



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:44 AM UTC

PDB ID : 6V1V / pdb_00006v1v
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

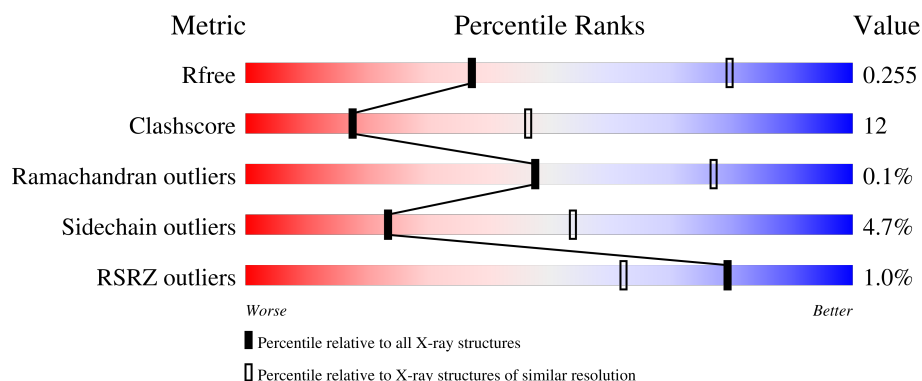
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 71% 22% 6%
1	B	796	2% 70% 23% 6%
1	C	796	68% 23% 7%
1	D	796	2% 67% 23% 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

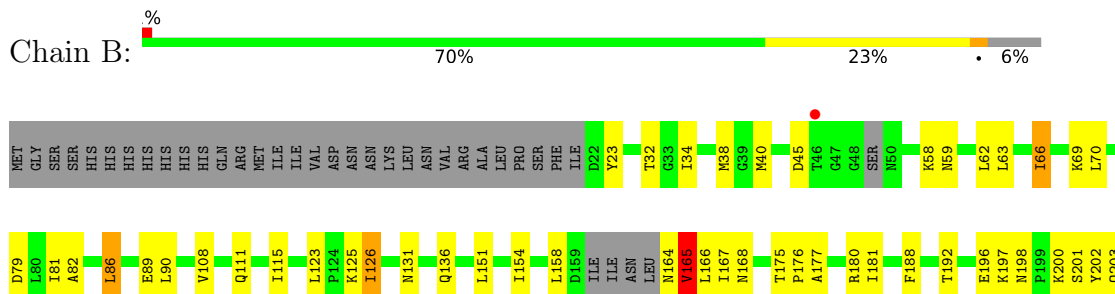
3 Residue-property plots

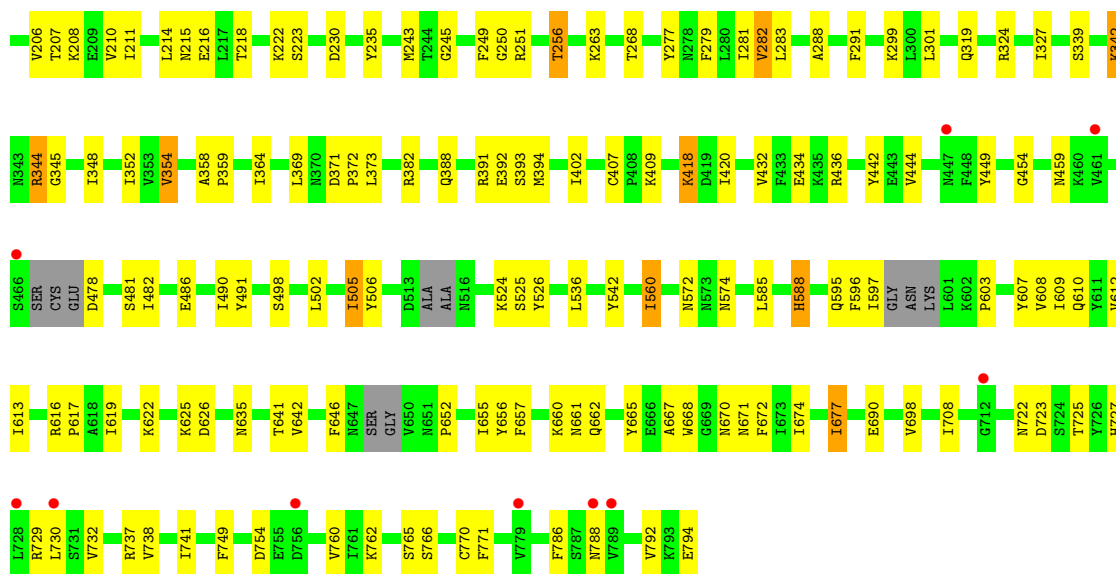
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Vegetative insecticidal protein



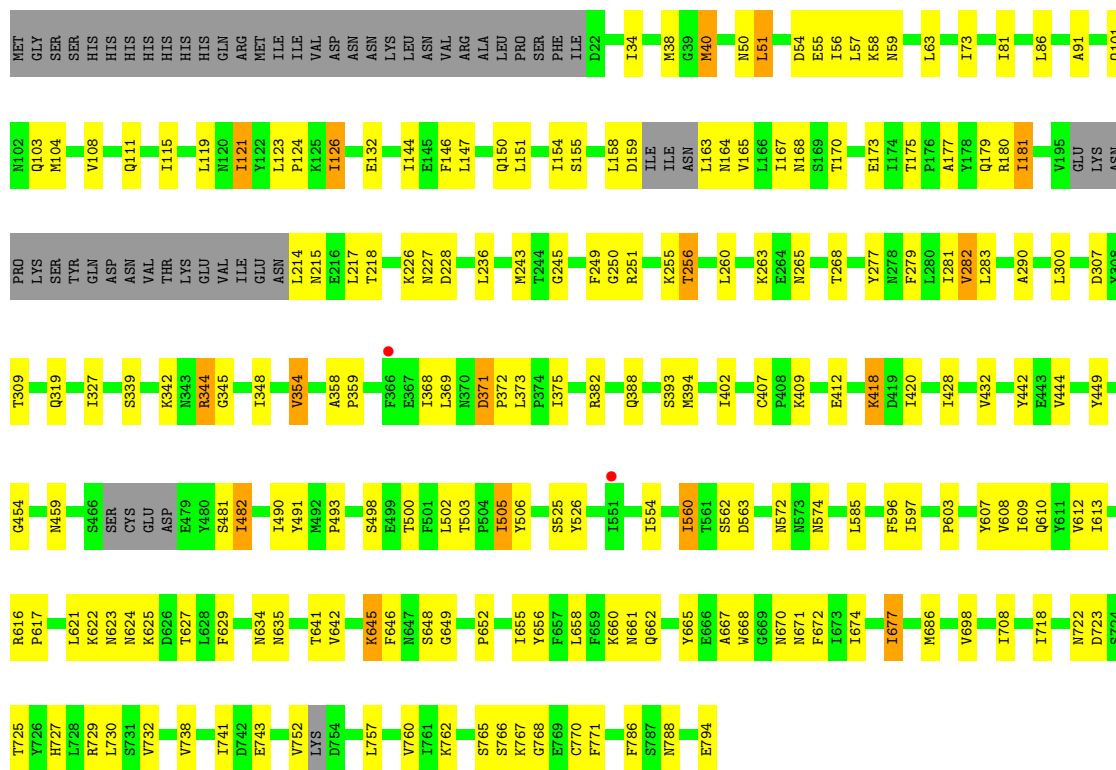
• Molecule 1: Vegetative insecticidal protein





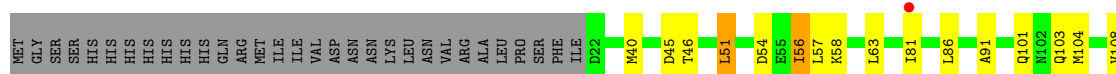
• Molecule 1: Vegetative insecticidal protein

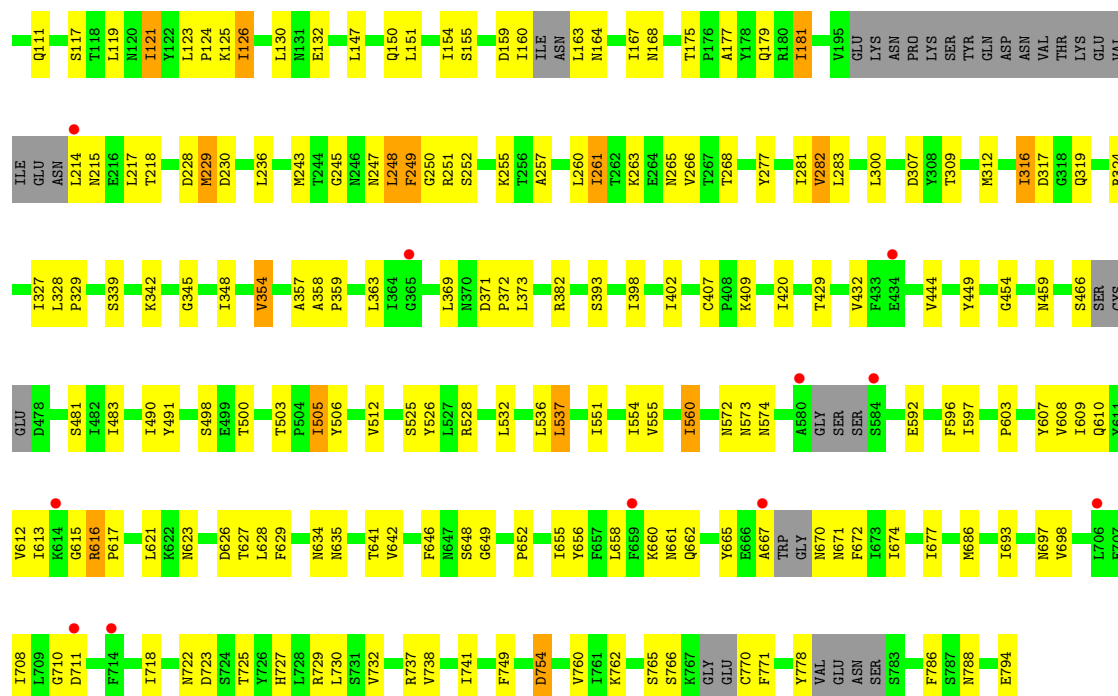
Chain C: 68% 23% 7%



• Molecule 1: Vegetative insecticidal protein

Chain D: 2% 67% 23% 8%





4 Data and refinement statistics

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 49.89 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.89-3.19) 98.3 (49.89-3.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.218 , 0.259 0.215 , 0.255	Depositor DCC
R_{free} test set	3538 reflections (4.79%)	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)	0.32 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.88	1/6105 (0.0%)	1.29	5/8254 (0.1%)
1	B	0.88	0/6087	1.30	9/8229 (0.1%)
1	C	0.89	0/5976	1.30	9/8082 (0.1%)
1	D	0.88	0/5919	1.33	20/7999 (0.3%)
All	All	0.88	1/24087 (0.0%)	1.31	43/32564 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	752	VAL	C-O	-5.37	1.18	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	573	ASN	N-CA-C	-7.95	103.58	113.20
1	B	588	HIS	CA-CB-CG	7.03	120.83	113.80
1	C	767	LYS	N-CA-C	-6.92	103.35	111.03
1	D	263	LYS	CA-C-N	6.82	129.74	120.54
1	D	263	LYS	C-N-CA	6.82	129.74	120.54
1	D	230	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	32	THR	CB-CA-C	6.09	121.84	110.70
1	C	624	ASN	CB-CA-C	5.85	118.59	110.16
1	D	615	GLY	CA-C-N	-5.70	116.70	122.74
1	D	615	GLY	C-N-CA	-5.70	116.70	122.74
1	D	121	ILE	CA-C-N	5.53	128.48	120.79
1	D	121	ILE	C-N-CA	5.53	128.48	120.79
1	D	282	VAL	CA-C-N	5.53	128.14	120.29
1	D	282	VAL	C-N-CA	5.53	128.14	120.29
1	B	486	GLU	CB-CA-C	5.50	118.91	109.51
1	A	282	VAL	O-C-N	5.42	127.22	121.91
1	C	165	VAL	N-CA-C	-5.40	107.16	111.81
1	D	159	ASP	N-CA-C	-5.40	107.35	114.04
1	C	319	GLN	CB-CA-C	5.39	119.73	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	VAL	CA-C-N	5.36	127.90	120.29
1	C	282	VAL	C-N-CA	5.36	127.90	120.29
1	B	263	LYS	N-CA-C	-5.32	103.94	110.65
1	B	319	GLN	CB-CA-C	5.31	119.61	110.79
1	B	165	VAL	N-CA-C	-5.30	107.25	111.81
1	B	282	VAL	CA-C-N	5.29	127.81	120.29
1	B	282	VAL	C-N-CA	5.29	127.81	120.29
1	B	459	ASN	N-CA-C	-5.26	106.99	113.41
1	D	249	PHE	CA-CB-CG	5.23	119.03	113.80
1	D	317	ASP	CA-C-O	-5.22	114.21	120.10
1	D	261	ILE	CA-C-N	5.17	127.72	120.28
1	D	261	ILE	C-N-CA	5.17	127.72	120.28
1	D	616	ARG	CB-CA-C	5.16	119.67	111.15
1	A	282	VAL	CA-C-N	5.14	127.59	120.29
1	A	282	VAL	C-N-CA	5.14	127.59	120.29
1	A	459	ASN	N-CA-C	-5.12	107.16	113.41
1	A	121	ILE	N-CA-C	-5.09	106.11	110.74
1	C	459	ASN	N-CA-C	-5.09	107.20	113.41
1	D	319	GLN	CB-CA-C	5.05	119.18	110.79
1	D	459	ASN	N-CA-C	-5.05	107.25	113.41
1	C	121	ILE	CA-C-N	5.01	127.26	120.65
1	C	121	ILE	C-N-CA	5.01	127.26	120.65
1	D	754	ASP	CA-CB-CG	5.00	117.61	112.60
1	D	263	LYS	CB-CA-C	5.00	118.49	110.29

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	126	0
1	B	5985	0	5950	146	0
1	C	5874	0	5847	173	0
1	D	5822	0	5811	178	0
All	All	23683	0	23578	585	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 (585) 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:B:70:LEU:HG	1:C:104:MET:HE1	1.09	1.06
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: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:A:229:MET:HE3	1:C:180:ARG:HD3	1.61	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:70:LEU:HG	1:C:104:MET:CE	2.04	0.80
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:HD23	1:A:537:LEU:O	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:A:177:ALA:O	1:A:181:ILE:HG12	1.87	0.74
1:C:394:MET:HE1	1:C:502:LEU:HD12	1.70	0.73
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:B:622:LYS:C	1:B:655:ILE:HG23	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:C:625:LYS:HG2	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:D:123:LEU:HD23	1:D:123:LEU:C	2.21	0.65
1:C:123:LEU:C	1:C:123:LEU:HD23	2.21	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:70:LEU:HD23	1:D:104:MET:HE1	1.77	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:D:328:LEU:C	1:D:328:LEU:HD13	2.22	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: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:A:394:MET:HE1	1:A:502:LEU:HD12	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:MET:HE2	1:D:132:GLU:HB3	1.82	0.62
1:A:164:ASN:CB	1:A:167:ILE:HD13	2.29	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:A:184:VAL:CG2	1:D:229:MET:HG2	2.31	0.61
1:B:166:LEU:HB3	1:B:251:ARG:CD	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:617:PRO:HB3	1:C:667:ALA:CB	2.29	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:A:155:SER:HB3	1:D:250:GLY:HA3	1.82	0.60
1:C:616:ARG:O	1:C:662:GLN:HG2	2.02	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:A:73:ILE:HD12	1:D:104:MET:CE	2.31	0.60
1:C:147:LEU:CD1	1:C:282:VAL:HG22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:652:PRO:C	1:B:655:ILE:CD1	2.77	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
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:554:ILE:CG1	1:D:674:ILE:CG2	2.72	0.58
1:D:648:SER:HB2	1:D:652:PRO:CG	2.33	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: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:560:ILE:N	1:C:670:ASN:HD22	1.99	0.57
1:C:661:ASN:ND2	1:C:665:TYR:O	2.37	0.57
1:B:619:ILE:HG23	1:B:657:PHE:CE1	2.40	0.57
1:B:652:PRO:C	1:B:655:ILE:HD12	2.30	0.56
1:A:310:GLN:HA	1:A:310:GLN:OE1	2.04	0.56
1:A:506:TYR:CD1	1:A:506:TYR:C	2.84	0.56
1:C:249:PHE:CE2	1:C:251:ARG:HB3	2.41	0.56
1:C:732:VAL:HG12	1:C:786:PHE:CD2	2.40	0.56
1:C:743:GLU:HG3	1:C:768:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:SER:HB2	1:C:770:CYS:SG	2.45	0.56
1:D:483:ILE:HD11	1:D:512:VAL:CG2	2.35	0.56
1:D:506:TYR:CD1	1:D:506:TYR:C	2.84	0.56
1:B:506:TYR:CD1	1:B:506:TYR:C	2.84	0.56
1:C:159:ASP:C	1:C:159:ASP:OD1	2.49	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
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:506:TYR:CD1	1:C:506:TYR:C	2.84	0.55
1:C:164:ASN:CB	1:C:167:ILE:HD13	2.31	0.55
1:B:574:ASN:OD1	1:B:588:HIS:HD2	1.91	0.54
1:A:62:LEU:HD21	1:D:63:LEU:HD21	1.89	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: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:51:LEU:HD12	1:D:56:ILE:CG1	2.33	0.54
1:D:249:PHE:HE2	1:D:251:ARG:HB3	1.72	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:69:LYS:HD3	1:D:104:MET:HG3	1.90	0.54
1:A:202:TYR:HA	1:A:206:VAL:HG23	1.88	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:208:LYS:N	1:C:50:ASN:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:HD3	1:B:256:THR:HG23	1.90	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: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:D:247:ASN:O	1:D:248:LEU:HB2	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
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:B:394:MET:HE1	1:B:502:LEU:HD12	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: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: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: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:O	1:B:690:GLU:HG2	2.10	0.51
1:C:616:ARG:HG2	1:C:635:ASN:HA	1.91	0.51
1:C:86:LEU:CD1	1:C:91:ALA:HB2	2.41	0.51
1:C:394:MET:CE	1:C:502:LEU:HD12	2.40	0.51
1:C:616:ARG:HD2	1:C:665:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:VAL:HG23	1:D:432:VAL:HG22	1.93	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
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:C:263:LYS:C	1:C:265:ASN:H	2.19	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: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: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:73:ILE:CG2	1:C:101:GLN:NE2	2.75	0.50
1:C:147:LEU:HD13	1:C:282:VAL:CG2	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:63:LEU:HD13	1:D:111:GLN:HB2	1.94	0.49
1:D:257:ALA:O	1:D:260:LEU:HB2	2.12	0.49
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:D:363:LEU:HD23	1:D:429:THR:C	2.38	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:73:ILE:CG2	1:C:101:GLN:HE22	2.25	0.48
1:C:155:SER:HA	1:C:158:LEU:HD12	1.95	0.48
1:A:178:TYR:CD1	1:D:248:LEU:HD11	2.48	0.48
1:A:612:VAL:HG21	1:A:671:ASN:HD22	1.79	0.48
1:B:38:MET:HE1	1:B:291:PHE:HB3	1.96	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: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:OD1	1:D:723:ASP:N	2.40	0.48
1:A:73:ILE:HD12	1:D:104:MET:HE3	1.96	0.48
1:B:62:LEU:O	1:B:66:ILE:HD12	2.14	0.48
1:B:175:THR:OG1	1:B:176:PRO:HD3	2.14	0.48
1:C:57:LEU:HD21	1:C:119:LEU:HD21	1.95	0.48
1:D:266:VAL:O	1:D:266:VAL:CG1	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:B:418:LYS:O	1:B:442:TYR:OH	2.31	0.47
1:B:730:LEU:C	1:B:730:LEU:HD12	2.39	0.47
1:D:181:ILE:CD1	1:D:236:LEU:HD12	2.44	0.47
1:A:38:MET:HE1	1:A:291:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:LEU:HD12	1:A:730:LEU:C	2.39	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:418:LYS:O	1:A:442:TYR:OH	2.32	0.47
1:C:418:LYS:O	1:C:442:TYR:OH	2.30	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:C:730:LEU:HD12	1:C:730:LEU:C	2.40	0.47
1:B:58:LYS:NZ	1:C:55:GLU:OE1	2.36	0.47
1:B:436:ARG:NH2	1:B:792:VAL:HG13	2.30	0.47
1:B:506:TYR:HB3	1:B:526:TYR:CE2	2.49	0.47
1:D:623:ASN:HB3	1:D:626:ASP:OD1	2.14	0.47
1:B:34:ILE:CG2	1:B:38:MET:HE3	2.45	0.47
1:D:730:LEU:HD12	1:D:730:LEU:C	2.40	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: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:HD23	1:B:123:LEU:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LEU:O	1:A:668:TRP:HA	2.15	0.46
1:B:249:PHE:O	1:D:155:SER:OG	2.26	0.46
1:B:619:ILE:CG2	1:B:657:PHE:CZ	2.98	0.46
1:C:40:MET:HE1	1:C:132:GLU:CB	2.46	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:59:ASN:ND2	1:C:59:ASN:OD1	2.48	0.45
1:B:449:TYR:CE1	1:B:454:GLY:HA2	2.51	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
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:572:ASN:C	1:D:574:ASN:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:613:ILE:HD12	1:D:613:ILE:O	2.17	0.44
1:A:34:ILE:CG2	1:A:38:MET:HE3	2.47	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:B:165:VAL:CG2	1:D:160:ILE:O	2.65	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: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: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
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:70:LEU:HA	1:D:104:MET:HE1	2.00	0.44
1:A:214:LEU:O	1:A:218:THR:HG23	2.18	0.44
1:B:86:LEU:HG	1:B:90:LEU:HD23	1.98	0.44
1:B:344:ARG:HD3	1:B:409:LYS:HE3	2.00	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: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: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:307:ASP:CG	1:C:309:THR:HG22	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:40:MET:CE	1:D:132:GLU:HB3	2.48	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:34:ILE:CG2	1:C:38:MET:HE3	2.49	0.43
1:C:86:LEU:HD12	1:C:91:ALA:HB2	2.01	0.43
1:D:307:ASP:CG	1:D:309:THR:HG22	2.43	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:C:741:ILE:HD11	1:C:771:PHE:HZ	1.84	0.43
1:B:168:ASN:HD21	1:D:168:ASN:CG	2.18	0.43
1:C:382:ARG:HB2	1:C:393:SER:OG	2.19	0.43
1:B:126:ILE:HD13	1:B:126:ILE:HA	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:58:LYS:HZ3	1:D:51:LEU:HA	1.85	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:HD12	1:C:236:LEU:HA	1.79	0.42
1:D:54:ASP:O	1:D:58:LYS:HG3	2.20	0.42
1:D:398:ILE:HG21	1:D:677:ILE:HD13	2.02	0.42
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.85	0.42
1:A:752:VAL:C	1:A:753:LYS:HG3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:40:MET:HE2	1:B:136:GLN:HE22	1.85	0.41
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:C:757:LEU:C	1:C:757:LEU:HD12	2.46	0.41
1:A:91:ALA:HB3	1:B:82:ALA:HB1	2.01	0.41
1:A:279:PHE:CE2	1:A:283:LEU:HD22	2.54	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
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:OD1	1:B:723:ASP:N	2.38	0.41
1:C:596:PHE:HA	1:C:656:TYR:CB	2.51	0.41
1:D:123:LEU:C	1:D:123:LEU:CD2	2.92	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:123:LEU:C	1:C:123:LEU:CD2	2.93	0.41
1:C:723:ASP:OD1	1:C:723:ASP:N	2.38	0.41
1:A:40:MET:HE2	1:A:136:GLN:HE22	1.86	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:A:73:ILE:CD1	1:D:104:MET:HE3	2.50	0.41
1:B:23:TYR:CE1	1:B:391:ARG:HB2	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/796 (93%)	691 (93%)	48 (6%)	1 (0%)	48	77
1	B	736/796 (92%)	693 (94%)	43 (6%)	0	100	100
1	C	729/796 (92%)	682 (94%)	46 (6%)	1 (0%)	48	77
1	D	715/796 (90%)	673 (94%)	41 (6%)	1 (0%)	48	77
All	All	2920/3184 (92%)	2739 (94%)	178 (6%)	3 (0%)	48	77

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 ⓘ

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%)	650 (96%)	30 (4%)	25	55
1	B	678/718 (94%)	643 (95%)	35 (5%)	21	51
1	C	663/718 (92%)	629 (95%)	34 (5%)	21	51
1	D	658/718 (92%)	630 (96%)	28 (4%)	26	56
All	All	2679/2872 (93%)	2552 (95%)	127 (5%)	23	54

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ILE
1	A	81	ILE
1	A	86	LEU
1	A	89	GLU
1	A	108	VAL
1	A	115	ILE
1	A	126	ILE
1	A	165	VAL
1	A	215	ASN
1	A	327	ILE
1	A	339	SER
1	A	354	VAL
1	A	373	LEU
1	A	388	GLN
1	A	402	ILE
1	A	418	LYS
1	A	466	SER
1	A	478	ASP
1	A	498	SER

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Mol	Chain	Res	Type
1	A	503	THR
1	A	505	ILE
1	A	524	LYS
1	A	554	ILE
1	A	560	ILE
1	A	597	ILE
1	A	609	ILE
1	A	613	ILE
1	A	627	THR
1	A	677	ILE
1	A	760	VAL
1	B	66	ILE
1	B	81	ILE
1	B	86	LEU
1	B	89	GLU
1	B	108	VAL
1	B	115	ILE
1	B	126	ILE
1	B	158	LEU
1	B	165	VAL
1	B	211	ILE
1	B	215	ASN
1	B	256	THR
1	B	299	LYS
1	B	327	ILE
1	B	339	SER
1	B	342	LYS
1	B	344	ARG
1	B	354	VAL
1	B	369	LEU
1	B	373	LEU
1	B	388	GLN
1	B	402	ILE
1	B	418	LYS
1	B	478	ASP
1	B	481	SER
1	B	482	ILE
1	B	490	ILE
1	B	498	SER
1	B	505	ILE
1	B	524	LYS
1	B	560	ILE

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Mol	Chain	Res	Type
1	B	609	ILE
1	B	613	ILE
1	B	677	ILE
1	B	760	VAL
1	C	40	MET
1	C	51	LEU
1	C	81	ILE
1	C	108	VAL
1	C	121	ILE
1	C	126	ILE
1	C	181	ILE
1	C	215	ASN
1	C	256	THR
1	C	260	LEU
1	C	327	ILE
1	C	339	SER
1	C	344	ARG
1	C	354	VAL
1	C	369	LEU
1	C	373	LEU
1	C	388	GLN
1	C	402	ILE
1	C	418	LYS
1	C	428	ILE
1	C	481	SER
1	C	482	ILE
1	C	490	ILE
1	C	498	SER
1	C	503	THR
1	C	505	ILE
1	C	554	ILE
1	C	560	ILE
1	C	609	ILE
1	C	613	ILE
1	C	627	THR
1	C	645	LYS
1	C	677	ILE
1	C	760	VAL
1	D	51	LEU
1	D	56	ILE
1	D	81	ILE
1	D	108	VAL

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Mol	Chain	Res	Type
1	D	126	ILE
1	D	181	ILE
1	D	215	ASN
1	D	248	LEU
1	D	316	ILE
1	D	327	ILE
1	D	339	SER
1	D	354	VAL
1	D	369	LEU
1	D	373	LEU
1	D	402	ILE
1	D	466	SER
1	D	490	ILE
1	D	498	SER
1	D	503	THR
1	D	505	ILE
1	D	537	LEU
1	D	551	ILE
1	D	560	ILE
1	D	609	ILE
1	D	627	THR
1	D	658	LEU
1	D	693	ILE
1	D	760	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	107	HIS
1	A	111	GLN
1	A	131	ASN
1	A	136	GLN
1	A	138	HIS
1	A	168	ASN
1	A	315	HIS
1	A	439	GLN
1	A	559	ASN
1	A	572	ASN
1	A	574	ASN
1	A	647	ASN
1	A	670	ASN

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Mol	Chain	Res	Type
1	A	671	ASN
1	B	61	ASN
1	B	74	ASN
1	B	85	ASN
1	B	101	GLN
1	B	107	HIS
1	B	131	ASN
1	B	136	GLN
1	B	138	HIS
1	B	213	ASN
1	B	227	ASN
1	B	237	GLN
1	B	315	HIS
1	B	334	ASN
1	B	439	GLN
1	B	559	ASN
1	B	572	ASN
1	B	588	HIS
1	B	623	ASN
1	B	635	ASN
1	B	670	ASN
1	B	671	ASN
1	C	74	ASN
1	C	101	GLN
1	C	102	ASN
1	C	138	HIS
1	C	168	ASN
1	C	215	ASN
1	C	315	HIS
1	C	319	GLN
1	C	370	ASN
1	C	516	ASN
1	C	559	ASN
1	C	574	ASN
1	C	647	ASN
1	C	662	GLN
1	C	670	ASN
1	C	671	ASN
1	C	722	ASN
1	D	74	ASN
1	D	85	ASN
1	D	102	ASN

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Mol	Chain	Res	Type
1	D	131	ASN
1	D	138	HIS
1	D	313	ASN
1	D	439	GLN
1	D	516	ASN
1	D	559	ASN
1	D	574	ASN
1	D	588	HIS
1	D	647	ASN
1	D	662	GLN
1	D	670	ASN
1	D	671	ASN
1	D	722	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	752/796 (94%)	-0.45	5 (0%) 84 69	58, 106, 163, 202	0
1	B	750/796 (94%)	-0.35	11 (1%) 72 51	59, 109, 183, 251	0
1	C	739/796 (92%)	-0.39	2 (0%) 90 81	63, 118, 172, 221	0
1	D	731/796 (91%)	-0.35	12 (1%) 70 50	64, 118, 176, 230	0
All	All	2972/3184 (93%)	-0.39	30 (1%) 79 62	58, 112, 174, 251	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	667	ALA	4.5
1	D	584	SER	4.3
1	D	714	PHE	3.6
1	C	551	ILE	3.5
1	D	214	LEU	3.5
1	B	756	ASP	3.2
1	B	447	ASN	3.0
1	D	434	GLU	2.9
1	A	455	SER	2.7
1	B	730	LEU	2.7
1	B	461	VAL	2.7
1	B	728	LEU	2.6
1	B	712	GLY	2.5
1	A	229	MET	2.4
1	D	614	LYS	2.4
1	A	731	SER	2.4
1	D	81	ILE	2.4
1	A	508	PHE	2.4
1	B	46	THR	2.4
1	A	652	PRO	2.4
1	B	789	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	580	ALA	2.3
1	D	711	ASP	2.2
1	B	466	SER	2.2
1	D	706	LEU	2.2
1	B	788	ASN	2.2
1	D	365	GLY	2.1
1	B	779	VAL	2.1
1	C	366	PHE	2.1
1	D	659	PHE	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 oligosaccharides 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.