



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:17 AM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

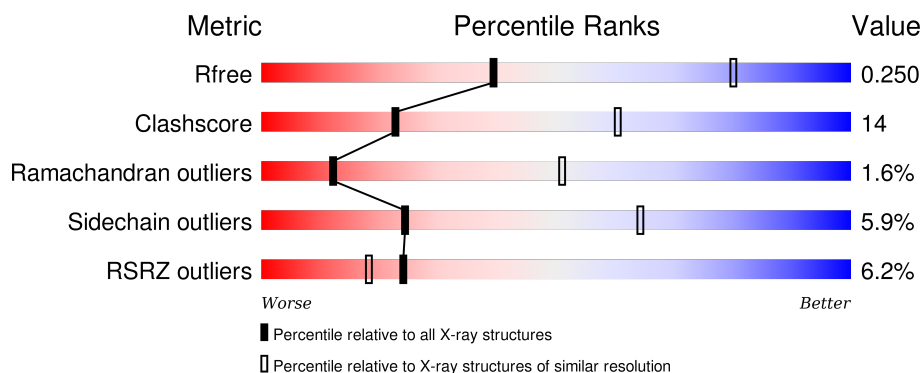
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	219	<div> <div></div> <div> <div>66%</div> <div>24%</div> <div>5%</div> <div>5%</div> </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></div> <div> <div>61%</div> <div>23%</div> <div>•</div> <div>12%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	219	
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

Continued on next page...

Continued from previous page...

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

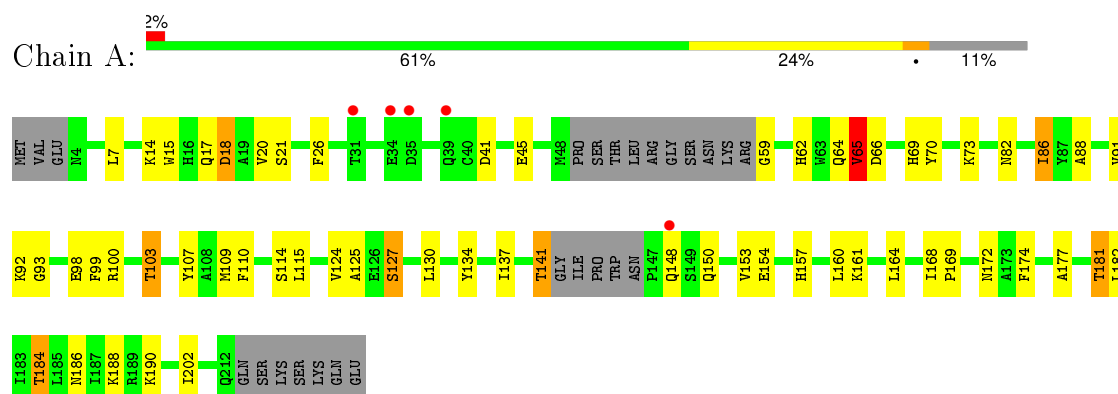
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

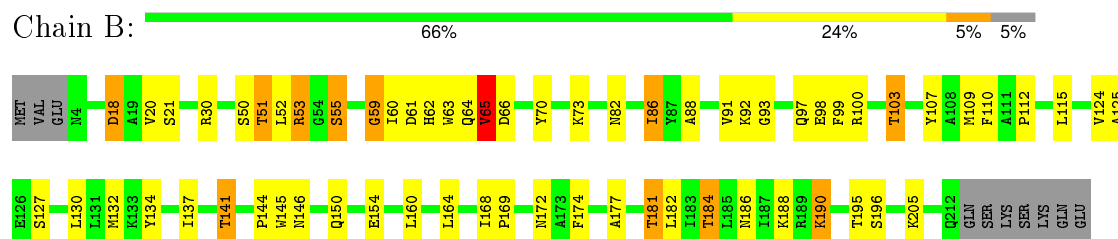
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

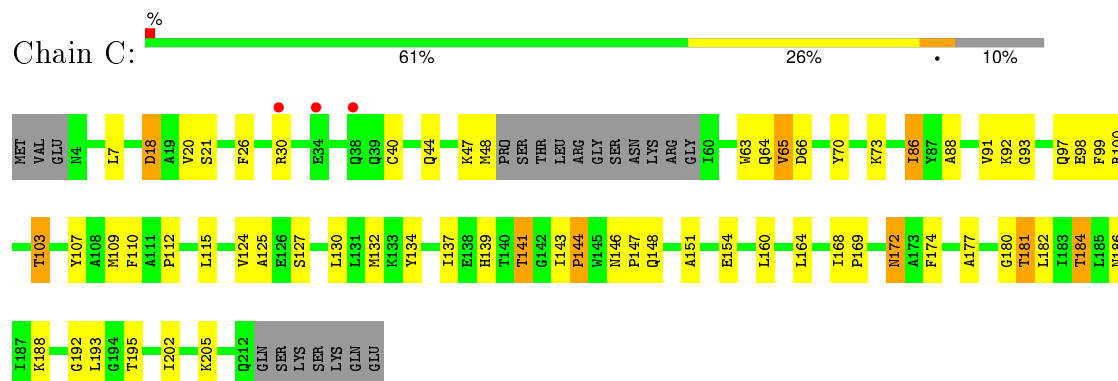
• Molecule 1: Integrase



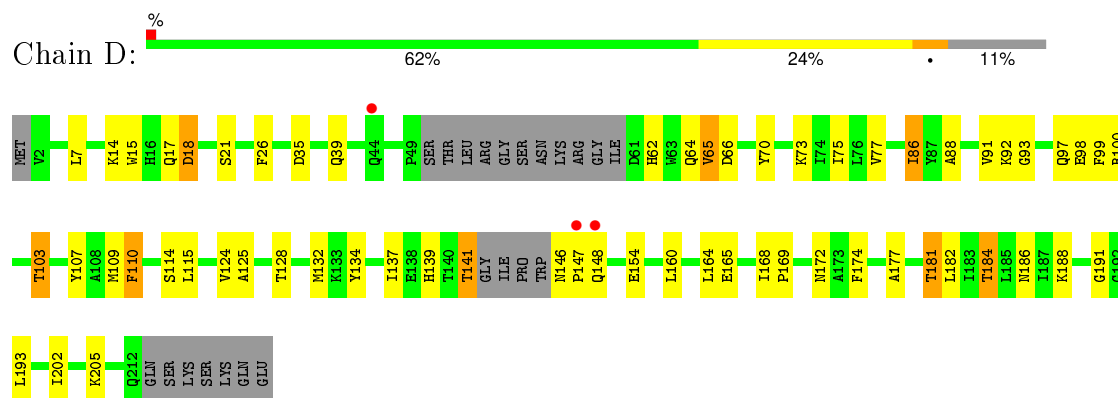
• Molecule 1: Integrase



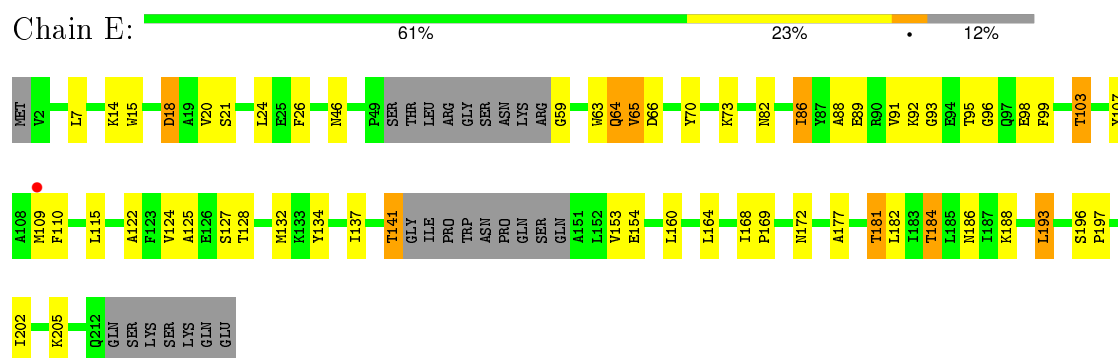
• Molecule 1: Integrase



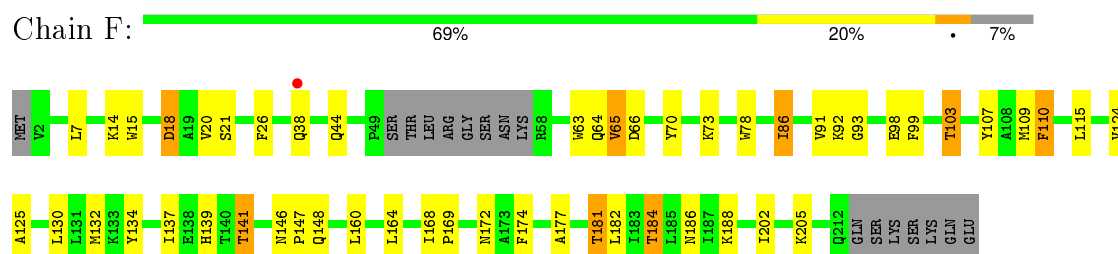
• Molecule 1: Integrase



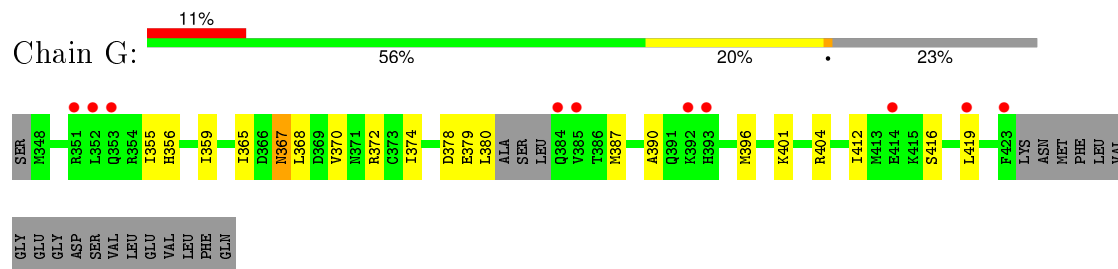
- Molecule 1: Integrase



- Molecule 1: Integrase

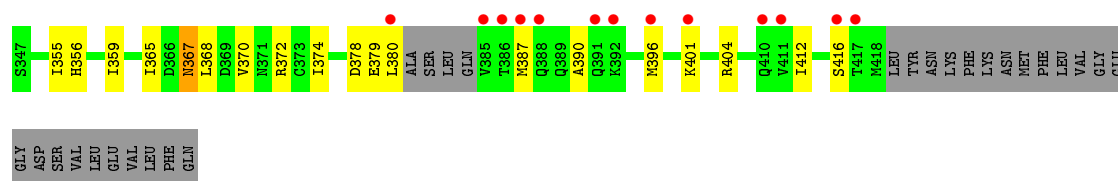


- Molecule 2: PC4 and SFRS1-interacting protein

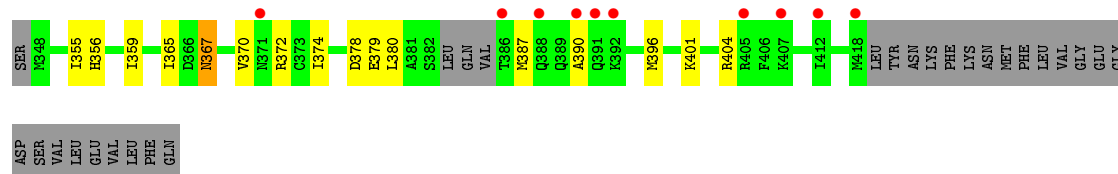


- Molecule 2: PC4 and SFRS1-interacting protein

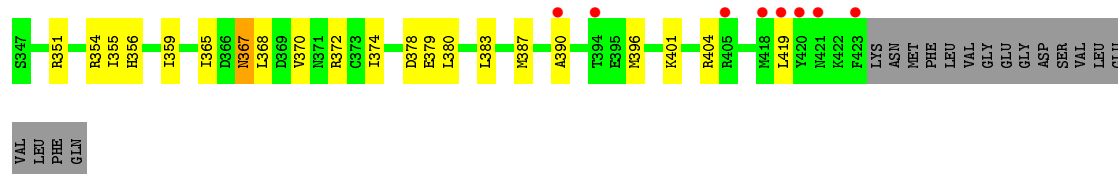




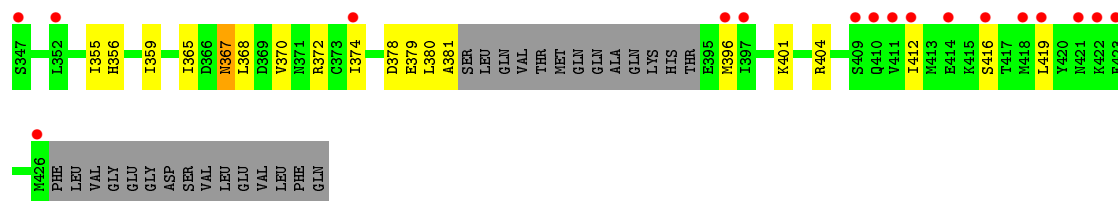
• Molecule 2: PC4 and SFRS1-interacting protein



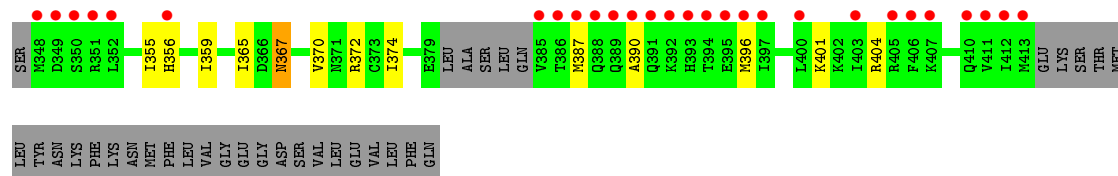
• Molecule 2: PC4 and SFRS1-interacting protein



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.253 0.206 , 0.250	Depositor DCC
R_{free} test set	1717 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.8	EDS
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 34296 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12792	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

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

Continued on next page...

Continued from previous page...

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:E:177:ALA:O	1:E:181:THR:HG23	1.93	0.68
1:D:184:THR:HA	1:D:188:LYS:HB2	1.76	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

Continued on next page...

Continued from previous page...

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
2:J:380:LEU:HD23	2:J:419:LEU:HD23	1.78	0.64
1:C:182:LEU:O	1:C:186:ASN:HB2	1.96	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:D:14:LYS:HG2	1:F:134:TYR:CE1	2.37	0.60
1:C:184:THR:HA	1:C:188:LYS:HB2	1.84	0.60
1:B:99:PHE:O	1:B:103:THR:HG23	2.02	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: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
1:F:168:ILE:HG12	1:F:169:PRO:HD3	1.84	0.58
1:B:86:ILE:HD11	1:B:160:LEU:HD13	1.84	0.58
1:A:134:TYR:CE1	2:H:365:ILE:HD13	2.38	0.58
2:I:355:ILE:O	2:I:359:ILE:HG13	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:380:LEU:HD23	2:G:419:LEU:HD23	1.84	0.58
1:C:30:ARG:HD2	1:D:35:ASP:OD2	2.04	0.58
1:A:107:TYR:HD1	1:A:137:ILE:HD11	1.69	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:188:LYS:HE2	1:E:15:TRP:CD1	2.39	0.57
1:D:107:TYR:HD1	1:D:137:ILE:HD11	1.68	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: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
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:B:134:TYR:CE1	2:G:365:ILE:HD13	2.39	0.56
1:E:168:ILE:N	1:E:169:PRO:CD	2.69	0.56
1:E:154:GLU:OE1	1:E:154:GLU:HA	2.05	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
2:J:401:LYS:HG3	2:J:404:ARG:HH21	1.70	0.55
1:B:55:SER:HB2	1:B:62:HIS:CE1	2.41	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:C:109:MET:HE1	1:D:110:PHE:CZ	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:65:VAL:CG2	1:E:115:LEU:HD11	2.37	0.54
2:K:378:ASP:C	2:K:380:LEU:H	2.10	0.54
1:E:59:GLY:O	1:E:82:ASN:HB2	2.07	0.54
2:I:356:HIS:CD2	2:I:396:MET:HA	2.43	0.54
1:F:65:VAL:CG2	1:F:115:LEU:HD11	2.37	0.54
1:E:109:MET:HE1	1:F:110:PHE:CZ	2.43	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

Continued on next page...

Continued from previous page...

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:D:164:LEU:HD23	1:D:181:THR:CG2	2.37	0.53
1:A:164:LEU:HD23	1:A:181:THR:CG2	2.39	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
1:B:134:TYR:CD1	1:F:14:LYS:HE3	2.44	0.52
1:A:107:TYR:CD1	1:A:137:ILE:HD11	2.45	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: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
1:C:107:TYR:HD1	1:C:137:ILE:HD11	1.74	0.51
2:J:401:LYS:HA	2:J:404:ARG:HD2	1.93	0.51
2:I:387:MET:HA	2:I:390:ALA:HB3	1.92	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
2:L:387:MET:HA	2:L:390:ALA:HB3	1.93	0.51
1:E:202:ILE:HD13	1:F:205:LYS:HB3	1.92	0.51
1:C:18:ASP:HB2	1:C:21:SER:H	1.75	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
2:J:351:ARG:HD3	2:J:383:LEU:HD11	1.93	0.51
1:D:154:GLU:HA	1:D:154:GLU:OE1	2.11	0.51
2:G:401:LYS:HA	2:G:404:ARG:HD2	1.92	0.50

Continued on next page...

Continued from previous page...

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: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
2:H:387:MET:HA	2:H:390:ALA:HB3	1.93	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
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:C:70:TYR:O	1:C:73:LYS:HB2	2.13	0.49
1:B:91:VAL:HG12	1:B:93:GLY:N	2.27	0.49
1:F:168:ILE:N	1:F:169:PRO:CD	2.76	0.49
1:C:164:LEU:HD23	1:C:181:THR:CG2	2.41	0.49
1:B:18:ASP:OD2	1:B:53:ARG:CZ	2.61	0.49
1:F:130:LEU:HD13	2:K:368:LEU:HD13	1.95	0.48
2:I:372:ARG:HG2	2:I:372:ARG:O	2.13	0.48
1:D:18:ASP:HB2	1:D:21:SER:H	1.78	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:D:168:ILE:N	1:D:169:PRO:CD	2.77	0.47
1:B:164:LEU:HD23	1:B:181:THR:CG2	2.41	0.47
1:E:24:LEU:HD21	1:E:193:LEU:HD21	1.96	0.47
2:I:365:ILE:C	2:I:367:ASN:H	2.18	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
1:A:70:TYR:O	1:A:73:LYS:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:365:ILE:C	2:G:367:ASN:H	2.18	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: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:D:132:MET:HE3	1:D:137:ILE:HB	1.97	0.47
1:B:145:TRP:CE3	1:B:146:ASN:HA	2.49	0.47
1:E:164:LEU:HD23	1:E:181:THR:CG2	2.42	0.46
2:L:401:LYS:HA	2:L:404:ARG:HD2	1.97	0.46
2:G:370:VAL:O	2:G:374:ILE:HG13	2.15	0.46
1:C:91:VAL:HG12	1:C:93:GLY:N	2.30	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: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:B:132:MET:HE3	1:B:137:ILE:HB	1.98	0.46
1:E:63:TRP:O	1:E:115:LEU:HD12	2.15	0.46
1:A:88:ALA:H	1:A:182:LEU:HD11	1.80	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: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
2:H:401:LYS:HA	2:H:404:ARG:HD2	1.98	0.45
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
1:D:164:LEU:O	1:D:168:ILE:HG23	2.16	0.45
1:F:99:PHE:O	1:F:103:THR:CG2	2.63	0.45
1:E:128:THR:O	1:E:132:MET:HG2	2.16	0.45
1:C:180:GLY:O	1:C:184:THR:HG23	2.15	0.45
1:C:88:ALA:H	1:C:182:LEU:HD11	1.81	0.45
1:B:70:TYR:O	1:B:73:LYS:HB2	2.16	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: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:K:380:LEU:HB3	2:K:419:LEU:HD21	1.99	0.45
2:G:378:ASP:C	2:G:380:LEU:N	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:CZ	1:B:127:SER:HB2	2.47	0.45
1:E:65:VAL:HG21	1:E:115:LEU:HD21	1.98	0.45
1:C:146:ASN:HA	1:C:147:PRO:HD3	1.89	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:B:109:MET:HB3	1:B:109:MET:HE3	1.80	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:F:107:TYR:CD1	1:F:137:ILE:HD11	2.50	0.44
1:D:17:GLN:HB3	1:D:21:SER:HB2	2.00	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:C:143:ILE:HA	1:C:144:PRO:HD2	1.88	0.43
1:A:7:LEU:HD22	1:A:26:PHE:CE1	2.54	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:D:128:THR:O	1:D:132:MET:HG2	2.18	0.43
1:F:132:MET:HE2	1:F:139:HIS:HB2	1.99	0.43
1:E:91:VAL:HG12	1:E:93:GLY:N	2.34	0.43
1:E:64:GLN:CD	1:E:153:VAL:HG21	2.39	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
1:C:202:ILE:HD13	1:D:205:LYS:HB3	2.00	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:F:164:LEU:O	1:F:168:ILE:HG23	2.19	0.43
2:K:412:ILE:O	2:K:416:SER:HB3	2.19	0.43
1:D:193:LEU:HD23	1:D:193:LEU:HA	1.62	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
1:E:7:LEU:HD22	1:E:26:PHE:CE1	2.53	0.43
1:F:18:ASP:HB3	1:F:20:VAL:H	1.82	0.43
1:D:62:HIS:HD1	1:D:114:SER:HB2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:HIS:O	1:A:161:LYS:HE2	2.19	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:F:63:TRP:O	1:F:115:LEU:HD12	2.19	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:D:91:VAL:HG13	1:D:98:GLU:CD	2.40	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:B:59:GLY:C	1:B:60:ILE:CD1	2.85	0.42
2:J:365:ILE:C	2:J:367:ASN:H	2.21	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:A:91:VAL:HG13	1:A:98:GLU:CD	2.39	0.42
2:J:378:ASP:C	2:J:380:LEU:N	2.73	0.42
1:A:150:GLN:O	1:A:154:GLU:HB2	2.20	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: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: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: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:A:62:HIS:HD1	1:A:114:SER:HB2	1.86	0.41
2:I:378:ASP:C	2:I:380:LEU:N	2.73	0.41
1:D:146:ASN:HA	1:D:147:PRO:HD3	1.77	0.41
1:C:154:GLU:OE1	1:C:154:GLU:HA	2.20	0.41
1:C:134:TYR:CE1	2:J:365:ILE:HD13	2.56	0.41
2:J:380:LEU:HB3	2:J:419:LEU:HD21	2.03	0.41
1:B:107:TYR:CD1	1:B:137:ILE:HD11	2.55	0.41
1:A:202:ILE:HD13	1:B:205:LYS:HB3	2.02	0.41
1:B:150:GLN:O	1:B:154:GLU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ILE:HD13	1:C:86:ILE:HG21	1.71	0.41
1:A:17:GLN:HB3	1:A:21:SER:HB2	2.01	0.41
1:E:18:ASP:CB	1:E:21:SER:H	2.34	0.41
1:C:205:LYS:HB3	1:D:202:ILE:HD13	2.03	0.41
1:F:65:VAL:HG13	1:F:78:TRP:CD2	2.56	0.40
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: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%)	17	59
1	B	207/219 (94%)	194 (94%)	11 (5%)	2 (1%)	19	61
1	C	194/219 (89%)	180 (93%)	10 (5%)	4 (2%)	9	44
1	D	190/219 (87%)	180 (95%)	8 (4%)	2 (1%)	17	59
1	E	187/219 (85%)	174 (93%)	11 (6%)	2 (1%)	17	59
1	F	199/219 (91%)	185 (93%)	12 (6%)	2 (1%)	19	61
2	G	69/95 (73%)	62 (90%)	5 (7%)	2 (3%)	6	35
2	H	64/95 (67%)	55 (86%)	7 (11%)	2 (3%)	5	33
2	I	64/95 (67%)	55 (86%)	7 (11%)	2 (3%)	5	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	75/95 (79%)	68 (91%)	5 (7%)	2 (3%)	6	37
2	K	63/95 (66%)	56 (89%)	5 (8%)	2 (3%)	5	32
2	L	57/95 (60%)	49 (86%)	7 (12%)	1 (2%)	11	49
All	All	1557/1884 (83%)	1438 (92%)	94 (6%)	25 (2%)	12	51

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%)	15	49
1	B	173/193 (90%)	157 (91%)	16 (9%)	11	41
1	C	164/193 (85%)	151 (92%)	13 (8%)	15	51
1	D	163/193 (84%)	151 (93%)	12 (7%)	17	54
1	E	161/193 (83%)	146 (91%)	15 (9%)	11	40
1	F	166/193 (86%)	153 (92%)	13 (8%)	16	51
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%)	24	64

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	194/219 (88%)	-0.12	5 (2%) 59 51	48, 74, 140, 210	0
1	B	209/219 (95%)	-0.21	0 100 100	42, 70, 114, 148	0
1	C	198/219 (90%)	-0.12	3 (1%) 76 68	46, 78, 121, 148	0
1	D	196/219 (89%)	-0.12	3 (1%) 76 68	53, 83, 135, 193	0
1	E	193/219 (88%)	-0.14	1 (0%) 91 89	54, 88, 138, 157	0
1	F	203/219 (92%)	-0.14	1 (0%) 91 89	46, 83, 122, 164	0
2	G	73/95 (76%)	0.83	10 (13%) 4 3	75, 127, 171, 193	0
2	H	68/95 (71%)	1.04	13 (19%) 2 1	82, 131, 175, 188	0
2	I	68/95 (71%)	0.97	10 (14%) 3 2	91, 145, 179, 209	0
2	J	77/95 (81%)	0.47	8 (10%) 8 6	76, 118, 158, 173	0
2	K	67/95 (70%)	1.23	17 (25%) 1 1	76, 141, 195, 211	0
2	L	61/95 (64%)	1.82	28 (45%) 0 0	97, 149, 190, 210	0
All	All	1607/1884 (85%)	0.16	99 (6%) 24 18	42, 88, 164, 211	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	386	THR	6.5
2	K	423	PHE	5.7
2	L	385	VAL	5.3
2	L	396	MET	5.2
2	I	391	GLN	5.0
2	G	423	PHE	4.9
2	L	387	MET	4.6
2	I	405	ARG	4.5
2	H	410	GLN	4.4
2	L	391	GLN	4.4
1	A	31	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	426	MET	4.3
2	K	419	LEU	4.2
2	L	393	HIS	4.2
2	K	410	GLN	4.2
2	J	405	ARG	4.0
2	I	390	ALA	3.9
2	I	386	THR	3.8
2	L	351	ARG	3.7
2	K	412	ILE	3.7
2	L	410	GLN	3.7
1	D	148	GLN	3.6
2	H	386	THR	3.6
2	G	352	LEU	3.6
2	I	418	MET	3.6
2	K	397	ILE	3.5
2	L	390	ALA	3.5
2	H	385	VAL	3.5
2	L	412	ILE	3.4
2	K	414	GLU	3.4
2	K	416	SER	3.4
2	K	418	MET	3.4
2	K	352	LEU	3.2
2	H	416	SER	3.2
2	K	409	SER	3.2
2	H	391	GLN	3.2
2	G	384	GLN	3.1
2	L	349	ASP	3.1
2	L	388	GLN	3.1
2	K	411	VAL	3.0
1	A	35	ASP	3.0
2	L	350	SER	2.9
2	J	420	TYR	2.9
2	L	397	ILE	2.9
2	G	385	VAL	2.9
2	L	405	ARG	2.9
2	L	352	LEU	2.9
1	A	148	GLN	2.8
2	L	389	GLN	2.8
2	J	419	LEU	2.7
2	K	347	SER	2.7
1	C	38	GLN	2.7
2	L	413	MET	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	348	MET	2.6
1	C	30	ARG	2.6
2	H	392	LYS	2.6
2	L	356	HIS	2.6
2	L	411	VAL	2.6
1	C	34	GLU	2.5
2	G	414	GLU	2.5
2	J	421	ASN	2.4
2	G	419	LEU	2.4
2	H	380	LEU	2.4
2	H	387	MET	2.4
2	I	412	ILE	2.4
2	L	403	ILE	2.3
2	I	392	LYS	2.3
2	L	406	PHE	2.3
2	I	371	ASN	2.3
2	L	394	THR	2.3
1	A	39	GLN	2.3
2	G	353	GLN	2.3
2	L	400	LEU	2.3
2	H	396	MET	2.3
1	D	147	PRO	2.2
2	G	392	LYS	2.2
2	K	396	MET	2.2
2	J	394	THR	2.2
2	G	351	ARG	2.2
2	I	407	LYS	2.2
2	L	407	LYS	2.2
2	K	421	ASN	2.2
2	J	418	MET	2.2
2	J	390	ALA	2.2
2	K	374	ILE	2.1
2	H	401	LYS	2.1
2	K	422	LYS	2.1
2	L	392	LYS	2.1
2	H	417	THR	2.1
1	F	38	GLN	2.1
2	H	411	VAL	2.1
2	J	423	PHE	2.1
1	A	34	GLU	2.1
1	D	44	GLN	2.1
2	H	388	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	388	GLN	2.1
2	G	393	HIS	2.0
2	L	395	GLU	2.0
1	E	109	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å 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.