Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:38 am BST

PDB ID	:	6V1V
Title	:	VIP3B (VIP3B_2160) adapted for crystallization
Authors	:	Evdokimov, A.G.; Zheng, M.; Moshiri, F.; Haas, J.; Lowder, C.
Deposited on	:	2019-11-21
Resolution	:	3.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

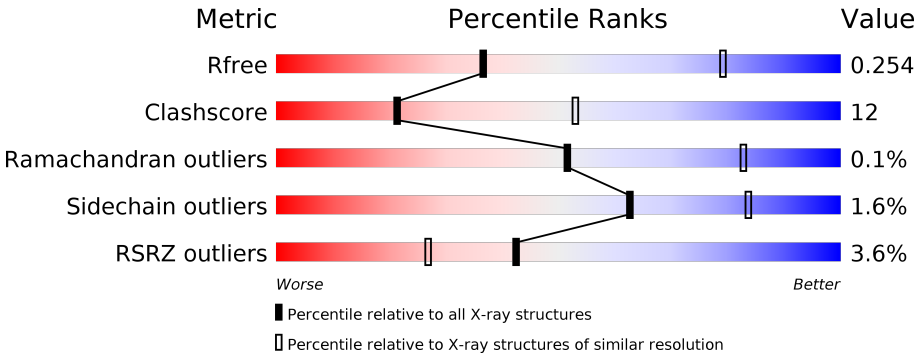
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 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 <=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	796	2% 74% 20% 6%
1	B	796	5% 73% 20% 6%
1	C	796	3% 70% 22% 7%
1	D	796	4% 69% 22% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23683 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 Vegetative insecticidal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	752	Total	C	N	O	S	0	0	0
			6002	3826	976	1185	15			
1	B	750	Total	C	N	O	S	0	0	0
			5985	3816	972	1182	15			
1	C	739	Total	C	N	O	S	0	0	0
			5874	3747	955	1157	15			
1	D	731	Total	C	N	O	S	0	0	0
			5822	3718	946	1143	15			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A290WPI2
A	-8	GLY	-	expression tag	UNP A0A290WPI2
A	-7	SER	-	expression tag	UNP A0A290WPI2
A	-6	SER	-	expression tag	UNP A0A290WPI2
A	-5	HIS	-	expression tag	UNP A0A290WPI2
A	-4	HIS	-	expression tag	UNP A0A290WPI2
A	-3	HIS	-	expression tag	UNP A0A290WPI2
A	-2	HIS	-	expression tag	UNP A0A290WPI2
A	-1	HIS	-	expression tag	UNP A0A290WPI2
A	0	HIS	-	expression tag	UNP A0A290WPI2
A	1	HIS	-	expression tag	UNP A0A290WPI2
A	?	-	TRP	deletion	UNP A0A290WPI2
A	?	-	LYS	deletion	UNP A0A290WPI2
A	?	-	GLU	deletion	UNP A0A290WPI2
A	?	-	LYS	deletion	UNP A0A290WPI2
A	?	-	SER	deletion	UNP A0A290WPI2
A	?	-	CYS	deletion	UNP A0A290WPI2
A	?	-	GLU	deletion	UNP A0A290WPI2
A	?	-	GLU	deletion	UNP A0A290WPI2
A	466	SER	ASP	engineered mutation	UNP A0A290WPI2
A	514	ALA	GLU	engineered mutation	UNP A0A290WPI2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	515	ALA	LYS	engineered mutation	UNP A0A290WPI2
A	517	ALA	GLN	engineered mutation	UNP A0A290WPI2
A	518	ALA	LYS	engineered mutation	UNP A0A290WPI2
A	?	-	ASP	deletion	UNP A0A290WPI2
A	?	-	THR	deletion	UNP A0A290WPI2
A	?	-	ILE	deletion	UNP A0A290WPI2
A	?	-	LYS	deletion	UNP A0A290WPI2
B	-9	MET	-	initiating methionine	UNP A0A290WPI2
B	-8	GLY	-	expression tag	UNP A0A290WPI2
B	-7	SER	-	expression tag	UNP A0A290WPI2
B	-6	SER	-	expression tag	UNP A0A290WPI2
B	-5	HIS	-	expression tag	UNP A0A290WPI2
B	-4	HIS	-	expression tag	UNP A0A290WPI2
B	-3	HIS	-	expression tag	UNP A0A290WPI2
B	-2	HIS	-	expression tag	UNP A0A290WPI2
B	-1	HIS	-	expression tag	UNP A0A290WPI2
B	0	HIS	-	expression tag	UNP A0A290WPI2
B	1	HIS	-	expression tag	UNP A0A290WPI2
B	?	-	TRP	deletion	UNP A0A290WPI2
B	?	-	LYS	deletion	UNP A0A290WPI2
B	?	-	GLU	deletion	UNP A0A290WPI2
B	?	-	LYS	deletion	UNP A0A290WPI2
B	?	-	SER	deletion	UNP A0A290WPI2
B	?	-	CYS	deletion	UNP A0A290WPI2
B	?	-	GLU	deletion	UNP A0A290WPI2
B	?	-	GLU	deletion	UNP A0A290WPI2
B	466	SER	ASP	engineered mutation	UNP A0A290WPI2
B	514	ALA	GLU	engineered mutation	UNP A0A290WPI2
B	515	ALA	LYS	engineered mutation	UNP A0A290WPI2
B	517	ALA	GLN	engineered mutation	UNP A0A290WPI2
B	518	ALA	LYS	engineered mutation	UNP A0A290WPI2
B	?	-	ASP	deletion	UNP A0A290WPI2
B	?	-	THR	deletion	UNP A0A290WPI2
B	?	-	ILE	deletion	UNP A0A290WPI2
B	?	-	LYS	deletion	UNP A0A290WPI2
C	-9	MET	-	initiating methionine	UNP A0A290WPI2
C	-8	GLY	-	expression tag	UNP A0A290WPI2
C	-7	SER	-	expression tag	UNP A0A290WPI2
C	-6	SER	-	expression tag	UNP A0A290WPI2
C	-5	HIS	-	expression tag	UNP A0A290WPI2
C	-4	HIS	-	expression tag	UNP A0A290WPI2
C	-3	HIS	-	expression tag	UNP A0A290WPI2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP A0A290WPI2
C	-1	HIS	-	expression tag	UNP A0A290WPI2
C	0	HIS	-	expression tag	UNP A0A290WPI2
C	1	HIS	-	expression tag	UNP A0A290WPI2
C	?	-	TRP	deletion	UNP A0A290WPI2
C	?	-	LYS	deletion	UNP A0A290WPI2
C	?	-	GLU	deletion	UNP A0A290WPI2
C	?	-	LYS	deletion	UNP A0A290WPI2
C	?	-	SER	deletion	UNP A0A290WPI2
C	?	-	CYS	deletion	UNP A0A290WPI2
C	?	-	GLU	deletion	UNP A0A290WPI2
C	?	-	GLU	deletion	UNP A0A290WPI2
C	466	SER	ASP	engineered mutation	UNP A0A290WPI2
C	514	ALA	GLU	engineered mutation	UNP A0A290WPI2
C	515	ALA	LYS	engineered mutation	UNP A0A290WPI2
C	517	ALA	GLN	engineered mutation	UNP A0A290WPI2
C	518	ALA	LYS	engineered mutation	UNP A0A290WPI2
C	?	-	ASP	deletion	UNP A0A290WPI2
C	?	-	THR	deletion	UNP A0A290WPI2
C	?	-	ILE	deletion	UNP A0A290WPI2
C	?	-	LYS	deletion	UNP A0A290WPI2
D	-9	MET	-	initiating methionine	UNP A0A290WPI2
D	-8	GLY	-	expression tag	UNP A0A290WPI2
D	-7	SER	-	expression tag	UNP A0A290WPI2
D	-6	SER	-	expression tag	UNP A0A290WPI2
D	-5	HIS	-	expression tag	UNP A0A290WPI2
D	-4	HIS	-	expression tag	UNP A0A290WPI2
D	-3	HIS	-	expression tag	UNP A0A290WPI2
D	-2	HIS	-	expression tag	UNP A0A290WPI2
D	-1	HIS	-	expression tag	UNP A0A290WPI2
D	0	HIS	-	expression tag	UNP A0A290WPI2
D	1	HIS	-	expression tag	UNP A0A290WPI2
D	?	-	TRP	deletion	UNP A0A290WPI2
D	?	-	LYS	deletion	UNP A0A290WPI2
D	?	-	GLU	deletion	UNP A0A290WPI2
D	?	-	LYS	deletion	UNP A0A290WPI2
D	?	-	SER	deletion	UNP A0A290WPI2
D	?	-	CYS	deletion	UNP A0A290WPI2
D	?	-	GLU	deletion	UNP A0A290WPI2
D	?	-	GLU	deletion	UNP A0A290WPI2
D	466	SER	ASP	engineered mutation	UNP A0A290WPI2
D	514	ALA	GLU	engineered mutation	UNP A0A290WPI2

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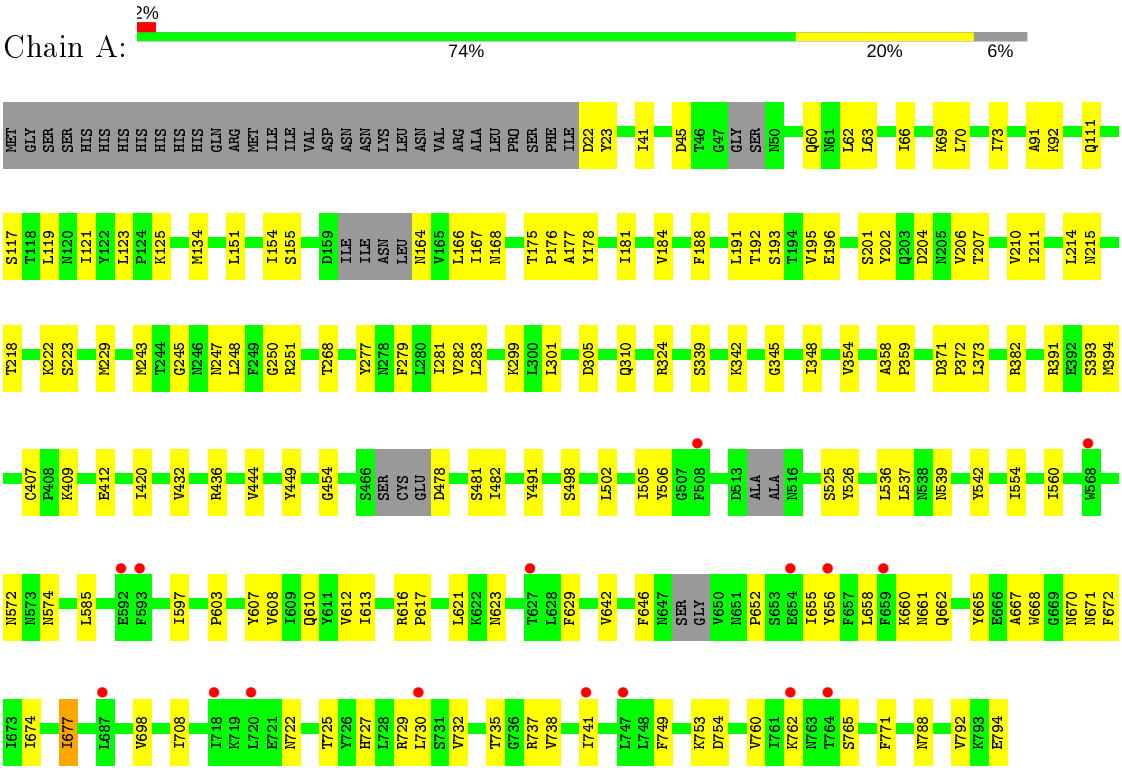
Chain	Residue	Modelled	Actual	Comment	Reference
D	515	ALA	LYS	engineered mutation	UNP A0A290WPI2
D	517	ALA	GLN	engineered mutation	UNP A0A290WPI2
D	518	ALA	LYS	engineered mutation	UNP A0A290WPI2
D	?	-	ASP	deletion	UNP A0A290WPI2
D	?	-	THR	deletion	UNP A0A290WPI2
D	?	-	ILE	deletion	UNP A0A290WPI2
D	?	-	LYS	deletion	UNP A0A290WPI2

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 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.

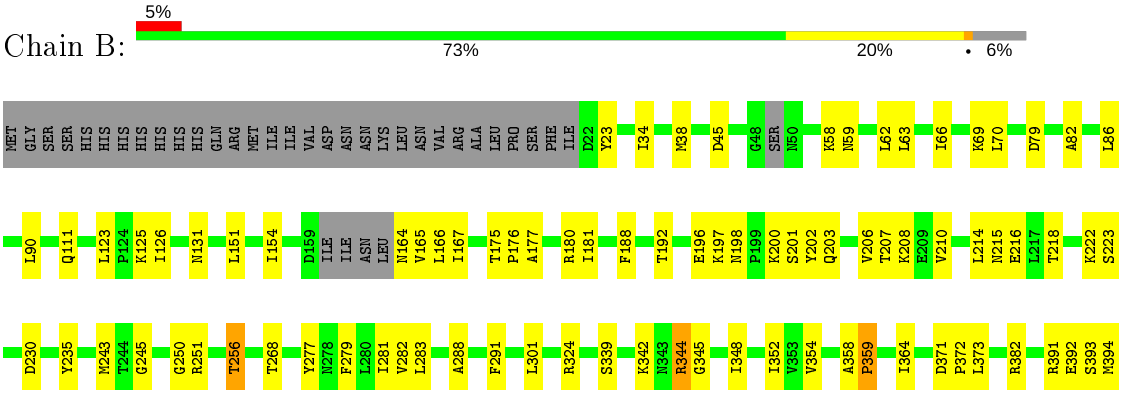
- Molecule 1: Vegetative insecticidal protein

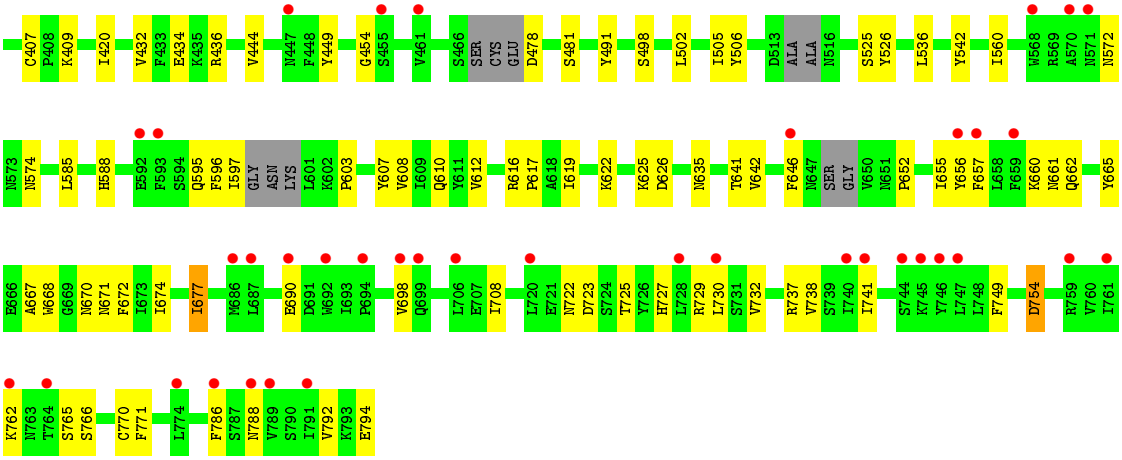
Chain A:



- Molecule 1: Vegetative insecticidal protein

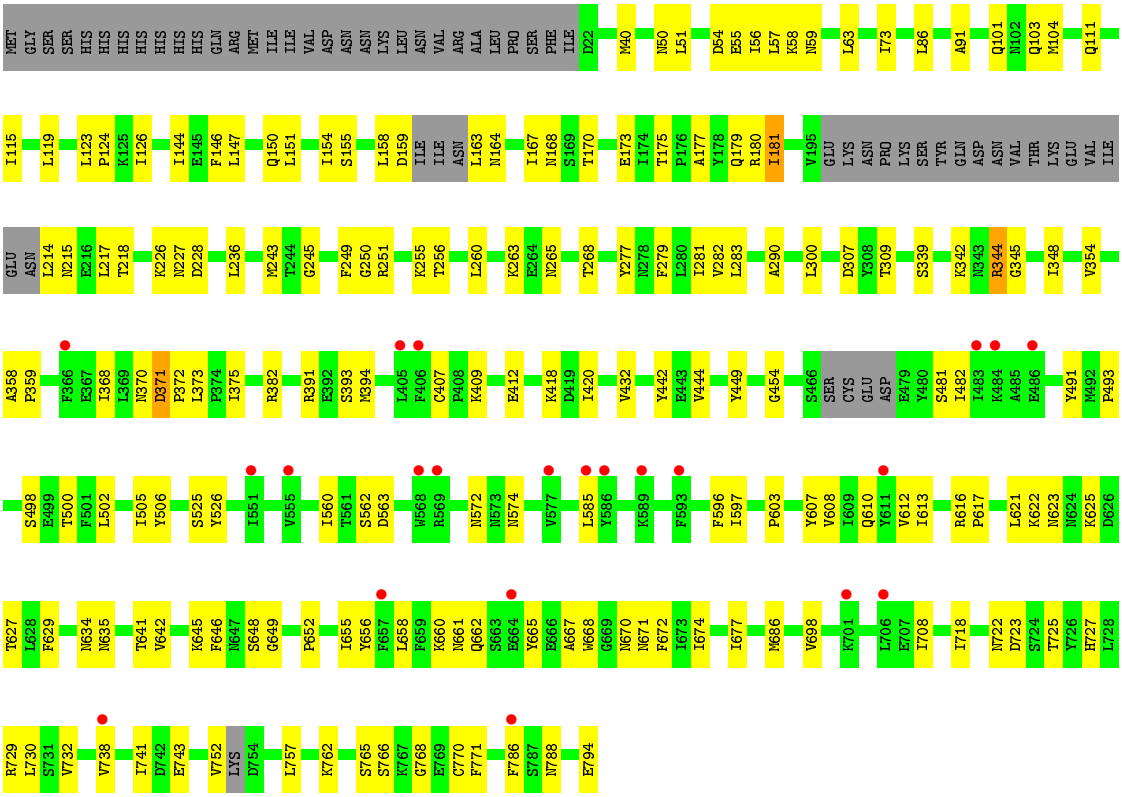
Chain B:





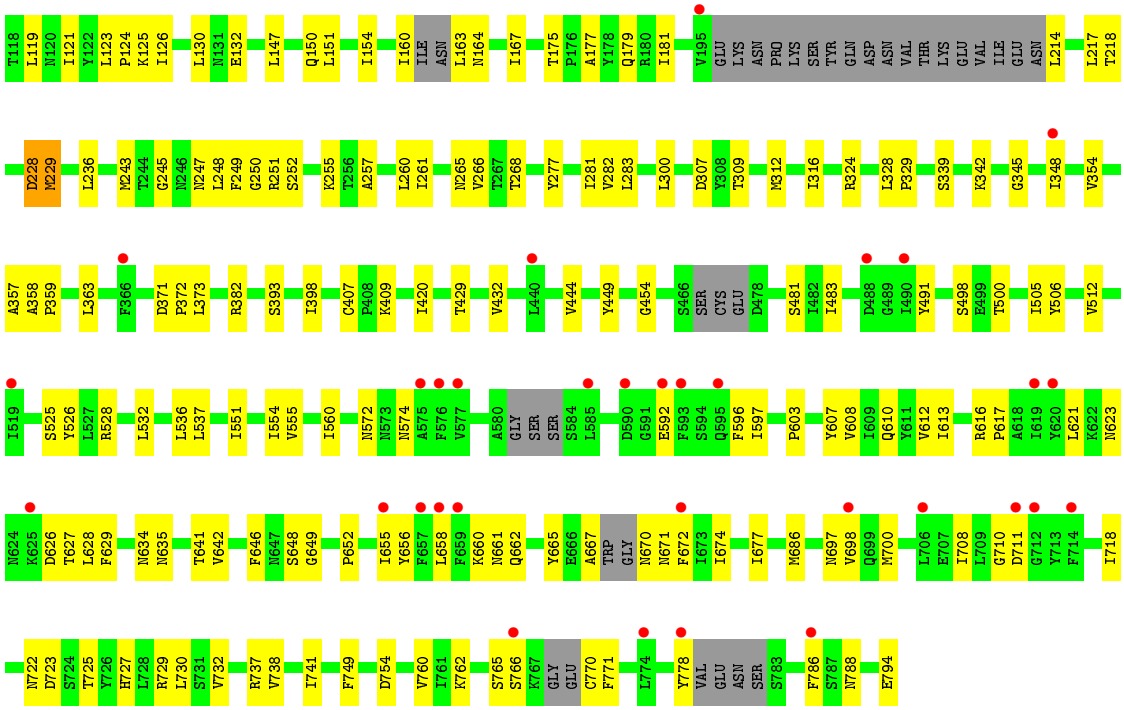
• Molecule 1: Vegetative insecticidal protein

Chain C:



• Molecule 1: Vegetative insecticidal protein

Chain D:


T118 L119 N120 I121 V122 L123 P124 K125 I126 L130 N131 E132 L147 Q150 L151 I154 I160 ILE ASN L163 N164 I167 T175 P176 A177 Y178 Q179 R180 I181 V195 GLU LYS ASN PRO LYS SER TYR GLN ASP ASN VAL THR LYS GLU VAL ILE GLU ASN L214 L217 T218
D228 M229 L236 M243 T244 G245 N246 N247 L248 P249 G250 R251 S252 K255 T256 A257 L260 I261 N265 V266 T267 T268 Y277 I281 V282 L283 L300 D307 Y308 T309 M312 I316 R324 L328 P329 S339 K342 G345 I348 V354
A357 A358 P359 L363 P366 D371 P372 L373 R382 S393 I398 C407 P408 K409 I420 T429 V432 L440 V444 Y449 G454 S466 SER CYS GLU D478 S481 I482 I483 D488 G489 I490 Y491 S498 E499 T500 I505 Y506 V512
I519 S525 Y526 L527 R528 L532 L536 L537 I551 I554 V555 I560 N572 N573 N574 A575 F576 V577 A580 GLY SER SER S584 L585 D590 G591 E592 F593 S594 Q595 F596 I597 P603 V607 V608 I609 Q610 Y611 V612 I613 R616 P617 A618 I619 Y620 L621 K622 N623
N624 K625 D626 T627 L628 F629 N634 N635 T641 V642 F646 N647 S648 G649 P652 I655 Y656 F657 L658 F659 K660 N661 Q662 Y665 E666 A667 TRP GLY N670 N671 F672 I673 I674 I677 M686 N697 V698 Q699 M700 L706 E707 I708 L709 G710 D711 G712 Y713 F714 I718
N722 D723 S724 T725 Y726 H727 L728 R729 L730 S731 V732 R737 V738 I741 F749 D754 V760 I761 K762 S765 S766 K767 GLY GLU C770 F771 L774 Y778 VAL GLU ASN SER S783 F786 S787 N788 E794

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	106.49Å 106.54Å 117.73Å 96.13° 70.93° 69.52°	Depositor
Resolution (Å)	49.89 – 3.19 49.84 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.89-3.19) 98.3 (49.84-3.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.218 , 0.259 0.215 , 0.254	Depositor DCC
R_{free} test set	3538 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	102.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23683	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.59	0/6105	0.79	0/8254
1	B	0.59	0/6087	0.80	0/8229
1	C	0.59	0/5976	0.80	0/8082
1	D	0.59	0/5919	0.81	1/7999 (0.0%)
All	All	0.59	0/24087	0.80	1/32564 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	228	ASP	CB-CA-C	5.03	120.45	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6002	0	5970	119	0
1	B	5985	0	5950	142	0
1	C	5874	0	5847	171	0
1	D	5822	0	5811	170	0
All	All	23683	0	23578	567	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 12.

All (567) 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:D:554:ILE:HG12	1:D:674:ILE:HG23	1.14	1.08
1:C:371:ASP:CB	1:C:372:PRO:HD3	1.83	1.07
1:C:371:ASP:HB3	1:C:372:PRO:HD3	1.09	1.04
1:B:652:PRO:HA	1:B:655:ILE:HD11	1.45	0.99
1:C:371:ASP:HB3	1:C:372:PRO:CD	1.91	0.99
1:D:312:MET:O	1:D:316:ILE:HD13	1.63	0.98
1:B:165:VAL:HG13	1:D:163:LEU:HD13	1.46	0.97
1:D:51:LEU:HD11	1:D:56:ILE:HG12	1.46	0.96
1:C:51:LEU:HD12	1:C:56:ILE:HG13	1.50	0.92
1:D:554:ILE:CG1	1:D:674:ILE:HG23	1.98	0.90
1:A:164:ASN:O	1:C:163:LEU:HD22	1.71	0.89
1:D:652:PRO:HA	1:D:655:ILE:CD1	2.01	0.89
1:B:70:LEU:HG	1:C:104:MET:CE	2.04	0.88
1:C:164:ASN:HB2	1:C:167:ILE:HD13	1.53	0.88
1:A:670:ASN:HA	1:A:672:PHE:CE1	2.08	0.88
1:B:595:GLN:O	1:B:656:TYR:HB2	1.72	0.88
1:C:371:ASP:CB	1:C:372:PRO:CD	2.48	0.88
1:D:554:ILE:HG12	1:D:674:ILE:CG2	2.03	0.88
1:C:175:THR:O	1:C:179:GLN:HG3	1.74	0.88
1:D:164:ASN:HB2	1:D:167:ILE:HD13	1.55	0.87
1:C:612:VAL:HG22	1:C:641:THR:HG22	1.57	0.87
1:B:670:ASN:HA	1:B:672:PHE:CE1	2.08	0.86
1:B:560:ILE:H	1:B:670:ASN:HD22	1.23	0.86
1:B:612:VAL:HG22	1:B:641:THR:HG22	1.58	0.85
1:C:560:ILE:H	1:C:670:ASN:HD22	1.22	0.85
1:A:560:ILE:H	1:A:670:ASN:HD22	1.23	0.85
1:B:164:ASN:HB2	1:B:167:ILE:HD13	1.59	0.85
1:B:596:PHE:HA	1:B:656:TYR:CB	2.07	0.85
1:D:612:VAL:HG22	1:D:641:THR:HG22	1.58	0.84
1:A:164:ASN:HB2	1:A:167:ILE:HD13	1.58	0.84
1:C:617:PRO:HB3	1:C:667:ALA:HB1	1.59	0.84
1:B:391:ARG:NH2	1:B:392:GLU:OE2	2.11	0.83
1:D:51:LEU:CD1	1:D:56:ILE:HG12	2.08	0.83
1:D:175:THR:O	1:D:179:GLN:HG3	1.79	0.82
1:D:560:ILE:H	1:D:670:ASN:HD22	1.23	0.82
1:C:170:THR:HA	1:C:173:GLU:HG2	1.61	0.81
1:C:51:LEU:CD1	1:C:56:ILE:HG13	2.10	0.81
1:B:164:ASN:O	1:D:163:LEU:HD22	1.80	0.81
1:B:596:PHE:HA	1:B:656:TYR:HB3	1.61	0.81
1:D:617:PRO:HB3	1:D:667:ALA:HB1	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:TYR:HD1	1:A:658:LEU:HD11	1.45	0.80
1:B:166:LEU:HB3	1:B:251:ARG:HD2	1.61	0.80
1:A:151:LEU:HD22	1:A:282:VAL:HG21	1.63	0.79
1:D:652:PRO:HA	1:D:655:ILE:HD12	1.64	0.79
1:C:146:PHE:CE1	1:C:147:LEU:HB3	2.18	0.78
1:A:537:LEU:O	1:A:537:LEU:HD23	1.84	0.78
1:A:207:THR:OG1	1:A:210:VAL:HG23	1.84	0.77
1:C:51:LEU:HD11	1:C:56:ILE:HG12	1.65	0.77
1:B:151:LEU:HD22	1:B:282:VAL:HG21	1.66	0.77
1:B:188:PHE:O	1:B:192:THR:HG23	1.86	0.76
1:A:188:PHE:O	1:A:192:THR:HG23	1.86	0.75
1:D:652:PRO:HA	1:D:655:ILE:HD11	1.67	0.75
1:C:146:PHE:CZ	1:C:147:LEU:HD23	2.21	0.75
1:B:70:LEU:HG	1:C:104:MET:HE3	1.68	0.75
1:A:177:ALA:O	1:A:181:ILE:HG12	1.87	0.74
1:B:371:ASP:HB3	1:B:372:PRO:HD3	1.68	0.73
1:B:177:ALA:O	1:B:181:ILE:HG12	1.88	0.73
1:C:730:LEU:HD11	1:C:757:LEU:HD21	1.69	0.73
1:C:51:LEU:CD1	1:C:56:ILE:CG1	2.67	0.72
1:D:697:ASN:HB3	1:D:710:GLY:HA3	1.70	0.72
1:D:328:LEU:HD11	1:D:528:ARG:HE	1.53	0.71
1:A:656:TYR:CD1	1:A:658:LEU:HD11	2.25	0.71
1:D:151:LEU:HD22	1:D:282:VAL:HG21	1.71	0.71
1:C:151:LEU:HD22	1:C:282:VAL:HG21	1.72	0.70
1:D:51:LEU:CD1	1:D:56:ILE:CG1	2.69	0.70
1:A:184:VAL:HG21	1:D:229:MET:HG2	1.72	0.70
1:C:372:PRO:HB3	1:C:645:LYS:HB3	1.73	0.70
1:D:628:LEU:HD21	1:D:648:SER:HA	1.74	0.69
1:B:625:LYS:HG3	1:B:626:ASP:H	1.56	0.68
1:B:652:PRO:HA	1:B:655:ILE:CD1	2.22	0.68
1:C:251:ARG:HH11	1:C:255:LYS:HG2	1.58	0.68
1:A:735:THR:HG23	1:A:753:LYS:HG2	1.74	0.68
1:C:607:TYR:HB2	1:C:646:PHE:CE1	2.30	0.67
1:D:652:PRO:CA	1:D:655:ILE:HD12	2.24	0.67
1:C:51:LEU:HD11	1:C:56:ILE:CG1	2.24	0.67
1:C:730:LEU:HD11	1:C:757:LEU:CD2	2.25	0.67
1:A:371:ASP:HB2	1:A:372:PRO:HD3	1.78	0.66
1:D:45:ASP:O	1:D:125:LYS:HD2	1.95	0.66
1:A:597:ILE:HD12	1:A:597:ILE:O	1.95	0.66
1:B:358:ALA:HB1	1:B:359:PRO:HD2	1.76	0.66
1:C:146:PHE:CE2	1:C:147:LEU:HD23	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:TYR:HB2	1:D:646:PHE:CE1	2.30	0.66
1:B:617:PRO:HB3	1:B:667:ALA:HB1	1.77	0.66
1:C:251:ARG:NH1	1:C:255:LYS:HG2	2.10	0.66
1:C:420:ILE:HD13	1:C:444:VAL:HG23	1.76	0.66
1:A:607:TYR:HB2	1:A:646:PHE:CE1	2.31	0.66
1:C:625:LYS:HG2	1:C:625:LYS:O	1.94	0.66
1:D:51:LEU:HD12	1:D:56:ILE:HG13	1.76	0.66
1:B:352:ILE:CD1	1:B:434:GLU:HG2	2.26	0.65
1:C:348:ILE:HG13	1:C:788:ASN:ND2	2.12	0.65
1:C:725:THR:HG23	1:C:762:LYS:HG2	1.78	0.65
1:D:420:ILE:HD13	1:D:444:VAL:HG23	1.79	0.65
1:C:752:VAL:HG11	1:C:757:LEU:CD2	2.26	0.65
1:A:617:PRO:HB3	1:A:667:ALA:HB1	1.77	0.65
1:D:167:ILE:HG12	1:D:260:LEU:HD21	1.78	0.65
1:B:622:LYS:O	1:B:655:ILE:HG23	1.97	0.65
1:D:697:ASN:HB3	1:D:710:GLY:CA	2.27	0.64
1:B:279:PHE:CE1	1:B:283:LEU:HD22	2.32	0.64
1:B:348:ILE:HG13	1:B:788:ASN:ND2	2.13	0.64
1:A:394:MET:HE1	1:A:502:LEU:HD12	1.80	0.64
1:A:202:TYR:CE1	1:A:210:VAL:HG12	2.33	0.64
1:B:607:TYR:HB2	1:B:646:PHE:CE1	2.32	0.64
1:C:181:ILE:HD13	1:C:236:LEU:CD1	2.28	0.63
1:A:348:ILE:HG13	1:A:788:ASN:ND2	2.12	0.63
1:C:648:SER:HB2	1:C:652:PRO:CG	2.29	0.63
1:D:358:ALA:HB1	1:D:359:PRO:HD2	1.78	0.63
1:B:622:LYS:C	1:B:655:ILE:HG23	2.18	0.63
1:C:572:ASN:HB2	1:C:574:ASN:H	1.64	0.63
1:C:251:ARG:HD2	1:C:256:THR:HG23	1.81	0.63
1:D:348:ILE:HG13	1:D:788:ASN:ND2	2.14	0.62
1:C:170:THR:HG22	1:C:173:GLU:OE2	2.00	0.62
1:B:652:PRO:CA	1:B:655:ILE:HD11	2.26	0.62
1:C:245:GLY:O	1:C:250:GLY:HA2	2.00	0.62
1:A:164:ASN:CB	1:A:167:ILE:HD13	2.29	0.62
1:B:70:LEU:HG	1:C:104:MET:HE1	1.79	0.62
1:C:358:ALA:HB1	1:C:359:PRO:HD2	1.82	0.61
1:A:358:ALA:HB1	1:A:359:PRO:HD2	1.81	0.61
1:D:363:LEU:HD23	1:D:429:THR:HA	1.83	0.61
1:A:22:ASP:HA	1:A:391:ARG:HH11	1.65	0.61
1:A:92:LYS:HE3	1:B:79:ASP:OD1	2.00	0.61
1:D:617:PRO:HB3	1:D:667:ALA:CB	2.31	0.61
1:B:166:LEU:HB3	1:B:251:ARG:CD	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:CG2	1:D:229:MET:HG2	2.31	0.61
1:D:481:SER:CB	1:D:512:VAL:HG11	2.30	0.61
1:B:420:ILE:HD13	1:B:444:VAL:HG23	1.82	0.61
1:D:616:ARG:O	1:D:662:GLN:HG2	2.01	0.61
1:C:123:LEU:HD23	1:C:123:LEU:C	2.21	0.61
1:C:617:PRO:HB3	1:C:667:ALA:CB	2.29	0.61
1:D:123:LEU:C	1:D:123:LEU:HD23	2.21	0.61
1:D:252:SER:OG	1:D:255:LYS:HB2	1.99	0.61
1:D:266:VAL:HG13	1:D:266:VAL:O	2.00	0.61
1:B:661:ASN:ND2	1:B:665:TYR:O	2.34	0.60
1:C:648:SER:HB2	1:C:652:PRO:CB	2.31	0.60
1:B:596:PHE:HA	1:B:656:TYR:HB2	1.82	0.60
1:B:619:ILE:CG2	1:B:657:PHE:CE1	2.84	0.60
1:C:616:ARG:O	1:C:662:GLN:HG2	2.02	0.60
1:A:155:SER:HB3	1:D:250:GLY:HA3	1.82	0.60
1:D:249:PHE:CE2	1:D:251:ARG:HB3	2.35	0.60
1:D:648:SER:HB2	1:D:652:PRO:CB	2.31	0.60
1:C:147:LEU:CD1	1:C:282:VAL:HG22	2.31	0.60
1:A:73:ILE:HD12	1:D:104:MET:CE	2.31	0.60
1:C:648:SER:HB2	1:C:652:PRO:HG3	1.83	0.60
1:D:592:GLU:HB2	1:D:660:LYS:HG3	1.84	0.60
1:A:23:TYR:CD2	1:A:542:TYR:HB3	2.37	0.60
1:B:741:ILE:HD11	1:B:771:PHE:CZ	2.37	0.60
1:A:420:ILE:HD13	1:A:444:VAL:HG23	1.84	0.60
1:B:196:GLU:HG2	1:B:201:SER:HB3	1.84	0.59
1:B:245:GLY:O	1:B:250:GLY:HA2	2.02	0.59
1:A:166:LEU:HD13	1:A:251:ARG:NH2	2.18	0.59
1:A:191:LEU:O	1:A:195:VAL:HG23	2.02	0.59
1:B:176:PRO:O	1:B:180:ARG:HG2	2.02	0.59
1:A:245:GLY:O	1:A:250:GLY:HA2	2.02	0.59
1:A:652:PRO:HA	1:A:655:ILE:HD11	1.85	0.59
1:A:196:GLU:HG2	1:A:201:SER:HB3	1.85	0.59
1:D:328:LEU:HD13	1:D:328:LEU:C	2.22	0.59
1:C:181:ILE:CD1	1:C:236:LEU:HD12	2.32	0.59
1:D:661:ASN:ND2	1:D:665:TYR:O	2.36	0.59
1:A:661:ASN:ND2	1:A:665:TYR:O	2.36	0.58
1:D:245:GLY:O	1:D:250:GLY:HA2	2.02	0.58
1:C:420:ILE:HD12	1:C:442:TYR:HE1	1.67	0.58
1:B:616:ARG:HD3	1:B:665:TYR:CD2	2.39	0.58
1:C:616:ARG:HA	1:C:634:ASN:O	2.04	0.58
1:B:616:ARG:O	1:B:662:GLN:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:CD1	1:C:282:VAL:CG2	2.82	0.58
1:D:181:ILE:HD13	1:D:236:LEU:CD1	2.34	0.58
1:D:741:ILE:HD11	1:D:771:PHE:CZ	2.38	0.58
1:C:656:TYR:CE1	1:C:658:LEU:HD11	2.38	0.58
1:A:45:ASP:O	1:A:125:LYS:HD3	2.04	0.58
1:B:23:TYR:CD2	1:B:542:TYR:HB3	2.39	0.58
1:C:648:SER:CB	1:C:652:PRO:HG3	2.34	0.58
1:D:648:SER:HB2	1:D:652:PRO:CG	2.33	0.58
1:D:554:ILE:CG1	1:D:674:ILE:CG2	2.72	0.58
1:A:371:ASP:CB	1:A:372:PRO:HD3	2.34	0.58
1:A:741:ILE:HD11	1:A:771:PHE:CZ	2.39	0.58
1:B:345:GLY:HA3	1:B:407:CYS:O	2.04	0.58
1:A:70:LEU:HA	1:D:104:MET:HE1	1.86	0.58
1:A:345:GLY:HA3	1:A:407:CYS:O	2.04	0.57
1:B:165:VAL:HG13	1:D:163:LEU:CD1	2.29	0.57
1:B:505:ILE:HG22	1:B:525:SER:HA	1.86	0.57
1:C:741:ILE:HD11	1:C:771:PHE:CZ	2.39	0.57
1:C:181:ILE:CD1	1:C:236:LEU:CD1	2.82	0.57
1:C:147:LEU:HD11	1:C:282:VAL:HG22	1.86	0.57
1:C:766:SER:CB	1:C:770:CYS:SG	2.93	0.57
1:D:160:ILE:O	1:D:163:LEU:N	2.38	0.57
1:D:483:ILE:HD11	1:D:512:VAL:HG23	1.85	0.57
1:D:648:SER:HB2	1:D:652:PRO:HG3	1.87	0.57
1:C:505:ILE:HG22	1:C:525:SER:HA	1.86	0.57
1:B:364:ILE:CG2	1:B:502:LEU:HB3	2.35	0.57
1:C:345:GLY:HA3	1:C:407:CYS:O	2.04	0.57
1:C:661:ASN:ND2	1:C:665:TYR:O	2.37	0.57
1:C:560:ILE:N	1:C:670:ASN:HD22	1.99	0.57
1:B:619:ILE:HG23	1:B:657:PHE:CE1	2.40	0.57
1:C:732:VAL:HG12	1:C:786:PHE:CD2	2.40	0.56
1:C:766:SER:HB2	1:C:770:CYS:SG	2.45	0.56
1:A:310:GLN:HA	1:A:310:GLN:OE1	2.04	0.56
1:C:249:PHE:CE2	1:C:251:ARG:HB3	2.41	0.56
1:C:743:GLU:HG3	1:C:768:GLY:O	2.05	0.56
1:D:483:ILE:HD11	1:D:512:VAL:CG2	2.35	0.56
1:D:646:PHE:CE1	1:D:674:ILE:HD11	2.41	0.56
1:D:345:GLY:HA3	1:D:407:CYS:O	2.04	0.56
1:D:481:SER:CB	1:D:512:VAL:CG1	2.84	0.56
1:D:371:ASP:HB2	1:D:372:PRO:HD3	1.88	0.56
1:A:616:ARG:O	1:A:662:GLN:HG2	2.05	0.56
1:C:342:LYS:HG3	1:C:491:TYR:CE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:ILE:O	1:C:770:CYS:HB2	2.06	0.55
1:B:69:LYS:NZ	1:C:103:GLN:HB3	2.22	0.55
1:C:73:ILE:HG22	1:C:101:GLN:NE2	2.21	0.55
1:D:164:ASN:CB	1:D:167:ILE:HD13	2.33	0.55
1:D:481:SER:HB2	1:D:512:VAL:CG1	2.37	0.55
1:D:648:SER:CB	1:D:652:PRO:HG3	2.36	0.55
1:D:123:LEU:HB3	1:D:124:PRO:HD3	1.87	0.55
1:D:505:ILE:HG22	1:D:525:SER:HA	1.88	0.55
1:D:555:VAL:HG23	1:D:674:ILE:HG22	1.89	0.55
1:D:698:VAL:HG12	1:D:708:ILE:HA	1.88	0.55
1:C:164:ASN:CB	1:C:167:ILE:HD13	2.31	0.55
1:D:247:ASN:O	1:D:248:LEU:HB2	2.08	0.54
1:B:574:ASN:OD1	1:B:588:HIS:HD2	1.91	0.54
1:B:698:VAL:HG12	1:B:708:ILE:HA	1.90	0.54
1:C:698:VAL:HG12	1:C:708:ILE:HA	1.89	0.54
1:D:371:ASP:CB	1:D:372:PRO:HD3	2.37	0.54
1:A:62:LEU:HD21	1:D:63:LEU:HD21	1.89	0.54
1:A:505:ILE:HG22	1:A:525:SER:HA	1.89	0.54
1:B:63:LEU:HD13	1:B:111:GLN:HB2	1.88	0.54
1:B:732:VAL:HG12	1:B:786:PHE:CD2	2.43	0.54
1:B:572:ASN:HB2	1:B:574:ASN:H	1.72	0.54
1:D:249:PHE:HE2	1:D:251:ARG:HB3	1.72	0.54
1:D:51:LEU:HD12	1:D:56:ILE:CG1	2.33	0.54
1:D:616:ARG:HB3	1:D:635:ASN:HA	1.89	0.54
1:D:616:ARG:HA	1:D:634:ASN:O	2.08	0.54
1:A:202:TYR:HA	1:A:206:VAL:HG23	1.88	0.54
1:A:69:LYS:HD3	1:D:104:MET:HG3	1.90	0.54
1:A:698:VAL:HG12	1:A:708:ILE:HA	1.89	0.54
1:B:164:ASN:CB	1:B:167:ILE:HD13	2.32	0.54
1:B:251:ARG:HD3	1:B:256:THR:HG23	1.90	0.54
1:B:208:LYS:N	1:C:50:ASN:OD1	2.40	0.54
1:D:481:SER:HB2	1:D:512:VAL:HG11	1.89	0.54
1:D:608:VAL:O	1:D:674:ILE:HA	2.08	0.54
1:D:560:ILE:N	1:D:670:ASN:HD22	2.00	0.54
1:A:572:ASN:HB2	1:A:574:ASN:H	1.73	0.53
1:B:652:PRO:C	1:B:655:ILE:CD1	2.77	0.53
1:C:623:ASN:HB2	1:C:655:ILE:HD13	1.91	0.53
1:A:608:VAL:O	1:A:674:ILE:HA	2.07	0.53
1:C:608:VAL:O	1:C:674:ILE:HA	2.08	0.53
1:C:146:PHE:CZ	1:C:147:LEU:HB3	2.43	0.53
1:D:670:ASN:HA	1:D:672:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:LEU:HD23	1:D:429:THR:CA	2.38	0.53
1:D:623:ASN:HB2	1:D:655:ILE:HG12	1.90	0.53
1:B:348:ILE:HA	1:B:729:ARG:HD2	1.90	0.53
1:A:63:LEU:HD13	1:A:111:GLN:HB2	1.91	0.53
1:C:752:VAL:HG11	1:C:757:LEU:HD22	1.91	0.53
1:D:277:TYR:CE2	1:D:281:ILE:HD11	2.44	0.53
1:D:348:ILE:HA	1:D:729:ARG:HD2	1.91	0.53
1:D:481:SER:HB3	1:D:512:VAL:HG11	1.89	0.53
1:C:368:ILE:HD13	1:C:493:PRO:HG2	1.90	0.52
1:B:202:TYR:HA	1:B:206:VAL:HG23	1.90	0.52
1:A:652:PRO:HA	1:A:655:ILE:CD1	2.39	0.52
1:C:670:ASN:HA	1:C:672:PHE:CE2	2.45	0.52
1:C:394:MET:CE	1:C:502:LEU:HD12	2.40	0.52
1:A:560:ILE:N	1:A:670:ASN:HD22	2.00	0.52
1:A:277:TYR:CE2	1:A:281:ILE:HD11	2.44	0.52
1:D:307:ASP:OD2	1:D:309:THR:HG22	2.09	0.52
1:B:277:TYR:CE2	1:B:281:ILE:HD11	2.44	0.52
1:B:652:PRO:C	1:B:655:ILE:HD12	2.30	0.52
1:B:608:VAL:O	1:B:674:ILE:HA	2.09	0.52
1:C:277:TYR:CE2	1:C:281:ILE:HD11	2.44	0.52
1:D:51:LEU:HD11	1:D:56:ILE:CG1	2.28	0.52
1:D:328:LEU:CD1	1:D:528:ARG:HE	2.21	0.52
1:D:732:VAL:HG12	1:D:786:PHE:CD2	2.44	0.52
1:A:506:TYR:C	1:A:506:TYR:CD1	2.84	0.52
1:B:154:ILE:HG12	1:B:268:THR:HG21	1.91	0.52
1:B:652:PRO:CA	1:B:655:ILE:CD1	2.86	0.52
1:B:207:THR:OG1	1:B:210:VAL:HG23	2.10	0.52
1:B:690:GLU:HG2	1:B:690:GLU:O	2.10	0.51
1:C:616:ARG:HG2	1:C:635:ASN:HA	1.91	0.51
1:C:616:ARG:HD2	1:C:665:TYR:CD2	2.46	0.51
1:C:86:LEU:CD1	1:C:91:ALA:HB2	2.41	0.51
1:D:354:VAL:HG23	1:D:432:VAL:HG22	1.93	0.51
1:D:506:TYR:CD1	1:D:506:TYR:C	2.84	0.51
1:B:506:TYR:C	1:B:506:TYR:CD1	2.84	0.51
1:C:159:ASP:OD1	1:C:159:ASP:C	2.49	0.51
1:D:342:LYS:HG2	1:D:491:TYR:CE1	2.45	0.51
1:B:216:GLU:HG2	1:C:227:ASN:OD1	2.10	0.51
1:C:307:ASP:OD2	1:C:309:THR:HG22	2.10	0.51
1:C:649:GLY:H	1:C:652:PRO:HB3	1.75	0.51
1:B:165:VAL:HG22	1:D:163:LEU:HB2	1.92	0.51
1:D:86:LEU:CD1	1:D:91:ALA:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ILE:HA	1:C:729:ARG:HD2	1.92	0.51
1:D:766:SER:HB2	1:D:770:CYS:HB2	1.92	0.51
1:A:537:LEU:HD22	1:A:539:ASN:ND2	2.26	0.51
1:A:732:VAL:O	1:A:754:ASP:HA	2.11	0.51
1:B:200:LYS:O	1:B:203:GLN:HG2	2.11	0.51
1:B:732:VAL:O	1:B:754:ASP:HA	2.12	0.50
1:D:57:LEU:HD21	1:D:119:LEU:HD21	1.93	0.50
1:A:572:ASN:HB2	1:A:574:ASN:HB2	1.93	0.50
1:C:123:LEU:HB3	1:C:124:PRO:HD3	1.93	0.50
1:C:181:ILE:HD13	1:C:236:LEU:HD13	1.92	0.50
1:C:249:PHE:HE2	1:C:251:ARG:HB3	1.75	0.50
1:C:616:ARG:HG2	1:C:635:ASN:HB2	1.94	0.50
1:B:725:THR:HG23	1:B:762:LYS:HG2	1.92	0.50
1:D:596:PHE:HA	1:D:656:TYR:CD2	2.47	0.50
1:D:646:PHE:CZ	1:D:674:ILE:HD11	2.46	0.50
1:B:560:ILE:N	1:B:670:ASN:HD22	1.99	0.50
1:C:506:TYR:CD1	1:C:506:TYR:C	2.84	0.50
1:D:697:ASN:HB3	1:D:710:GLY:N	2.26	0.50
1:C:170:THR:HA	1:C:173:GLU:CG	2.36	0.50
1:C:394:MET:HE1	1:C:502:LEU:HD12	1.93	0.50
1:B:342:LYS:HG3	1:B:491:TYR:CE1	2.47	0.50
1:A:154:ILE:HG12	1:A:268:THR:HG21	1.94	0.50
1:C:147:LEU:HD13	1:C:282:VAL:CG2	2.40	0.50
1:C:73:ILE:CG2	1:C:101:GLN:NE2	2.75	0.50
1:D:612:VAL:HG21	1:D:671:ASN:HD22	1.76	0.50
1:D:730:LEU:HD21	1:D:738:VAL:HG21	1.94	0.50
1:A:247:ASN:O	1:A:248:LEU:HB3	2.11	0.50
1:D:357:ALA:HB2	1:D:363:LEU:HD22	1.94	0.49
1:D:612:VAL:HG23	1:D:671:ASN:HB2	1.94	0.49
1:A:166:LEU:HD13	1:A:251:ARG:HH21	1.77	0.49
1:A:725:THR:HG23	1:A:762:LYS:HG2	1.94	0.49
1:B:612:VAL:HG21	1:B:671:ASN:HD22	1.78	0.49
1:A:70:LEU:CA	1:D:104:MET:HE1	2.41	0.49
1:A:41:ILE:CG2	1:A:299:LYS:HG3	2.42	0.49
1:B:612:VAL:HG23	1:B:671:ASN:HB2	1.94	0.49
1:C:562:SER:OG	1:C:563:ASP:N	2.45	0.49
1:A:62:LEU:O	1:A:66:ILE:HD12	2.12	0.49
1:B:45:ASP:O	1:B:125:LYS:HD3	2.11	0.49
1:C:612:VAL:HG23	1:C:671:ASN:HB2	1.94	0.49
1:D:257:ALA:O	1:D:260:LEU:HB2	2.12	0.49
1:D:63:LEU:HD13	1:D:111:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:LYS:HG2	1:C:661:ASN:H	1.77	0.49
1:A:394:MET:CE	1:A:502:LEU:HD12	2.42	0.49
1:C:612:VAL:HG21	1:C:671:ASN:HD22	1.77	0.49
1:A:243:MET:SD	1:A:283:LEU:HD23	2.53	0.49
1:C:420:ILE:HD12	1:C:442:TYR:CE1	2.47	0.49
1:B:625:LYS:HG3	1:B:626:ASP:N	2.26	0.48
1:C:181:ILE:HD11	1:C:236:LEU:HD12	1.95	0.48
1:C:727:HIS:NE2	1:C:794:GLU:OE2	2.39	0.48
1:A:612:VAL:HG23	1:A:671:ASN:HB2	1.95	0.48
1:B:766:SER:HB2	1:B:770:CYS:HB2	1.95	0.48
1:C:155:SER:HA	1:C:158:LEU:HD12	1.95	0.48
1:C:73:ILE:CG2	1:C:101:GLN:HE22	2.25	0.48
1:A:612:VAL:HG21	1:A:671:ASN:HD22	1.79	0.48
1:B:597:ILE:HD12	1:B:656:TYR:HA	1.95	0.48
1:D:177:ALA:O	1:D:181:ILE:HG13	2.13	0.48
1:A:178:TYR:CD1	1:D:248:LEU:HD11	2.48	0.48
1:D:506:TYR:HB3	1:D:526:TYR:CE2	2.48	0.48
1:C:597:ILE:HD11	1:C:621:LEU:CD2	2.44	0.48
1:D:723:ASP:N	1:D:723:ASP:OD1	2.40	0.48
1:B:175:THR:OG1	1:B:176:PRO:HD3	2.14	0.48
1:B:62:LEU:O	1:B:66:ILE:HD12	2.14	0.48
1:C:57:LEU:HD21	1:C:119:LEU:HD21	1.95	0.48
1:D:266:VAL:CG1	1:D:266:VAL:O	2.62	0.48
1:B:23:TYR:CE2	1:B:542:TYR:HB3	2.48	0.48
1:B:223:SER:CB	1:C:228:ASP:HB2	2.44	0.48
1:C:371:ASP:HB2	1:C:372:PRO:CD	2.41	0.48
1:A:348:ILE:HA	1:A:729:ARG:HD2	1.95	0.47
1:B:727:HIS:NE2	1:B:794:GLU:OE2	2.39	0.47
1:A:175:THR:OG1	1:A:176:PRO:HD3	2.14	0.47
1:A:229:MET:CE	1:C:180:ARG:HD3	2.44	0.47
1:D:181:ILE:CD1	1:D:236:LEU:HD12	2.44	0.47
1:B:352:ILE:HD12	1:B:434:GLU:HG2	1.97	0.47
1:A:168:ASN:ND2	1:C:168:ASN:ND2	2.62	0.47
1:D:130:LEU:HD13	1:D:217:LEU:HD21	1.96	0.47
1:D:532:LEU:O	1:D:537:LEU:HD22	2.14	0.47
1:D:725:THR:HG23	1:D:762:LYS:HG2	1.96	0.47
1:A:23:TYR:CE2	1:A:542:TYR:HB3	2.49	0.47
1:A:506:TYR:HB3	1:A:526:TYR:CE2	2.49	0.47
1:B:572:ASN:HB2	1:B:574:ASN:HB2	1.96	0.47
1:B:652:PRO:O	1:B:655:ILE:HD12	2.15	0.47
1:B:506:TYR:HB3	1:B:526:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ARG:NH2	1:B:792:VAL:HG13	2.30	0.47
1:B:58:LYS:NZ	1:C:55:GLU:OE1	2.36	0.47
1:D:623:ASN:HB3	1:D:626:ASP:OD1	2.14	0.47
1:D:732:VAL:O	1:D:754:ASP:HA	2.14	0.47
1:B:222:LYS:HA	1:B:301:LEU:HD11	1.96	0.47
1:B:394:MET:HE1	1:B:502:LEU:HD12	1.96	0.47
1:C:572:ASN:HB2	1:C:574:ASN:HB2	1.96	0.47
1:A:206:VAL:HG21	1:A:211:ILE:HD11	1.97	0.46
1:B:730:LEU:HD21	1:B:738:VAL:HG21	1.97	0.46
1:A:616:ARG:NH2	1:A:665:TYR:CE2	2.83	0.46
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.77	0.46
1:C:147:LEU:O	1:C:151:LEU:HB2	2.16	0.46
1:C:585:LEU:O	1:C:668:TRP:HA	2.16	0.46
1:B:603:PRO:HA	1:B:652:PRO:CG	2.45	0.46
1:C:732:VAL:CG1	1:C:786:PHE:CE2	2.98	0.46
1:D:167:ILE:CG1	1:D:260:LEU:HD21	2.44	0.46
1:B:243:MET:SD	1:B:283:LEU:HD23	2.56	0.46
1:C:263:LYS:C	1:C:265:ASN:H	2.19	0.46
1:D:117:SER:O	1:D:121:ILE:HG12	2.16	0.46
1:A:41:ILE:HG22	1:A:299:LYS:HG3	1.98	0.46
1:B:732:VAL:CG1	1:B:786:PHE:CE2	2.99	0.46
1:C:354:VAL:HG23	1:C:432:VAL:HG22	1.97	0.46
1:D:217:LEU:HG	1:D:300:LEU:CD2	2.45	0.46
1:A:608:VAL:HB	1:A:677:ILE:HD11	1.97	0.46
1:A:722:ASN:HB2	1:A:765:SER:HB3	1.98	0.46
1:B:585:LEU:O	1:B:668:TRP:HA	2.16	0.46
1:D:732:VAL:CG1	1:D:786:PHE:CE2	2.99	0.46
1:A:585:LEU:O	1:A:668:TRP:HA	2.15	0.46
1:B:619:ILE:CG2	1:B:657:PHE:CZ	2.98	0.46
1:C:597:ILE:HD11	1:C:621:LEU:HD21	1.98	0.46
1:D:160:ILE:HD11	1:D:265:ASN:HB2	1.97	0.46
1:A:730:LEU:HD21	1:A:738:VAL:HG21	1.98	0.45
1:C:147:LEU:HD13	1:C:282:VAL:HG23	1.99	0.45
1:C:506:TYR:HB3	1:C:526:TYR:CE2	2.51	0.45
1:A:603:PRO:HA	1:A:652:PRO:CG	2.46	0.45
1:B:449:TYR:CE1	1:B:454:GLY:HA2	2.51	0.45
1:B:59:ASN:ND2	1:C:59:ASN:OD1	2.48	0.45
1:B:608:VAL:HB	1:B:677:ILE:HD11	1.97	0.45
1:D:147:LEU:O	1:D:151:LEU:HB2	2.17	0.45
1:A:123:LEU:HD13	1:A:202:TYR:CD2	2.52	0.45
1:B:617:PRO:HA	1:B:661:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LYS:HE3	1:C:228:ASP:OD2	2.16	0.45
1:D:181:ILE:CD1	1:D:236:LEU:CD1	2.94	0.45
1:C:344:ARG:HD3	1:C:409:LYS:HE3	1.98	0.45
1:C:722:ASN:HB2	1:C:765:SER:HB3	1.98	0.45
1:D:167:ILE:HG12	1:D:260:LEU:CD2	2.43	0.45
1:D:722:ASN:HB2	1:D:765:SER:HB3	1.98	0.45
1:C:342:LYS:HG3	1:C:491:TYR:CD1	2.51	0.45
1:C:279:PHE:CE2	1:C:283:LEU:HD22	2.52	0.45
1:D:697:ASN:HB3	1:D:710:GLY:H	1.82	0.45
1:D:727:HIS:NE2	1:D:794:GLU:OE2	2.40	0.45
1:A:449:TYR:CE2	1:A:454:GLY:HA2	2.51	0.45
1:A:610:GLN:HA	1:A:642:VAL:O	2.17	0.45
1:B:394:MET:CE	1:B:502:LEU:HD12	2.47	0.45
1:B:722:ASN:HB2	1:B:765:SER:HB2	1.99	0.45
1:D:86:LEU:HD12	1:D:91:ALA:HB2	1.98	0.45
1:D:617:PRO:HA	1:D:661:ASN:HA	1.99	0.45
1:A:436:ARG:NH2	1:A:792:VAL:HG13	2.32	0.45
1:A:117:SER:HB2	1:A:121:ILE:HD13	1.98	0.44
1:B:188:PHE:CE2	1:B:192:THR:HG21	2.52	0.44
1:B:342:LYS:HG3	1:B:491:TYR:CD1	2.52	0.44
1:D:603:PRO:HA	1:D:652:PRO:CG	2.47	0.44
1:D:730:LEU:HA	1:D:788:ASN:O	2.17	0.44
1:B:730:LEU:HA	1:B:788:ASN:O	2.17	0.44
1:C:217:LEU:HG	1:C:300:LEU:CD2	2.47	0.44
1:D:613:ILE:O	1:D:613:ILE:HD12	2.17	0.44
1:A:342:LYS:HG3	1:A:491:TYR:CE1	2.52	0.44
1:A:660:LYS:HG2	1:A:661:ASN:H	1.82	0.44
1:B:354:VAL:HG23	1:B:432:VAL:HG22	1.99	0.44
1:B:616:ARG:NH2	1:B:635:ASN:HB2	2.32	0.44
1:C:418:LYS:O	1:C:442:TYR:OH	2.30	0.44
1:B:206:VAL:O	1:C:50:ASN:ND2	2.49	0.44
1:C:54:ASP:O	1:C:58:LYS:HG3	2.17	0.44
1:C:730:LEU:HA	1:C:788:ASN:O	2.17	0.44
1:B:165:VAL:CG2	1:D:160:ILE:O	2.65	0.44
1:D:154:ILE:HG12	1:D:268:THR:HG21	2.00	0.44
1:D:449:TYR:CE2	1:D:454:GLY:HA2	2.52	0.44
1:B:364:ILE:HG21	1:B:502:LEU:HB3	1.99	0.44
1:C:177:ALA:O	1:C:181:ILE:HG13	2.16	0.44
1:D:363:LEU:HD23	1:D:429:THR:C	2.38	0.44
1:A:299:LYS:HD3	1:A:305:ASP:OD1	2.17	0.44
1:A:412:GLU:OE1	1:A:482:ILE:HD11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:LEU:HB2	1:A:629:PHE:HB3	1.99	0.44
1:A:730:LEU:HA	1:A:788:ASN:O	2.18	0.44
1:C:150:GLN:OE1	1:C:500:THR:HB	2.18	0.44
1:C:610:GLN:HA	1:C:642:VAL:O	2.18	0.44
1:D:348:ILE:HG13	1:D:788:ASN:HD22	1.82	0.44
1:A:214:LEU:O	1:A:218:THR:HG23	2.18	0.44
1:B:344:ARG:HD3	1:B:409:LYS:HE3	2.00	0.44
1:B:86:LEU:HG	1:B:90:LEU:HD23	1.98	0.44
1:C:394:MET:HE2	1:C:502:LEU:CD1	2.47	0.44
1:D:175:THR:O	1:D:179:GLN:CG	2.58	0.44
1:D:342:LYS:HG2	1:D:491:TYR:HE1	1.81	0.44
1:A:229:MET:HB3	1:C:180:ARG:HD3	1.99	0.43
1:A:229:MET:HE3	1:C:180:ARG:HD3	2.00	0.43
1:D:40:MET:CE	1:D:132:GLU:HB3	2.48	0.43
1:D:610:GLN:HA	1:D:642:VAL:O	2.18	0.43
1:B:610:GLN:HA	1:B:642:VAL:O	2.18	0.43
1:B:619:ILE:CG2	1:B:657:PHE:HE1	2.29	0.43
1:B:38:MET:HE2	1:B:291:PHE:HB3	2.01	0.43
1:C:154:ILE:HG12	1:C:268:THR:HG21	2.00	0.43
1:D:214:LEU:O	1:D:218:THR:HG23	2.18	0.43
1:D:251:ARG:HH11	1:D:255:LYS:HB3	1.83	0.43
1:A:324:ARG:HG3	1:A:536:LEU:HD13	2.01	0.43
1:C:214:LEU:O	1:C:218:THR:HG23	2.18	0.43
1:C:730:LEU:HD21	1:C:738:VAL:HG21	1.98	0.43
1:D:649:GLY:H	1:D:652:PRO:HB3	1.82	0.43
1:C:621:LEU:HB2	1:C:629:PHE:HB3	1.99	0.43
1:D:382:ARG:HB2	1:D:393:SER:OG	2.19	0.43
1:D:686:MET:HB3	1:D:718:ILE:HD11	2.00	0.43
1:C:449:TYR:CE2	1:C:454:GLY:HA2	2.53	0.43
1:A:196:GLU:HB3	1:A:202:TYR:CZ	2.53	0.43
1:B:34:ILE:HG13	1:B:288:ALA:HB1	2.00	0.43
1:C:86:LEU:HD12	1:C:91:ALA:HB2	2.01	0.43
1:D:621:LEU:HB2	1:D:629:PHE:HB3	1.99	0.43
1:C:603:PRO:HA	1:C:652:PRO:CG	2.48	0.43
1:D:150:GLN:OE1	1:D:500:THR:HB	2.18	0.43
1:B:214:LEU:O	1:B:218:THR:HG23	2.19	0.43
1:B:324:ARG:HG3	1:B:536:LEU:HD13	2.01	0.43
1:B:382:ARG:HB2	1:B:393:SER:OG	2.19	0.43
1:B:730:LEU:HD12	1:B:730:LEU:C	2.39	0.43
1:C:741:ILE:HD11	1:C:771:PHE:HZ	1.84	0.43
1:A:730:LEU:HD12	1:A:730:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ARG:HB2	1:C:393:SER:OG	2.19	0.43
1:B:126:ILE:HA	1:B:126:ILE:HD13	1.84	0.42
1:B:223:SER:HB2	1:C:228:ASP:HB2	2.00	0.42
1:B:660:LYS:HG2	1:B:661:ASN:H	1.83	0.42
1:C:63:LEU:HD13	1:C:111:GLN:HB2	2.01	0.42
1:A:737:ARG:HD2	1:A:749:PHE:CZ	2.54	0.42
1:C:126:ILE:HD13	1:C:126:ILE:HA	1.85	0.42
1:D:46:THR:HG22	1:D:125:LYS:HB2	2.00	0.42
1:D:711:ASP:HB2	1:D:778:TYR:HD2	1.84	0.42
1:A:623:ASN:HB2	1:A:655:ILE:HG13	2.01	0.42
1:D:324:ARG:HG3	1:D:536:LEU:HD13	2.02	0.42
1:A:134:MET:SD	1:A:193:SER:HA	2.60	0.42
1:B:616:ARG:HH21	1:B:635:ASN:HB2	1.84	0.42
1:C:73:ILE:HG21	1:C:101:GLN:HE22	1.85	0.42
1:C:144:ILE:O	1:C:147:LEU:HG	2.19	0.42
1:C:236:LEU:HA	1:C:236:LEU:HD12	1.79	0.42
1:D:398:ILE:HG21	1:D:677:ILE:HD13	2.02	0.42
1:D:54:ASP:O	1:D:58:LYS:HG3	2.20	0.42
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.85	0.42
1:B:223:SER:OG	1:C:228:ASP:HB2	2.20	0.42
1:C:243:MET:SD	1:C:283:LEU:HD23	2.59	0.42
1:C:375:ILE:HD11	1:C:677:ILE:HD13	2.02	0.42
1:B:70:LEU:HD23	1:B:70:LEU:HA	1.85	0.42
1:C:111:GLN:O	1:C:115:ILE:HD13	2.19	0.42
1:C:412:GLU:OE1	1:C:482:ILE:HD11	2.19	0.42
1:C:730:LEU:HD12	1:C:730:LEU:C	2.40	0.42
1:D:572:ASN:HB3	1:D:574:ASN:H	1.85	0.42
1:B:348:ILE:HG13	1:B:788:ASN:HD22	1.83	0.42
1:A:354:VAL:HG23	1:A:432:VAL:HG22	2.01	0.42
1:A:727:HIS:NE2	1:A:794:GLU:OE2	2.39	0.42
1:C:236:LEU:HD11	1:C:290:ALA:CB	2.50	0.42
1:D:101:GLN:HE21	1:D:101:GLN:HB2	1.65	0.41
1:A:69:LYS:NZ	1:D:103:GLN:HB3	2.36	0.41
1:B:131:ASN:HA	1:B:197:LYS:HE2	2.02	0.41
1:A:279:PHE:CE2	1:A:283:LEU:HD22	2.54	0.41
1:A:91:ALA:HB3	1:B:82:ALA:HB1	2.01	0.41
1:A:166:LEU:CD1	1:A:251:ARG:NH2	2.84	0.41
1:A:299:LYS:NZ	1:A:305:ASP:OD1	2.53	0.41
1:A:345:GLY:O	1:A:409:LYS:HB3	2.20	0.41
1:D:342:LYS:CG	1:D:491:TYR:HE1	2.34	0.41
1:A:188:PHE:CE2	1:A:192:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HA	1:A:301:LEU:HD11	2.02	0.41
1:C:616:ARG:HG2	1:C:635:ASN:CB	2.50	0.41
1:D:737:ARG:HD2	1:D:749:PHE:CZ	2.55	0.41
1:B:723:ASP:N	1:B:723:ASP:OD1	2.38	0.41
1:C:596:PHE:HA	1:C:656:TYR:CB	2.51	0.41
1:B:572:ASN:CB	1:B:574:ASN:H	2.34	0.41
1:B:737:ARG:HD2	1:B:749:PHE:CZ	2.55	0.41
1:C:723:ASP:OD1	1:C:723:ASP:N	2.38	0.41
1:A:195:VAL:HG12	1:A:202:TYR:OH	2.21	0.41
1:C:277:TYR:O	1:C:281:ILE:HG13	2.21	0.41
1:B:198:ASN:OD1	1:B:200:LYS:HG2	2.21	0.41
1:B:230:ASP:OD1	1:B:235:TYR:HE2	2.02	0.41
1:B:23:TYR:CE1	1:B:391:ARG:HB2	2.56	0.41
1:D:730:LEU:C	1:D:730:LEU:HD12	2.40	0.41
1:C:616:ARG:HG2	1:C:635:ASN:CA	2.50	0.41
1:C:622:LYS:HG2	1:C:623:ASN:N	2.36	0.41
1:D:126:ILE:HD13	1:D:126:ILE:HA	1.85	0.41
1:D:243:MET:SD	1:D:283:LEU:HD23	2.61	0.41
1:D:316:ILE:CD1	1:D:316:ILE:N	2.84	0.41
1:D:342:LYS:HE3	1:D:491:TYR:HE1	1.85	0.41
1:A:223:SER:HB2	1:D:228:ASP:HB2	2.03	0.41
1:B:619:ILE:HG23	1:B:657:PHE:CZ	2.56	0.40
1:C:623:ASN:HB2	1:C:655:ILE:CD1	2.51	0.40
1:C:686:MET:HB3	1:C:718:ILE:HD11	2.03	0.40
1:A:60:GLN:OE1	1:A:119:LEU:CD1	2.70	0.40
1:C:616:ARG:HD2	1:C:665:TYR:CE2	2.56	0.40
1:D:261:ILE:HA	1:D:266:VAL:HG11	2.03	0.40
1:D:345:GLY:O	1:D:409:LYS:HB3	2.21	0.40
1:D:597:ILE:O	1:D:597:ILE:CG2	2.70	0.40
1:A:277:TYR:O	1:A:281:ILE:HG13	2.22	0.40
1:B:198:ASN:OD1	1:B:200:LYS:CG	2.70	0.40
1:D:700:MET:CG	1:D:700:MET:O	2.69	0.40
1:A:382:ARG:HB2	1:A:393:SER:OG	2.21	0.40
1:C:617:PRO:HA	1:C:661:ASN:HA	2.02	0.40
1:D:328:LEU:HB3	1:D:329:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	740/796 (93%)	691 (93%)	48 (6%)	1 (0%)	51 83
1	B	736/796 (92%)	693 (94%)	43 (6%)	0	100 100
1	C	729/796 (92%)	682 (94%)	46 (6%)	1 (0%)	51 83
1	D	715/796 (90%)	673 (94%)	41 (6%)	1 (0%)	51 83
All	All	2920/3184 (92%)	2739 (94%)	178 (6%)	3 (0%)	51 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	371	ASP
1	D	229	MET
1	A	204	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	680/718 (95%)	670 (98%)	10 (2%)	65 85
1	B	678/718 (94%)	667 (98%)	11 (2%)	62 83
1	C	663/718 (92%)	650 (98%)	13 (2%)	55 79
1	D	658/718 (92%)	650 (99%)	8 (1%)	71 87
All	All	2679/2872 (93%)	2637 (98%)	42 (2%)	62 83

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	339	SER
1	A	373	LEU
1	A	478	ASP
1	A	481	SER
1	A	498	SER
1	A	554	ILE
1	A	613	ILE
1	A	677	ILE
1	A	760	VAL
1	B	215	ASN
1	B	256	THR
1	B	339	SER
1	B	344	ARG
1	B	359	PRO
1	B	373	LEU
1	B	478	ASP
1	B	481	SER
1	B	498	SER
1	B	677	ILE
1	B	754	ASP
1	C	40	MET
1	C	181	ILE
1	C	215	ASN
1	C	260	LEU
1	C	339	SER
1	C	344	ARG
1	C	370	ASN
1	C	373	LEU
1	C	391	ARG
1	C	481	SER
1	C	498	SER
1	C	613	ILE
1	C	627	THR
1	D	56	ILE
1	D	339	SER
1	D	373	LEU
1	D	498	SER
1	D	551	ILE
1	D	627	THR
1	D	658	LEU
1	D	760	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	111	GLN
1	A	168	ASN
1	A	572	ASN
1	A	574	ASN
1	A	670	ASN
1	A	788	ASN
1	B	74	ASN
1	B	101	GLN
1	B	107	HIS
1	B	213	ASN
1	B	572	ASN
1	B	588	HIS
1	B	623	ASN
1	B	670	ASN
1	C	74	ASN
1	C	101	GLN
1	C	102	ASN
1	C	168	ASN
1	C	370	ASN
1	C	574	ASN
1	C	647	ASN
1	C	670	ASN
1	C	788	ASN
1	D	74	ASN
1	D	102	ASN
1	D	574	ASN
1	D	647	ASN
1	D	670	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	752/796 (94%)	-0.02	16 (2%)	63	49	58, 106, 163, 202	0
1	B	750/796 (94%)	0.07	38 (5%)	28	15	59, 109, 183, 251	0
1	C	739/796 (92%)	-0.03	22 (2%)	50	34	63, 118, 172, 221	0
1	D	731/796 (91%)	0.13	32 (4%)	34	20	64, 118, 176, 230	0
All	All	2972/3184 (93%)	0.04	108 (3%)	42	27	58, 112, 174, 251	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	577	VAL	6.2
1	D	585	LEU	6.1
1	B	786	PHE	5.0
1	D	659	PHE	4.7
1	D	657	PHE	4.7
1	D	714	PHE	4.7
1	B	686	MET	4.5
1	D	786	PHE	4.5
1	A	720	LEU	4.4
1	B	745	LYS	4.4
1	B	447	ASN	4.3
1	B	747	LEU	4.3
1	D	766	SER	4.2
1	C	406	PHE	4.1
1	B	692	TRP	3.8
1	D	593	PHE	3.7
1	D	672	PHE	3.7
1	B	761	ILE	3.6
1	B	657	PHE	3.6
1	D	706	LEU	3.6
1	B	741	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	577	VAL	3.4
1	D	658	LEU	3.4
1	B	744	SER	3.3
1	D	576	PHE	3.3
1	A	568	TRP	3.3
1	D	620	TYR	3.3
1	B	659	PHE	3.3
1	A	592	GLU	3.2
1	B	656	TYR	3.2
1	D	195	VAL	3.1
1	A	747	LEU	3.1
1	D	619	ILE	3.0
1	B	455	SER	3.0
1	C	786	PHE	3.0
1	C	405	LEU	3.0
1	A	593	PHE	2.9
1	D	778	TYR	2.9
1	C	483	ILE	2.9
1	D	440	LEU	2.9
1	D	595	GLN	2.9
1	B	788	ASN	2.9
1	C	657	PHE	2.8
1	B	461	VAL	2.8
1	B	791	ILE	2.8
1	C	589	LYS	2.8
1	B	728	LEU	2.8
1	A	741	ILE	2.8
1	B	746	TYR	2.8
1	B	740	ILE	2.7
1	A	687	LEU	2.7
1	B	592	GLU	2.7
1	C	484	LYS	2.6
1	A	654	GLU	2.6
1	B	698	VAL	2.5
1	D	711	ASP	2.5
1	B	789	VAL	2.5
1	B	706	LEU	2.5
1	C	593	PHE	2.5
1	C	585	LEU	2.5
1	B	571	ASN	2.5
1	B	759	ARG	2.5
1	C	706	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	593	PHE	2.5
1	D	348	ILE	2.5
1	B	764	THR	2.4
1	A	656	TYR	2.4
1	C	611	TYR	2.4
1	B	730	LEU	2.4
1	D	698	VAL	2.4
1	D	625	LYS	2.4
1	B	690	GLU	2.3
1	C	568	TRP	2.3
1	D	655	ILE	2.3
1	A	718	ILE	2.3
1	B	687	LEU	2.3
1	B	720	LEU	2.2
1	B	568	TRP	2.2
1	C	738	VAL	2.2
1	C	701	LYS	2.2
1	B	762	LYS	2.2
1	B	699	GLN	2.2
1	C	486	GLU	2.2
1	D	592	GLU	2.2
1	A	508	PHE	2.2
1	C	586	TYR	2.2
1	D	575	ALA	2.2
1	C	664	GLU	2.2
1	A	764	THR	2.2
1	B	694	PRO	2.1
1	A	627	THR	2.1
1	B	774	LEU	2.1
1	A	762	LYS	2.1
1	C	551	ILE	2.1
1	D	590	ASP	2.1
1	D	488	ASP	2.1
1	D	490	ILE	2.1
1	A	659	PHE	2.1
1	B	646	PHE	2.1
1	B	570	ALA	2.1
1	D	519	ILE	2.1
1	D	774	LEU	2.1
1	C	366	PHE	2.0
1	C	555	VAL	2.0
1	D	712	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	366	PHE	2.0
1	A	730	LEU	2.0
1	C	569	ARG	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.