



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:48 am BST

PDB ID : 3HPG  
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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

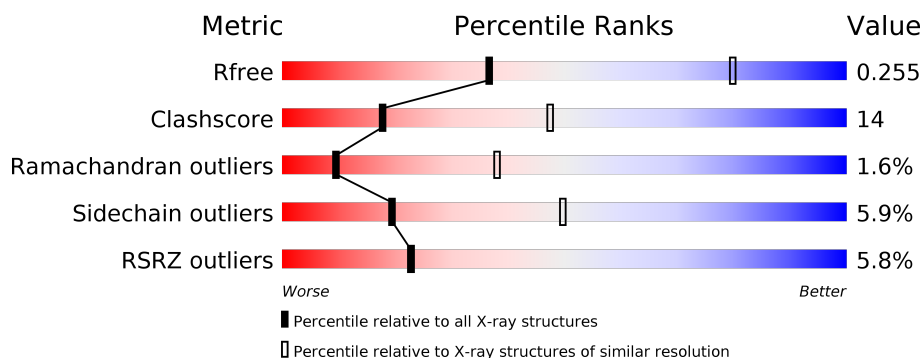
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 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	<div> <div>2%</div> <div> <div>61%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	219	<div> <div>66%</div> <div>24%</div> <div>5%</div> <div>5%</div> </div>
1	C	219	<div> <div>%</div> <div> <div>61%</div> <div>26%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	219	<div> <div>%</div> <div> <div>62%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	219	<div> <div>61%</div> <div>23%</div> <div>•</div> <div>12%</div> </div>
1	F	219	<div> <div>69%</div> <div>20%</div> <div>•</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	95	
2	H	95	
2	I	95	
2	J	95	
2	K	95	
2	L	95	

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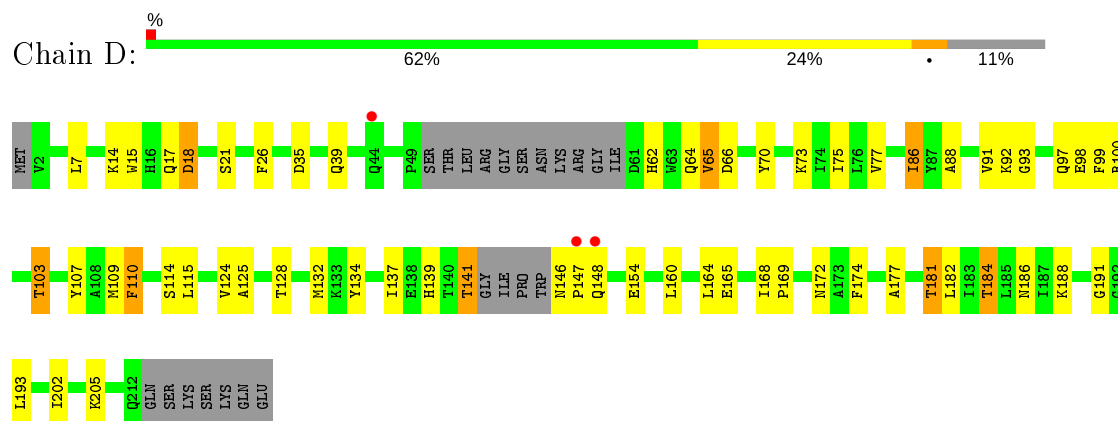
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Chain	Residue	Modelled	Actual	Comment	Reference
K	440	PHE	-	EXPRESSION TAG	UNP O75475
K	441	GLN	-	EXPRESSION TAG	UNP O75475
L	436	LEU	-	EXPRESSION TAG	UNP O75475
L	437	GLU	-	EXPRESSION TAG	UNP O75475
L	438	VAL	-	EXPRESSION TAG	UNP O75475
L	439	LEU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

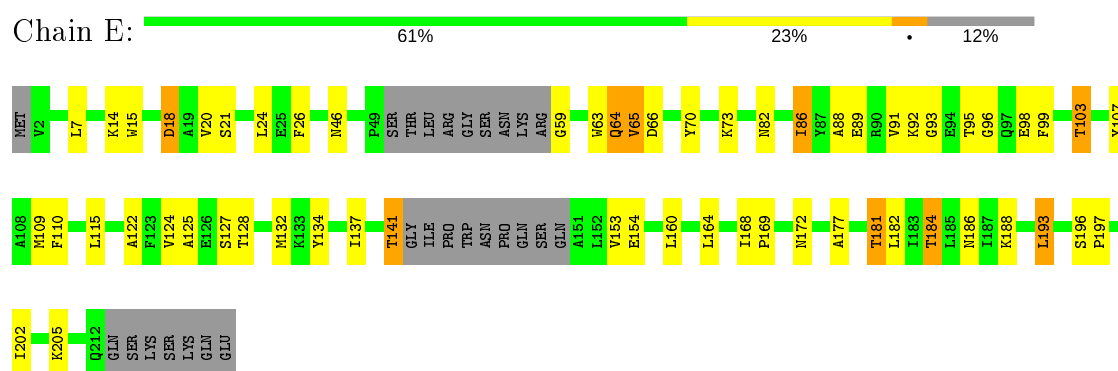
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

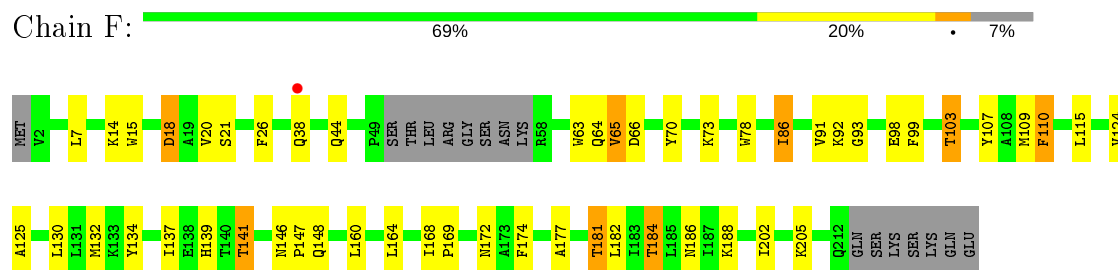




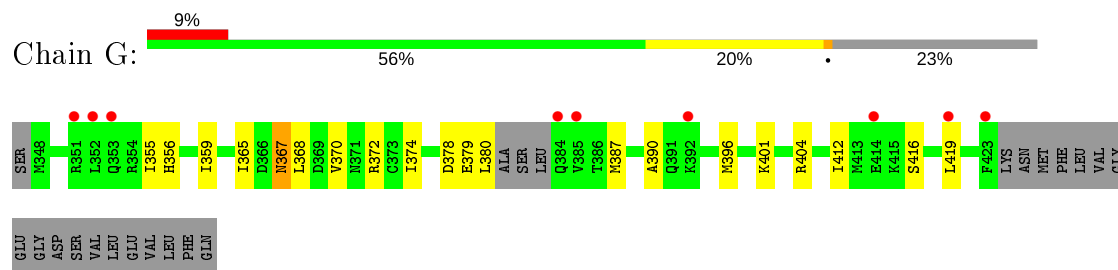
- Molecule 1: Integrase



- Molecule 1: Integrase



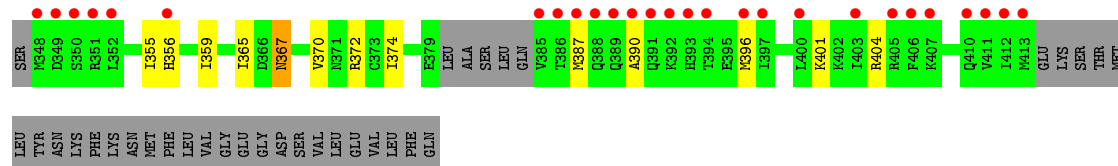
- Molecule 2: PC4 and SFRS1-interacting protein



- Molecule 2: PC4 and SFRS1-interacting protein







## 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 38.68 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.67-3.28) 99.7 (38.68-3.27)	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 0.215 , 0.255	Depositor DCC
$R_{free}$ test set	1731 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> )	0.32 , 63.8	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	0.58	0/1561	0.68	1/2116 (0.0%)
1	B	0.61	0/1682	0.72	1/2285 (0.0%)
1	C	0.56	0/1596	0.66	0/2166
1	D	0.51	0/1578	0.64	0/2142
1	E	0.52	0/1560	0.65	0/2115
1	F	0.56	0/1627	0.67	0/2213
2	G	0.40	0/607	0.50	0/807
2	H	0.40	0/554	0.51	0/736
2	I	0.36	0/552	0.50	0/733
2	J	0.40	0/633	0.53	0/844
2	K	0.40	0/553	0.50	0/733
2	L	0.37	0/501	0.49	0/666
All	All	0.52	0/13004	0.63	2/17556 (0.0%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	VAL	CB-CA-C	-5.20	101.52	111.40
1	B	65	VAL	CB-CA-C	-5.19	101.54	111.40

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	47	0
1	B	1644	0	1574	62	0
1	C	1562	0	1495	53	0
1	D	1545	0	1471	52	0
1	E	1528	0	1466	49	0
1	F	1590	0	1508	47	0
2	G	604	0	636	16	0
2	H	553	0	585	12	0
2	I	551	0	581	11	0
2	J	629	0	663	18	0
2	K	551	0	585	15	0
2	L	500	0	529	8	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	345	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 14.

All (345) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:184:THR:HA	1:E:188:LYS:HB2	1.75	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:59:GLY:C	1:B:60:ILE:HD13	2.19	0.61
1:E:20:VAL:CG1	1:E:193:LEU:HD11	2.30	0.61
1:A:168:ILE:HG12	1:A:169:PRO:HD3	1.81	0.61
1:B:150:GLN:HA	1:B:150:GLN:OE1	2.00	0.61
1:B:59:GLY:O	1:B:82:ASN:ND2	2.34	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: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
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
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:F:86:ILE:HD11	1:F:160:LEU:HD13	1.84	0.58
1:D:134:TYR:CZ	2:I:365:ILE:HD13	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:355:ILE:O	2:H:359:ILE:HG13	2.04	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
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
2:L:355:ILE:O	2:L:359:ILE:HG13	2.04	0.57
1:E:168:ILE:HG12	1:E:169:PRO:HD3	1.87	0.57
1:D:15:TRP:CE3	1:E:184:THR:HG22	2.40	0.57
2:G:378:ASP:C	2:G:380:LEU:H	2.08	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:E:154:GLU:OE1	1:E:154:GLU:HA	2.05	0.56
1:E:168:ILE:N	1:E:169:PRO:CD	2.69	0.56
1:B:134:TYR:CE1	2:G:365:ILE:HD13	2.39	0.56
2:H:401:LYS:HG3	2:H:404:ARG:HH21	1.70	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
1:C:109:MET:HE1	1:D:110:PHE:CZ	2.41	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
2:J:378:ASP:C	2:J:380:LEU:H	2.11	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
2:K:378:ASP:C	2:K:380:LEU:H	2.10	0.54
1:E:109:MET:HE1	1:F:110:PHE:CZ	2.43	0.54
1:F:65:VAL:CG2	1:F:115:LEU:HD11	2.37	0.54
1:E:110:PHE:CZ	1:F:109:MET:HE1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:378:ASP:C	2:I:380:LEU:H	2.11	0.54
2:I:401:LYS:HG3	2:I:404:ARG:HH21	1.72	0.54
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:H:378:ASP:C	2:H:380:LEU:H	2.12	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: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:168:ILE:N	1:B:169:PRO:CD	2.73	0.52
1:B:65:VAL:CG2	1:B:115:LEU:HD11	2.39	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
1:A:107:TYR:CD1	1:A:137:ILE:HD11	2.45	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:C:30:ARG:HD2	1:D:35:ASP:CG	2.31	0.51
1:C:110:PHE:CZ	1:D:109:MET:HE1	2.45	0.51
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: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: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
1:C:132:MET:HE3	1:C:137:ILE:HB	1.93	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:HA	1:D:154:GLU:OE1	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
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:109:MET:HE1	1:B:110:PHE:CZ	2.47	0.50
1:A:18:ASP:HB2	1:A:21:SER:H	1.77	0.50
1:A:154:GLU:OE1	1:A:154:GLU:HA	2.11	0.50
1:B:107:TYR:HD1	1:B:137:ILE:HD11	1.77	0.50
1:B:59:GLY:O	1:B:60:ILE:HD13	2.12	0.49
1:A:41:ASP:O	1:A:45:GLU:HG3	2.12	0.49
2:H:356:HIS:CD2	2:H:396:MET:HA	2.47	0.49
1:C:134:TYR:CZ	2:J:365:ILE:HD13	2.48	0.49
2:L:370:VAL:O	2:L:374:ILE:HG13	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
2:I:372:ARG:HG2	2:I:372:ARG:O	2.13	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: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
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:H:372:ARG:O	2:H:372:ARG:HG2	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
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
2:I:365:ILE:C	2:I:367:ASN:H	2.18	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
1:A:70:TYR:O	1:A:73:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:365:ILE:C	2:G:367:ASN:H	2.18	0.47
2:I:401:LYS:HA	2:I:404:ARG:HD2	1.96	0.47
1:B:18:ASP:HB2	1:B:21:SER:H	1.79	0.47
1:E:196:SER:HB2	1:E:197:PRO:HD2	1.96	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
1:B:145:TRP:CE3	1:B:146:ASN:HA	2.49	0.47
1:D:132:MET:HE3	1:D:137:ILE:HB	1.97	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:100:ARG:CZ	1:A:127:SER:HB2	2.46	0.46
1:A:91:VAL:HG12	1:A:93:GLY:N	2.31	0.46
2:H:365:ILE:C	2:H:367:ASN:H	2.19	0.46
2:K:372:ARG:O	2:K:372:ARG:HG2	2.16	0.46
1:B:132:MET:HE3	1:B:137:ILE:HB	1.98	0.46
1:B:154:GLU:HA	1:B:154:GLU:OE1	2.16	0.46
2:K:365:ILE:C	2:K:367:ASN:H	2.18	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:D:132:MET:HE2	1:D:139:HIS:HB2	1.98	0.46
1:D:7:LEU:HD22	1:D:26:PHE:CE1	2.51	0.46
1:B:107:TYR:CD1	1:B:112:PRO:HD2	2.51	0.46
1:B:30:ARG:NH2	1:B:60:ILE:HD11	2.30	0.46
1:B:91:VAL:HG13	1:B:98:GLU:CD	2.36	0.45
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
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
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: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:B:100:ARG:CZ	1:B:127:SER:HB2	2.47	0.45
1:B:88:ALA:H	1:B:182:LEU:HD11	1.80	0.45
1:A:15:TRP:HE3	1:F:184:THR:HG22	1.82	0.45
2:G:378:ASP:C	2:G:380:LEU:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:380:LEU:HB3	2:K:419:LEU:HD21	1.99	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
1:B:109:MET:HB3	1:B:109:MET:HE3	1.80	0.44
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:CD2	1:F:70:TYR:O	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: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:A:110:PHE:CZ	1:B:109:MET:HE1	2.52	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:F:132:MET:HE3	1:F:137:ILE:HB	1.98	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: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:132:MET:HE2	1:F:139:HIS:HB2	1.99	0.43
1:F:124:VAL:CG2	1:F:141:THR:HG21	2.46	0.43
1:E:64:GLN:CD	1:E:153:VAL:HG21	2.39	0.43
1:E:91:VAL:HG12	1:E:93:GLY:N	2.34	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:HG2	2:J:372:ARG:O	2.18	0.43
2:L:365:ILE:C	2:L:367:ASN:H	2.22	0.43
1:A:15:TRP:CE3	1:F:184:THR:HG22	2.54	0.43
1:D:97:GLN:HA	1:D:100:ARG:NH1	2.33	0.43
1:E:132:MET:HE3	1:E:137:ILE:HB	1.99	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:164:LEU:O	1:F:168:ILE:HG23	2.19	0.43
1:F:73:LYS:HD3	1:F:174:PHE:CD1	2.54	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:D:62:HIS:HD1	1:D:114:SER:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:ASP:HB3	1:F:20:VAL:H	1.82	0.43
2:K:378:ASP:C	2:K:380:LEU:N	2.73	0.42
1:B:86:ILE:HG21	1:B:86:ILE:HD13	1.67	0.42
1:C:91:VAL:HG13	1:C:98:GLU:CD	2.39	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:D:91:VAL:HG13	1:D:98:GLU:CD	2.40	0.42
1:E:96:GLY:HA2	1:E:122:ALA:HB1	2.00	0.42
1:B:59:GLY:C	1:B:60:ILE:CD1	2.85	0.42
1:D:65:VAL:HG21	1:D:115:LEU:HD21	2.02	0.42
2:J:365:ILE:C	2:J:367:ASN:H	2.21	0.42
1:A:91:VAL:HG13	1:A:98:GLU:CD	2.39	0.42
1:E:88:ALA:H	1:E:182:LEU:HD11	1.85	0.42
1:A:184:THR:HG22	1:F:15:TRP:HE3	1.85	0.42
1:A:150:GLN:O	1:A:154:GLU:HB2	2.20	0.42
2:J:378:ASP:C	2:J:380:LEU:N	2.73	0.42
2:L:372:ARG:HG2	2:L:372:ARG:O	2.20	0.42
1:C:40:CYS:O	1:C:44:GLN:HG2	2.20	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:100:ARG:CZ	1:C:127:SER:HB2	2.50	0.41
1:C:97:GLN:HA	1:C:100:ARG:NH1	2.35	0.41
1:C:132:MET:HE2	1:C:139:HIS:HB2	2.01	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
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:100:ARG:NE	1:A:127:SER:HB2	2.35	0.41
1:A:73:LYS:HD3	1:A:174:PHE:CD1	2.55	0.41
1:A:62:HIS:HD1	1:A:114:SER:HB2	1.86	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
2:I:378:ASP:C	2:I:380:LEU:N	2.73	0.41
1:A:202:ILE:HD13	1:B:205:LYS:HB3	2.02	0.41
1:C:134:TYR:CE1	2:J:365:ILE:HD13	2.56	0.41
1:B:107:TYR:CD1	1:B:137:ILE:HD11	2.55	0.41
2:J:380:LEU:HB3	2:J:419:LEU:HD21	2.03	0.41
1:A:17:GLN:HB3	1:A:21:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLN:O	1:B:154:GLU:HB2	2.21	0.41
1:C:205:LYS:HB3	1:D:202:ILE:HD13	2.03	0.41
1:C:86:ILE:HG21	1:C:86:ILE:HD13	1.71	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:F:146:ASN:HA	1:F:147:PRO:HD3	1.89	0.40
1:F:65:VAL:HG13	1:F:78:TRP:CD2	2.56	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
2:J:354:ARG:HG2	2:J:354:ARG:O	2.21	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
1:C:172:ASN:HD22	1:C:172:ASN:C	2.24	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%)	14	46
1	B	207/219 (94%)	194 (94%)	11 (5%)	2 (1%)	15	48
1	C	194/219 (89%)	180 (93%)	10 (5%)	4 (2%)	7	33
1	D	190/219 (87%)	180 (95%)	8 (4%)	2 (1%)	14	46
1	E	187/219 (85%)	174 (93%)	11 (6%)	2 (1%)	14	46
1	F	199/219 (91%)	185 (93%)	12 (6%)	2 (1%)	15	48
2	G	69/95 (73%)	62 (90%)	5 (7%)	2 (3%)	4	25
2	H	64/95 (67%)	55 (86%)	7 (11%)	2 (3%)	4	24
2	I	64/95 (67%)	55 (86%)	7 (11%)	2 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	75/95 (79%)	68 (91%)	5 (7%)	2 (3%)	5	26
2	K	63/95 (66%)	56 (89%)	5 (8%)	2 (3%)	4	23
2	L	57/95 (60%)	49 (86%)	7 (12%)	1 (2%)	8	36
All	All	1557/1884 (83%)	1438 (92%)	94 (6%)	25 (2%)	9	38

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
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%)	148 (92%)	13 (8%)	11	36
1	B	173/193 (90%)	157 (91%)	16 (9%)	9	31
1	C	164/193 (85%)	151 (92%)	13 (8%)	12	37
1	D	163/193 (84%)	151 (93%)	12 (7%)	13	40
1	E	161/193 (83%)	146 (91%)	15 (9%)	9	30
1	F	166/193 (86%)	153 (92%)	13 (8%)	12	38
2	G	70/89 (79%)	70 (100%)	0	100	100
2	H	65/89 (73%)	65 (100%)	0	100	100
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%)	1300 (94%)	82 (6%)	19	50

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	65	VAL
1	A	66	ASP
1	A	86	ILE
1	A	92	LYS
1	A	103	THR
1	A	127	SER
1	A	141	THR
1	A	148	GLN
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	53	ARG
1	B	55	SER
1	B	64	GLN
1	B	65	VAL
1	B	66	ASP

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Mol	Chain	Res	Type
1	B	86	ILE
1	B	92	LYS
1	B	103	THR
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	86	ILE
1	C	92	LYS
1	C	103	THR
1	C	141	THR
1	C	148	GLN
1	C	172	ASN
1	C	181	THR
1	C	184	THR
1	C	193	LEU
1	C	195	THR
1	D	64	GLN
1	D	65	VAL
1	D	66	ASP
1	D	86	ILE
1	D	92	LYS
1	D	103	THR
1	D	110	PHE
1	D	141	THR
1	D	148	GLN
1	D	172	ASN
1	D	181	THR
1	D	184	THR
1	E	64	GLN
1	E	65	VAL
1	E	66	ASP
1	E	86	ILE
1	E	89	GLU
1	E	92	LYS
1	E	95	THR
1	E	98	GLU

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Mol	Chain	Res	Type
1	E	103	THR
1	E	127	SER
1	E	141	THR
1	E	172	ASN
1	E	181	THR
1	E	184	THR
1	E	193	LEU
1	F	64	GLN
1	F	65	VAL
1	F	66	ASP
1	F	86	ILE
1	F	92	LYS
1	F	98	GLU
1	F	103	THR
1	F	110	PHE
1	F	141	THR
1	F	148	GLN
1	F	172	ASN
1	F	181	THR
1	F	184	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	172	ASN
1	E	46	ASN
1	F	172	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 carbohydrates 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

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.14	5 (2%) 56 52	48, 74, 140, 210	0
1	B	209/219 (95%)	-0.23	0 100 100	42, 70, 114, 148	0
1	C	198/219 (90%)	-0.14	3 (1%) 73 71	46, 78, 121, 148	0
1	D	196/219 (89%)	-0.14	3 (1%) 73 71	53, 83, 135, 193	0
1	E	193/219 (88%)	-0.16	0 100 100	54, 88, 138, 157	0
1	F	203/219 (92%)	-0.16	1 (0%) 91 91	46, 83, 122, 164	0
2	G	73/95 (76%)	0.78	9 (12%) 4 4	75, 127, 171, 193	0
2	H	68/95 (71%)	0.99	13 (19%) 1 1	82, 131, 175, 188	0
2	I	68/95 (71%)	0.94	10 (14%) 2 2	91, 145, 179, 209	0
2	J	77/95 (81%)	0.44	7 (9%) 9 10	76, 118, 158, 173	0
2	K	67/95 (70%)	1.18	16 (23%) 0 0	76, 141, 195, 211	0
2	L	61/95 (64%)	1.76	27 (44%) 0 0	97, 149, 190, 210	0
All	All	1607/1884 (85%)	0.13	94 (5%) 23 23	42, 88, 164, 211	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	386	THR	6.4
2	K	423	PHE	5.6
2	L	385	VAL	5.1
2	L	396	MET	5.0
2	I	391	GLN	4.9
2	G	423	PHE	4.7
2	L	387	MET	4.6
2	H	410	GLN	4.4
2	L	391	GLN	4.4
1	A	31	THR	4.3
2	I	405	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
2	L	393	HIS	4.1
2	K	426	MET	4.1
2	K	410	GLN	4.1
2	K	419	LEU	4.1
2	I	390	ALA	3.9
2	J	405	ARG	3.9
2	K	412	ILE	3.7
2	L	410	GLN	3.6
2	I	386	THR	3.6
2	L	351	ARG	3.6
1	D	148	GLN	3.5
2	G	352	LEU	3.5
2	I	418	MET	3.5
2	K	397	ILE	3.5
2	L	390	ALA	3.5
2	H	386	THR	3.4
2	K	414	GLU	3.3
2	L	412	ILE	3.3
2	H	385	VAL	3.3
2	K	418	MET	3.2
2	K	416	SER	3.2
2	K	352	LEU	3.2
2	K	409	SER	3.2
2	H	416	SER	3.1
2	H	391	GLN	3.1
2	G	384	GLN	3.0
2	L	388	GLN	3.0
2	K	411	VAL	3.0
2	L	349	ASP	2.9
1	A	35	ASP	2.9
1	A	148	GLN	2.8
2	G	385	VAL	2.8
2	L	352	LEU	2.8
2	J	420	TYR	2.8
2	L	397	ILE	2.8
2	L	350	SER	2.8
2	L	405	ARG	2.8
2	L	389	GLN	2.7
2	J	419	LEU	2.7
1	C	38	GLN	2.6
2	K	347	SER	2.6
2	L	413	MET	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	348	MET	2.5
1	C	30	ARG	2.5
2	H	392	LYS	2.5
2	L	411	VAL	2.5
2	L	356	HIS	2.5
1	C	34	GLU	2.4
2	G	414	GLU	2.4
2	J	421	ASN	2.4
2	I	412	ILE	2.4
2	I	371	ASN	2.3
2	L	403	ILE	2.3
2	H	387	MET	2.3
2	H	380	LEU	2.3
2	L	400	LEU	2.3
1	A	39	GLN	2.3
2	G	419	LEU	2.3
2	G	353	GLN	2.3
2	L	406	PHE	2.2
2	L	394	THR	2.2
2	I	392	LYS	2.2
2	I	407	LYS	2.2
2	H	396	MET	2.1
1	D	147	PRO	2.1
2	L	407	LYS	2.1
1	D	44	GLN	2.1
2	H	388	GLN	2.1
2	G	392	LYS	2.1
2	K	421	ASN	2.1
2	H	411	VAL	2.1
2	K	374	ILE	2.1
2	K	422	LYS	2.1
2	J	394	THR	2.1
2	J	390	ALA	2.1
2	G	351	ARG	2.1
2	L	392	LYS	2.1
1	F	38	GLN	2.1
2	J	418	MET	2.1
2	H	401	LYS	2.0
2	I	388	GLN	2.0
2	H	417	THR	2.0
1	A	34	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	220	1/1	0.98	0.16	78,78,78,78	0
3	ZN	E	220	1/1	0.98	0.13	88,88,88,88	0
3	ZN	C	220	1/1	0.98	0.17	77,77,77,77	0
3	ZN	A	220	1/1	0.99	0.15	98,98,98,98	0
3	ZN	D	220	1/1	0.99	0.13	72,72,72,72	0
3	ZN	F	220	1/1	1.00	0.13	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.