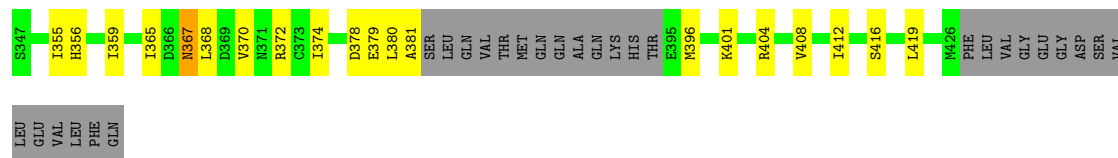
• Molecule 2: PC4 and SFRS1-interacting protein

Chain J: 56% 24% 19%



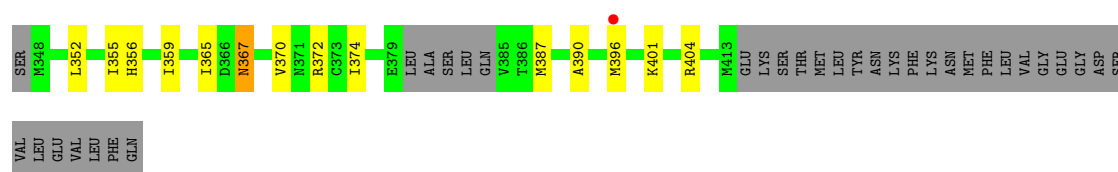
• Molecule 2: PC4 and SFRS1-interacting protein

Chain K: 49% 20% 29%



• Molecule 2: PC4 and SFRS1-interacting protein

Chain L: 49% 14% 36%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.10Å 148.90Å 91.08Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	38.67 – 3.28 38.67 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.67-3.28) 99.8 (38.67-3.28)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.212 , 0.253 0.211 , 0.250	Depositor DCC
$R_{free}$ test set	1723 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 93.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.333 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:  
ZN

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	0.74	0/1561	1.01	3/2116 (0.1%)
1	B	0.83	0/1682	1.10	9/2285 (0.4%)
1	C	0.74	0/1596	1.02	8/2166 (0.4%)
1	D	0.71	0/1578	0.99	4/2142 (0.2%)
1	E	0.71	0/1560	0.98	4/2115 (0.2%)
1	F	0.73	0/1627	1.00	2/2213 (0.1%)
2	G	0.56	0/607	0.79	0/807
2	H	0.53	0/554	0.82	0/736
2	I	0.46	0/552	0.79	0/733
2	J	0.54	0/633	0.87	2/844 (0.2%)
2	K	0.53	0/553	0.81	1/733 (0.1%)
2	L	0.49	0/501	0.81	0/666
All	All	0.69	0/13004	0.97	33/17556 (0.2%)

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	B	0	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	GLY	N-CA-C	7.23	120.70	111.37
1	A	110	PHE	CA-C-N	-7.05	113.94	123.46
1	A	110	PHE	C-N-CA	-7.05	113.94	123.46
1	B	110	PHE	CA-C-N	-7.04	113.96	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	PHE	C-N-CA	-7.04	113.96	123.46
2	J	381	ALA	N-CA-C	-6.90	104.73	113.43
1	D	110	PHE	CA-C-N	-6.11	115.21	123.46
1	D	110	PHE	C-N-CA	-6.11	115.21	123.46
1	A	65	VAL	CB-CA-C	-6.11	101.52	110.81
1	B	65	VAL	CB-CA-C	-6.10	101.54	110.81
1	B	111	ALA	CA-C-N	6.04	125.95	119.85
1	B	111	ALA	C-N-CA	6.04	125.95	119.85
1	C	47	LYS	N-CA-C	6.04	120.47	111.96
1	C	110	PHE	CA-C-N	-5.91	115.49	123.46
1	C	110	PHE	C-N-CA	-5.91	115.49	123.46
1	F	110	PHE	CA-C-N	-5.87	115.53	123.46
1	F	110	PHE	C-N-CA	-5.87	115.53	123.46
1	B	193	LEU	N-CA-C	-5.86	105.98	113.02
1	B	58	ARG	N-CA-C	-5.79	101.96	110.52
1	C	65	VAL	CB-CA-C	-5.73	102.10	110.81
1	E	110	PHE	CA-C-N	-5.66	115.82	123.46
1	E	110	PHE	C-N-CA	-5.66	115.82	123.46
1	B	200	ILE	CB-CA-C	-5.56	104.85	111.97
1	C	143	ILE	CA-C-N	5.44	126.64	119.84
1	C	143	ILE	C-N-CA	5.44	126.64	119.84
1	D	111	ALA	CA-C-N	5.22	125.12	119.85
1	D	111	ALA	C-N-CA	5.22	125.12	119.85
2	K	408	VAL	N-CA-C	5.22	115.36	110.30
1	E	137	ILE	N-CA-C	5.19	115.37	108.11
1	C	110	PHE	N-CA-C	-5.18	102.52	110.14
2	J	408	VAL	N-CA-C	5.12	115.27	110.30
1	E	65	VAL	CB-CA-C	-5.11	103.04	110.81
1	C	84	GLY	N-CA-C	-5.03	108.34	115.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	GLY	Peptide

## 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	1529	0	1463	52	0
1	B	1644	0	1574	64	0
1	C	1562	0	1495	55	0
1	D	1545	0	1471	56	0
1	E	1528	0	1466	54	0
1	F	1590	0	1508	51	0
2	G	604	0	636	17	0
2	H	553	0	585	14	0
2	I	551	0	581	12	0
2	J	629	0	663	20	0
2	K	551	0	585	16	0
2	L	500	0	529	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	12792	0	12556	370	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 15.

All (370) 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:144:PRO:HB2	1:B:150:GLN:NE2	1.84	0.93
1:C:47:LYS:O	1:C:48:MET:HB2	1.73	0.88
1:B:134:TYR:CE1	1:F:14:LYS:HG2	2.10	0.86
1:F:164:LEU:HD23	1:F:181:THR:HG21	1.59	0.84
1:B:134:TYR:CZ	2:G:365:ILE:HD13	2.13	0.83
1:D:164:LEU:HD23	1:D:181:THR:HG21	1.64	0.79
1:D:65:VAL:HG22	1:D:115:LEU:HD11	1.63	0.79
1:A:164:LEU:HD23	1:A:181:THR:HG21	1.65	0.77
1:B:182:LEU:O	1:B:186:ASN:HB2	1.85	0.76
1:B:164:LEU:HD23	1:B:181:THR:HG21	1.69	0.74
1:E:65:VAL:HG22	1:E:115:LEU:HD11	1.71	0.73
1:C:164:LEU:HD23	1:C:181:THR:HG21	1.68	0.72
1:E:164:LEU:HD23	1:E:181:THR:HG21	1.70	0.72
1:E:99:PHE:O	1:E:103:THR:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:O	1:A:186:ASN:HB2	1.90	0.72
1:B:65:VAL:HG22	1:B:115:LEU:HD11	1.72	0.72
1:A:99:PHE:O	1:A:103:THR:HG23	1.90	0.71
1:C:99:PHE:O	1:C:103:THR:HG23	1.91	0.71
1:B:20:VAL:HB	1:B:53:ARG:HH11	1.56	0.70
1:C:65:VAL:HG22	1:C:115:LEU:HD11	1.73	0.70
1:D:99:PHE:O	1:D:103:THR:HG23	1.91	0.70
1:B:30:ARG:CZ	1:B:60:ILE:HG13	2.21	0.70
1:B:20:VAL:HB	1:B:53:ARG:NH1	2.07	0.69
1:D:124:VAL:HG22	1:D:141:THR:HG21	1.75	0.69
1:D:182:LEU:O	1:D:186:ASN:HB2	1.92	0.69
1:F:65:VAL:HG22	1:F:115:LEU:HD11	1.73	0.69
1:A:184:THR:HA	1:A:188:LYS:HB2	1.74	0.69
1:E:182:LEU:O	1:E:186:ASN:HB2	1.92	0.69
1:E:184:THR:HA	1:E:188:LYS:HB2	1.75	0.69
1:F:170:MET:HE2	2:L:365:ILE:HD11	1.73	0.69
1:C:134:TYR:CE1	1:E:14:LYS:HG2	2.28	0.69
1:F:124:VAL:HG22	1:F:141:THR:HG21	1.75	0.68
1:D:184:THR:HA	1:D:188:LYS:HB2	1.76	0.68
1:E:177:ALA:O	1:E:181:THR:HG23	1.93	0.68
1:C:177:ALA:O	1:C:181:THR:HG23	1.93	0.68
1:F:177:ALA:O	1:F:181:THR:HG23	1.93	0.67
1:A:65:VAL:HG22	1:A:115:LEU:HD11	1.74	0.67
1:B:184:THR:HA	1:B:188:LYS:HB2	1.75	0.67
1:F:184:THR:HA	1:F:188:LYS:HB2	1.74	0.67
1:B:130:LEU:HD13	2:G:368:LEU:HD13	1.77	0.67
1:B:177:ALA:O	1:B:181:THR:HG23	1.95	0.66
1:A:177:ALA:O	1:A:181:THR:HG23	1.95	0.66
1:B:59:GLY:C	1:B:60:ILE:HD13	2.19	0.66
1:E:124:VAL:HG22	1:E:141:THR:HG21	1.75	0.66
1:F:182:LEU:O	1:F:186:ASN:HB2	1.95	0.66
1:F:38:GLN:HA	1:F:44:GLN:HE21	1.61	0.66
1:D:177:ALA:O	1:D:181:THR:HG23	1.95	0.66
1:F:38:GLN:HA	1:F:44:GLN:NE2	2.10	0.65
1:A:124:VAL:HG22	1:A:141:THR:HG21	1.77	0.65
1:B:18:ASP:OD2	1:B:53:ARG:NH1	2.30	0.64
1:C:182:LEU:O	1:C:186:ASN:HB2	1.96	0.64
2:J:380:LEU:HD23	2:J:419:LEU:HD23	1.78	0.64
1:A:153:VAL:HG13	1:A:157:HIS:ND1	2.12	0.64
1:D:15:TRP:CD1	1:E:188:LYS:HE2	2.33	0.64
1:F:99:PHE:O	1:F:103:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:HG22	1:C:141:THR:HG21	1.80	0.63
1:A:15:TRP:CD1	1:F:188:LYS:HE2	2.33	0.63
1:B:124:VAL:HG22	1:B:141:THR:HG21	1.81	0.63
1:F:134:TYR:CZ	2:K:365:ILE:HD13	2.33	0.62
2:K:380:LEU:HD23	2:K:419:LEU:HD23	1.79	0.62
1:E:107:TYR:HD1	1:E:137:ILE:HD11	1.65	0.62
1:D:65:VAL:CG2	1:D:115:LEU:HD11	2.30	0.62
1:E:20:VAL:CG1	1:E:193:LEU:HD11	2.30	0.61
2:G:378:ASP:C	2:G:380:LEU:H	2.08	0.61
1:A:168:ILE:HG12	1:A:169:PRO:HD3	1.81	0.61
1:B:59:GLY:O	1:B:82:ASN:ND2	2.34	0.61
1:B:150:GLN:HA	1:B:150:GLN:OE1	2.00	0.61
1:D:165:GLU:HG2	1:E:46:ASN:ND2	2.16	0.61
1:A:14:LYS:HG2	1:E:134:TYR:CE1	2.36	0.61
1:A:132:MET:HE3	1:A:137:ILE:HB	1.83	0.60
1:B:99:PHE:O	1:B:103:THR:HG23	2.02	0.60
1:C:184:THR:HA	1:C:188:LYS:HB2	1.84	0.60
1:D:14:LYS:HG2	1:F:134:TYR:CE1	2.37	0.60
1:C:65:VAL:CG2	1:C:115:LEU:HD11	2.31	0.60
1:B:51:THR:OG1	1:B:52:LEU:N	2.35	0.59
1:C:86:ILE:HD11	1:C:160:LEU:HD13	1.83	0.59
1:C:47:LYS:O	1:C:48:MET:CB	2.49	0.59
2:J:378:ASP:C	2:J:380:LEU:H	2.11	0.59
1:C:130:LEU:HD13	2:J:368:LEU:HD13	1.84	0.59
2:G:355:ILE:O	2:G:359:ILE:HG13	2.03	0.59
2:K:378:ASP:C	2:K:380:LEU:H	2.10	0.59
1:D:15:TRP:HE3	1:E:184:THR:HG22	1.68	0.59
1:D:86:ILE:HD11	1:D:160:LEU:HD13	1.84	0.59
1:B:134:TYR:CZ	1:F:14:LYS:HG2	2.38	0.58
1:D:134:TYR:CZ	2:I:365:ILE:HD13	2.38	0.58
1:F:86:ILE:HD11	1:F:160:LEU:HD13	1.84	0.58
2:I:378:ASP:C	2:I:380:LEU:H	2.11	0.58
1:B:86:ILE:HD11	1:B:160:LEU:HD13	1.84	0.58
1:F:168:ILE:HG12	1:F:169:PRO:HD3	1.84	0.58
1:A:134:TYR:CE1	2:H:365:ILE:HD13	2.38	0.58
2:G:380:LEU:HD23	2:G:419:LEU:HD23	1.84	0.58
2:I:355:ILE:O	2:I:359:ILE:HG13	2.03	0.58
1:A:107:TYR:HD1	1:A:137:ILE:HD11	1.69	0.58
1:C:30:ARG:HD2	1:D:35:ASP:OD2	2.04	0.58
1:A:188:LYS:HE2	1:F:15:TRP:CD1	2.39	0.58
1:C:30:ARG:HG2	1:D:39:GLN:NE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:355:ILE:O	2:H:359:ILE:HG13	2.04	0.57
1:C:109:MET:HE1	1:D:110:PHE:CZ	2.39	0.57
1:D:107:TYR:HD1	1:D:137:ILE:HD11	1.68	0.57
1:D:188:LYS:HE2	1:E:15:TRP:CD1	2.39	0.57
1:E:109:MET:HE1	1:F:110:PHE:CZ	2.39	0.57
2:G:401:LYS:HG3	2:G:404:ARG:HH21	1.68	0.57
1:F:164:LEU:HD23	1:F:181:THR:CG2	2.32	0.57
1:C:132:MET:HE3	1:C:137:ILE:HB	1.86	0.57
2:L:355:ILE:O	2:L:359:ILE:HG13	2.04	0.57
1:E:132:MET:HE3	1:E:137:ILE:HB	1.86	0.57
1:D:15:TRP:CE3	1:E:184:THR:HG22	2.40	0.57
1:E:168:ILE:HG12	1:E:169:PRO:HD3	1.87	0.57
1:D:132:MET:HE3	1:D:137:ILE:HB	1.88	0.56
1:C:30:ARG:HD2	1:D:35:ASP:CG	2.31	0.56
1:D:168:ILE:HG12	1:D:169:PRO:HD3	1.86	0.56
1:D:191:GLY:HA2	1:E:24:LEU:CD1	2.34	0.56
1:B:134:TYR:CE1	2:G:365:ILE:HD13	2.39	0.56
1:E:154:GLU:HA	1:E:154:GLU:OE1	2.05	0.56
1:E:168:ILE:N	1:E:169:PRO:CD	2.69	0.56
2:H:401:LYS:HG3	2:H:404:ARG:HH21	1.70	0.56
2:H:378:ASP:C	2:H:380:LEU:H	2.12	0.56
1:A:130:LEU:HD13	2:H:368:LEU:HD13	1.88	0.56
1:B:55:SER:HB2	1:B:62:HIS:CE1	2.41	0.55
2:J:401:LYS:HG3	2:J:404:ARG:HH21	1.70	0.55
1:C:168:ILE:HG12	1:C:169:PRO:HD3	1.87	0.55
2:K:381:ALA:HB2	2:K:419:LEU:HD11	1.88	0.55
1:F:107:TYR:HD1	1:F:137:ILE:HD11	1.71	0.55
2:G:356:HIS:CD2	2:G:396:MET:HA	2.41	0.55
1:A:65:VAL:CG2	1:A:115:LEU:HD11	2.36	0.55
1:A:86:ILE:HD11	1:A:160:LEU:HD13	1.88	0.55
1:B:168:ILE:HG12	1:B:169:PRO:HD3	1.88	0.55
1:F:132:MET:HE3	1:F:137:ILE:HB	1.89	0.54
1:E:59:GLY:O	1:E:82:ASN:HB2	2.07	0.54
1:E:65:VAL:CG2	1:E:115:LEU:HD11	2.37	0.54
2:I:356:HIS:CD2	2:I:396:MET:HA	2.43	0.54
1:E:110:PHE:CZ	1:F:109:MET:HE1	2.43	0.54
1:F:65:VAL:CG2	1:F:115:LEU:HD11	2.37	0.54
2:L:401:LYS:HG3	2:L:404:ARG:HH21	1.72	0.54
1:B:190:LYS:HE3	1:B:196:SER:HB3	1.90	0.54
2:I:401:LYS:HG3	2:I:404:ARG:HH21	1.72	0.54
1:F:170:MET:HE2	2:L:365:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:SER:HB2	1:B:62:HIS:HE1	1.71	0.53
1:A:168:ILE:N	1:A:169:PRO:CD	2.71	0.53
2:J:355:ILE:O	2:J:359:ILE:HG13	2.09	0.53
1:F:18:ASP:HB2	1:F:21:SER:H	1.74	0.53
1:A:164:LEU:HD23	1:A:181:THR:CG2	2.39	0.53
1:C:110:PHE:CZ	1:D:109:MET:HE1	2.44	0.53
1:D:164:LEU:HD23	1:D:181:THR:CG2	2.37	0.53
1:E:20:VAL:HG13	1:E:193:LEU:HD11	1.91	0.53
1:E:107:TYR:CD1	1:E:137:ILE:HD11	2.44	0.52
2:K:401:LYS:HG3	2:K:404:ARG:HH21	1.74	0.52
1:B:130:LEU:HD12	2:G:368:LEU:HB3	1.90	0.52
1:D:88:ALA:H	1:D:182:LEU:HD11	1.75	0.52
1:B:65:VAL:CG2	1:B:115:LEU:HD11	2.39	0.52
1:B:168:ILE:N	1:B:169:PRO:CD	2.73	0.52
2:K:356:HIS:CD2	2:K:396:MET:HA	2.45	0.52
1:B:30:ARG:NH2	1:B:60:ILE:CD1	2.73	0.52
2:G:365:ILE:C	2:G:367:ASN:H	2.18	0.52
1:A:107:TYR:CD1	1:A:137:ILE:HD11	2.45	0.52
1:B:132:MET:HE3	1:B:137:ILE:HB	1.92	0.52
1:B:134:TYR:CD1	1:F:14:LYS:HE3	2.44	0.52
1:D:107:TYR:CD1	1:D:137:ILE:HD11	2.45	0.52
1:C:99:PHE:O	1:C:103:THR:CG2	2.58	0.52
1:A:99:PHE:O	1:A:103:THR:CG2	2.59	0.51
1:C:107:TYR:HD1	1:C:137:ILE:HD11	1.74	0.51
1:E:86:ILE:HD11	1:E:160:LEU:HD13	1.92	0.51
2:J:356:HIS:CD2	2:J:396:MET:HA	2.44	0.51
2:I:365:ILE:C	2:I:367:ASN:H	2.18	0.51
2:I:387:MET:HA	2:I:390:ALA:HB3	1.92	0.51
2:J:401:LYS:HA	2:J:404:ARG:HD2	1.93	0.51
1:D:170:MET:HE2	2:J:365:ILE:CD1	2.41	0.51
1:E:59:GLY:N	1:E:82:ASN:HD22	2.09	0.51
2:K:355:ILE:O	2:K:359:ILE:HG13	2.11	0.51
2:H:365:ILE:C	2:H:367:ASN:H	2.19	0.51
1:C:18:ASP:HB2	1:C:21:SER:H	1.75	0.51
1:E:202:ILE:HD13	1:F:205:LYS:HB3	1.92	0.51
2:L:387:MET:HA	2:L:390:ALA:HB3	1.93	0.51
2:G:387:MET:HA	2:G:390:ALA:HB3	1.92	0.51
1:B:18:ASP:HB3	1:B:20:VAL:H	1.76	0.51
1:D:154:GLU:OE1	1:D:154:GLU:HA	2.11	0.51
2:J:351:ARG:HD3	2:J:383:LEU:HD11	1.93	0.51
2:G:401:LYS:HA	2:G:404:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:NE	1:B:60:ILE:HG13	2.26	0.50
2:J:370:VAL:O	2:J:374:ILE:HG13	2.11	0.50
1:B:91:VAL:HG13	1:B:98:GLU:CD	2.36	0.50
2:H:387:MET:HA	2:H:390:ALA:HB3	1.93	0.50
2:K:401:LYS:HA	2:K:404:ARG:HD2	1.94	0.50
2:L:356:HIS:CD2	2:L:396:MET:HA	2.46	0.50
1:A:110:PHE:CZ	1:B:109:MET:HE1	2.46	0.50
1:A:18:ASP:HB2	1:A:21:SER:H	1.77	0.50
1:A:109:MET:HE1	1:B:110:PHE:CZ	2.47	0.50
1:A:154:GLU:OE1	1:A:154:GLU:HA	2.11	0.50
2:G:378:ASP:C	2:G:380:LEU:N	2.70	0.50
1:B:59:GLY:C	1:B:60:ILE:CD1	2.85	0.50
1:B:107:TYR:HD1	1:B:137:ILE:HD11	1.77	0.50
2:K:365:ILE:C	2:K:367:ASN:H	2.18	0.50
1:A:41:ASP:O	1:A:45:GLU:HG3	2.12	0.49
1:C:134:TYR:CZ	2:J:365:ILE:HD13	2.48	0.49
2:H:356:HIS:CD2	2:H:396:MET:HA	2.47	0.49
2:L:370:VAL:O	2:L:374:ILE:HG13	2.12	0.49
1:B:59:GLY:O	1:B:60:ILE:HD13	2.12	0.49
1:B:91:VAL:HG12	1:B:93:GLY:N	2.27	0.49
1:C:70:TYR:O	1:C:73:LYS:HB2	2.13	0.49
1:C:164:LEU:HD23	1:C:181:THR:CG2	2.41	0.49
1:F:168:ILE:N	1:F:169:PRO:CD	2.76	0.49
1:B:18:ASP:OD2	1:B:53:ARG:CZ	2.61	0.49
1:D:18:ASP:HB2	1:D:21:SER:H	1.78	0.48
1:F:130:LEU:HD13	2:K:368:LEU:HD13	1.95	0.48
1:D:99:PHE:O	1:D:103:THR:CG2	2.61	0.48
1:C:168:ILE:N	1:C:169:PRO:CD	2.77	0.48
1:E:109:MET:HE2	1:F:109:MET:HE2	1.95	0.48
1:A:153:VAL:HG13	1:A:157:HIS:CE1	2.48	0.48
1:E:205:LYS:HB3	1:F:202:ILE:HD13	1.95	0.48
1:D:91:VAL:HG12	1:D:93:GLY:N	2.28	0.48
1:E:64:GLN:CD	1:E:153:VAL:HG21	2.39	0.48
2:J:387:MET:HA	2:J:390:ALA:HB3	1.94	0.48
1:C:18:ASP:CB	1:C:21:SER:H	2.27	0.48
2:I:370:VAL:O	2:I:374:ILE:HG13	2.14	0.48
2:L:365:ILE:C	2:L:367:ASN:H	2.22	0.48
2:H:372:ARG:HG2	2:H:372:ARG:O	2.14	0.48
1:A:59:GLY:N	1:A:82:ASN:HD22	2.11	0.48
2:H:370:VAL:O	2:H:374:ILE:HG13	2.14	0.48
1:B:164:LEU:HD23	1:B:181:THR:CG2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ILE:N	1:D:169:PRO:CD	2.77	0.47
1:E:24:LEU:HD21	1:E:193:LEU:HD21	1.96	0.47
1:E:196:SER:HB2	1:E:197:PRO:CD	2.44	0.47
1:E:20:VAL:HG11	1:E:193:LEU:HD11	1.97	0.47
2:G:372:ARG:O	2:G:372:ARG:HG2	2.13	0.47
2:K:378:ASP:C	2:K:380:LEU:N	2.73	0.47
1:A:70:TYR:O	1:A:73:LYS:HB2	2.15	0.47
1:C:91:VAL:HG13	1:C:98:GLU:CD	2.39	0.47
1:B:18:ASP:HB2	1:B:21:SER:H	1.79	0.47
2:I:401:LYS:HA	2:I:404:ARG:HD2	1.96	0.47
1:E:196:SER:HB2	1:E:197:PRO:HD2	1.96	0.47
1:A:91:VAL:HG13	1:A:98:GLU:CD	2.39	0.47
1:B:63:TRP:O	1:B:115:LEU:HD12	2.14	0.47
1:E:18:ASP:HB2	1:E:21:SER:H	1.80	0.47
2:J:365:ILE:C	2:J:367:ASN:H	2.21	0.47
1:B:145:TRP:CE3	1:B:146:ASN:HA	2.49	0.47
1:C:91:VAL:HG12	1:C:93:GLY:N	2.30	0.46
1:E:164:LEU:HD23	1:E:181:THR:CG2	2.42	0.46
2:G:370:VAL:O	2:G:374:ILE:HG13	2.15	0.46
2:L:401:LYS:HA	2:L:404:ARG:HD2	1.97	0.46
1:A:91:VAL:HG12	1:A:93:GLY:N	2.31	0.46
1:A:100:ARG:CZ	1:A:127:SER:HB2	2.46	0.46
2:I:372:ARG:O	2:I:372:ARG:HG2	2.13	0.46
1:D:91:VAL:HG13	1:D:98:GLU:CD	2.40	0.46
1:B:154:GLU:OE1	1:B:154:GLU:HA	2.16	0.46
2:H:352:LEU:HD22	2:H:396:MET:HE1	1.97	0.46
1:A:88:ALA:H	1:A:182:LEU:HD11	1.80	0.46
1:E:63:TRP:O	1:E:115:LEU:HD12	2.15	0.46
1:E:70:TYR:O	1:E:73:LYS:HB2	2.16	0.46
1:A:132:MET:HE2	1:A:139:HIS:HB2	1.98	0.46
1:D:7:LEU:HD22	1:D:26:PHE:CE1	2.51	0.46
2:I:378:ASP:C	2:I:380:LEU:N	2.73	0.46
1:B:30:ARG:NH2	1:B:60:ILE:HD11	2.30	0.46
1:B:107:TYR:CD1	1:B:112:PRO:HD2	2.51	0.46
1:D:70:TYR:O	1:D:73:LYS:HB2	2.16	0.45
2:H:401:LYS:HA	2:H:404:ARG:HD2	1.98	0.45
2:J:378:ASP:C	2:J:380:LEU:N	2.73	0.45
1:C:180:GLY:O	1:C:184:THR:HG23	2.15	0.45
1:D:164:LEU:O	1:D:168:ILE:HG23	2.16	0.45
1:E:128:THR:O	1:E:132:MET:HG2	2.16	0.45
1:F:99:PHE:O	1:F:103:THR:CG2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:TYR:O	1:B:73:LYS:HB2	2.16	0.45
1:C:88:ALA:H	1:C:182:LEU:HD11	1.81	0.45
1:A:109:MET:HE2	1:B:109:MET:HE2	1.97	0.45
1:C:63:TRP:O	1:C:115:LEU:HD12	2.16	0.45
1:C:147:PRO:O	1:C:151:ALA:HB2	2.16	0.45
1:A:15:TRP:HE3	1:F:184:THR:HG22	1.82	0.45
1:B:88:ALA:H	1:B:182:LEU:HD11	1.80	0.45
1:B:100:ARG:CZ	1:B:127:SER:HB2	2.47	0.45
2:K:380:LEU:HB3	2:K:419:LEU:HD21	1.99	0.45
1:C:172:ASN:C	1:C:172:ASN:HD22	2.24	0.45
1:C:146:ASN:HA	1:C:147:PRO:HD3	1.89	0.45
1:E:65:VAL:HG21	1:E:115:LEU:HD21	1.98	0.45
2:K:372:ARG:O	2:K:372:ARG:HG2	2.16	0.45
1:B:60:ILE:HG22	1:B:61:ASP:N	2.32	0.44
1:D:14:LYS:HG2	1:F:134:TYR:CZ	2.52	0.44
1:F:70:TYR:O	1:F:70:TYR:CD2	2.70	0.44
1:C:107:TYR:CD1	1:C:137:ILE:HD11	2.51	0.44
2:J:383:LEU:HD23	2:J:383:LEU:HA	1.64	0.44
1:D:18:ASP:CB	1:D:21:SER:H	2.31	0.44
1:E:91:VAL:HG13	1:E:98:GLU:CD	2.42	0.44
2:J:352:LEU:HD22	2:J:396:MET:HE1	1.99	0.44
2:L:352:LEU:HD22	2:L:396:MET:HE1	2.00	0.44
1:B:59:GLY:C	1:B:60:ILE:CG1	2.88	0.44
1:E:202:ILE:HD13	1:F:205:LYS:CB	2.48	0.44
1:D:17:GLN:HB3	1:D:21:SER:HB2	2.00	0.44
1:F:107:TYR:CD1	1:F:137:ILE:HD11	2.50	0.44
1:C:7:LEU:O	1:C:7:LEU:HD23	2.17	0.44
2:K:370:VAL:O	2:K:374:ILE:HG13	2.17	0.44
1:D:7:LEU:C	1:D:7:LEU:HD23	2.42	0.43
1:A:7:LEU:HD22	1:A:26:PHE:CE1	2.54	0.43
1:C:143:ILE:HA	1:C:144:PRO:HD2	1.88	0.43
1:C:7:LEU:HD23	1:C:7:LEU:C	2.44	0.43
1:D:128:THR:O	1:D:132:MET:HG2	2.18	0.43
1:E:99:PHE:O	1:E:103:THR:CG2	2.62	0.43
1:F:124:VAL:CG2	1:F:141:THR:HG21	2.46	0.43
1:E:91:VAL:HG12	1:E:93:GLY:N	2.34	0.43
2:I:352:LEU:HD22	2:I:396:MET:HE1	2.00	0.43
1:C:202:ILE:HD13	1:D:205:LYS:HB3	2.00	0.43
1:D:124:VAL:CG2	1:D:141:THR:HG21	2.48	0.43
2:J:372:ARG:O	2:J:372:ARG:HG2	2.18	0.43
1:A:15:TRP:CE3	1:F:184:THR:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLN:HA	1:D:100:ARG:NH1	2.33	0.43
1:D:132:MET:HE2	1:D:139:HIS:HB2	2.00	0.43
1:F:91:VAL:HG12	1:F:93:GLY:N	2.33	0.43
1:D:193:LEU:HD23	1:D:193:LEU:HA	1.62	0.43
1:E:7:LEU:HD22	1:E:26:PHE:CE1	2.53	0.43
1:F:73:LYS:HD3	1:F:174:PHE:CD1	2.54	0.43
1:F:164:LEU:O	1:F:168:ILE:HG23	2.19	0.43
2:H:412:ILE:O	2:H:416:SER:HB3	2.19	0.43
2:K:412:ILE:O	2:K:416:SER:HB3	2.19	0.43
1:A:69:HIS:O	1:A:161:LYS:HE2	2.19	0.43
1:A:118:ASP:C	1:A:120:GLY:H	2.27	0.43
1:F:18:ASP:HB3	1:F:20:VAL:H	1.82	0.43
1:B:86:ILE:HG21	1:B:86:ILE:HD13	1.67	0.42
2:H:378:ASP:C	2:H:380:LEU:N	2.74	0.42
1:C:107:TYR:CD1	1:C:112:PRO:HD2	2.54	0.42
1:B:73:LYS:HD3	1:B:174:PHE:CD1	2.54	0.42
1:C:7:LEU:HD22	1:C:26:PHE:CE1	2.54	0.42
1:F:63:TRP:O	1:F:115:LEU:HD12	2.19	0.42
1:B:70:TYR:O	1:B:70:TYR:CD2	2.73	0.42
1:E:96:GLY:HA2	1:E:122:ALA:HB1	2.00	0.42
1:D:65:VAL:HG21	1:D:115:LEU:HD21	2.02	0.42
1:A:184:THR:HG22	1:F:15:TRP:HE3	1.85	0.42
1:E:88:ALA:H	1:E:182:LEU:HD11	1.85	0.42
1:C:109:MET:HE2	1:D:109:MET:HE2	2.02	0.42
1:A:150:GLN:O	1:A:154:GLU:HB2	2.20	0.42
1:C:40:CYS:O	1:C:44:GLN:HG2	2.20	0.42
1:E:124:VAL:O	1:E:125:ALA:C	2.63	0.42
1:B:60:ILE:HG22	1:B:61:ASP:H	1.85	0.41
1:F:7:LEU:HD22	1:F:26:PHE:CE1	2.55	0.41
1:C:97:GLN:HA	1:C:100:ARG:NH1	2.35	0.41
1:C:100:ARG:CZ	1:C:127:SER:HB2	2.50	0.41
1:D:73:LYS:HD3	1:D:174:PHE:CD1	2.56	0.41
1:D:75:ILE:HG22	1:D:77:VAL:HG23	2.02	0.41
2:G:352:LEU:HD22	2:G:396:MET:HE1	2.01	0.41
1:F:132:MET:HE2	1:F:139:HIS:HB2	2.02	0.41
1:C:18:ASP:HB3	1:C:20:VAL:H	1.85	0.41
1:C:73:LYS:HD3	1:C:174:PHE:CD1	2.55	0.41
1:A:73:LYS:HD3	1:A:174:PHE:CD1	2.55	0.41
1:A:100:ARG:NE	1:A:127:SER:HB2	2.35	0.41
1:C:118:ASP:C	1:C:120:GLY:H	2.29	0.41
1:A:62:HIS:HD1	1:A:114:SER:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ASP:C	1:D:120:GLY:H	2.28	0.41
1:C:154:GLU:OE1	1:C:154:GLU:HA	2.20	0.41
1:D:146:ASN:HA	1:D:147:PRO:HD3	1.77	0.41
1:A:202:ILE:HD13	1:B:205:LYS:HB3	2.02	0.41
1:B:107:TYR:CD1	1:B:137:ILE:HD11	2.55	0.41
1:C:134:TYR:CE1	2:J:365:ILE:HD13	2.56	0.41
1:E:167:LEU:C	1:E:169:PRO:HD2	2.46	0.41
1:F:91:VAL:HG13	1:F:98:GLU:CD	2.45	0.41
2:J:380:LEU:HB3	2:J:419:LEU:HD21	2.03	0.41
2:L:372:ARG:O	2:L:372:ARG:HG2	2.20	0.41
1:A:17:GLN:HB3	1:A:21:SER:HB2	2.01	0.41
1:B:150:GLN:O	1:B:154:GLU:HB2	2.21	0.41
1:C:86:ILE:HG21	1:C:86:ILE:HD13	1.71	0.41
1:C:205:LYS:HB3	1:D:202:ILE:HD13	2.03	0.41
1:E:18:ASP:CB	1:E:21:SER:H	2.34	0.41
1:A:18:ASP:HB3	1:A:20:VAL:H	1.86	0.40
1:D:64:GLN:CD	1:D:153:VAL:HG21	2.46	0.40
1:F:65:VAL:HG13	1:F:78:TRP:CD2	2.56	0.40
1:F:146:ASN:HA	1:F:147:PRO:HD3	1.89	0.40
1:A:167:LEU:C	1:A:169:PRO:HD2	2.47	0.40
1:A:177:ALA:O	1:A:181:THR:CG2	2.68	0.40
1:A:164:LEU:O	1:A:168:ILE:HG23	2.21	0.40
1:B:97:GLN:HA	1:B:100:ARG:NH1	2.37	0.40
1:E:170:MET:HE2	2:K:365:ILE:CD1	2.51	0.40
2:J:354:ARG:O	2:J:354:ARG:HG2	2.21	0.40
1:B:124:VAL:O	1:B:125:ALA:C	2.64	0.40
2:G:412:ILE:O	2:G:416:SER:HB3	2.21	0.40
1:C:164:LEU:O	1:C:168:ILE:HG23	2.21	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	188/219 (86%)	180 (96%)	6 (3%)	2 (1%)	12	40
1	B	207/219 (94%)	194 (94%)	11 (5%)	2 (1%)	13	42
1	C	194/219 (89%)	180 (93%)	10 (5%)	4 (2%)	5	27
1	D	190/219 (87%)	180 (95%)	8 (4%)	2 (1%)	12	40
1	E	187/219 (85%)	174 (93%)	11 (6%)	2 (1%)	12	40
1	F	199/219 (91%)	185 (93%)	12 (6%)	2 (1%)	13	42
2	G	69/95 (73%)	62 (90%)	5 (7%)	2 (3%)	3	21
2	H	64/95 (67%)	55 (86%)	7 (11%)	2 (3%)	3	20
2	I	64/95 (67%)	55 (86%)	7 (11%)	2 (3%)	3	20
2	J	75/95 (79%)	68 (91%)	5 (7%)	2 (3%)	4	22
2	K	63/95 (66%)	56 (89%)	5 (8%)	2 (3%)	3	19
2	L	57/95 (60%)	49 (86%)	7 (12%)	1 (2%)	7	30
All	All	1557/1884 (83%)	1438 (92%)	94 (6%)	25 (2%)	8	32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	F	18	ASP
1	B	18	ASP
1	B	125	ALA
1	C	125	ALA
1	D	18	ASP
1	E	18	ASP
1	E	125	ALA
2	H	367	ASN
2	I	367	ASN
2	J	367	ASN
2	K	367	ASN
2	L	367	ASN
1	A	125	ALA
1	C	18	ASP
1	C	192	GLY
1	D	125	ALA
1	F	125	ALA
2	G	367	ASN
2	J	379	GLU
2	K	379	GLU
2	G	379	GLU

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Mol	Chain	Res	Type
2	H	379	GLU
1	C	144	PRO
2	I	379	GLU

### 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	161/193 (83%)	145 (90%)	16 (10%)	6	24
1	B	173/193 (90%)	156 (90%)	17 (10%)	6	25
1	C	164/193 (85%)	148 (90%)	16 (10%)	6	25
1	D	163/193 (84%)	151 (93%)	12 (7%)	11	34
1	E	161/193 (83%)	147 (91%)	14 (9%)	8	29
1	F	166/193 (86%)	152 (92%)	14 (8%)	9	30
2	G	70/89 (79%)	70 (100%)	0	100	100
2	H	65/89 (73%)	64 (98%)	1 (2%)	60	77
2	I	64/89 (72%)	64 (100%)	0	100	100
2	J	73/89 (82%)	73 (100%)	0	100	100
2	K	64/89 (72%)	64 (100%)	0	100	100
2	L	58/89 (65%)	58 (100%)	0	100	100
All	All	1382/1692 (82%)	1292 (94%)	90 (6%)	14	40

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	66	ASP
1	A	73	LYS
1	A	86	ILE
1	A	89	GLU
1	A	98	GLU
1	A	103	THR

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Mol	Chain	Res	Type
1	A	127	SER
1	A	137	ILE
1	A	141	THR
1	A	148	GLN
1	A	153	VAL
1	A	172	ASN
1	A	181	THR
1	A	184	THR
1	A	190	LYS
1	B	50	SER
1	B	51	THR
1	B	55	SER
1	B	65	VAL
1	B	66	ASP
1	B	73	LYS
1	B	86	ILE
1	B	89	GLU
1	B	92	LYS
1	B	103	THR
1	B	137	ILE
1	B	141	THR
1	B	172	ASN
1	B	181	THR
1	B	184	THR
1	B	190	LYS
1	B	195	THR
1	C	64	GLN
1	C	65	VAL
1	C	66	ASP
1	C	73	LYS
1	C	86	ILE
1	C	92	LYS
1	C	95	THR
1	C	98	GLU
1	C	103	THR
1	C	137	ILE
1	C	141	THR
1	C	148	GLN
1	C	181	THR
1	C	184	THR
1	C	193	LEU
1	C	195	THR

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Mol	Chain	Res	Type
1	D	65	VAL
1	D	66	ASP
1	D	86	ILE
1	D	89	GLU
1	D	95	THR
1	D	98	GLU
1	D	103	THR
1	D	141	THR
1	D	148	GLN
1	D	172	ASN
1	D	181	THR
1	D	184	THR
1	E	65	VAL
1	E	66	ASP
1	E	86	ILE
1	E	89	GLU
1	E	95	THR
1	E	98	GLU
1	E	103	THR
1	E	127	SER
1	E	137	ILE
1	E	141	THR
1	E	172	ASN
1	E	181	THR
1	E	184	THR
1	E	193	LEU
1	F	65	VAL
1	F	66	ASP
1	F	73	LYS
1	F	86	ILE
1	F	89	GLU
1	F	95	THR
1	F	98	GLU
1	F	103	THR
1	F	114	SER
1	F	141	THR
1	F	148	GLN
1	F	172	ASN
1	F	181	THR
1	F	184	THR
2	H	397	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	46	ASN
1	A	157	HIS
1	B	46	ASN
1	B	56	ASN
1	B	129	GLN
1	C	172	ASN
1	E	46	ASN
1	E	172	ASN
1	F	12	HIS
1	F	172	ASN
2	I	367	ASN
2	K	367	ASN

### 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, 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	194/219 (88%)	-0.31	1 (0%) 87 79	48, 74, 140, 210	0
1	B	209/219 (95%)	-0.26	2 (0%) 79 67	42, 70, 114, 148	0
1	C	198/219 (90%)	-0.23	1 (0%) 87 79	46, 78, 121, 148	0
1	D	196/219 (89%)	-0.24	3 (1%) 71 57	53, 83, 135, 193	0
1	E	193/219 (88%)	-0.16	2 (1%) 79 67	54, 88, 138, 157	0
1	F	203/219 (92%)	-0.19	2 (0%) 79 67	46, 83, 122, 164	0
2	G	73/95 (76%)	0.20	1 (1%) 73 59	75, 127, 171, 193	0
2	H	68/95 (71%)	0.27	0 100 100	82, 131, 175, 188	0
2	I	68/95 (71%)	0.30	1 (1%) 71 57	91, 145, 178, 209	0
2	J	77/95 (81%)	-0.03	0 100 100	76, 118, 158, 173	0
2	K	67/95 (70%)	0.33	0 100 100	76, 141, 195, 211	0
2	L	61/95 (64%)	0.40	1 (1%) 70 56	97, 149, 190, 210	0
All	All	1607/1884 (85%)	-0.11	14 (0%) 81 70	42, 88, 164, 211	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	212	GLN	3.9
1	C	60	ILE	3.0
1	D	136	GLY	3.0
1	E	151	ALA	2.8
2	L	396	MET	2.7
1	A	152	LEU	2.7
1	F	38	GLN	2.6
2	I	358	GLU	2.4
2	G	351	ARG	2.4
1	B	82	ASN	2.3
1	D	126	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	59	GLY	2.2
1	D	97	GLN	2.1
1	B	64	GLN	2.1

## 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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	B	220	1/1	0.99	0.04	78,78,78,78	0
3	ZN	C	220	1/1	0.99	0.04	77,77,77,77	0
3	ZN	E	220	1/1	0.99	0.04	88,88,88,88	0
3	ZN	D	220	1/1	1.00	0.03	72,72,72,72	0
3	ZN	A	220	1/1	1.00	0.04	98,98,98,98	0
3	ZN	F	220	1/1	1.00	0.02	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.