



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2019 – 01:09 PM EST

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	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

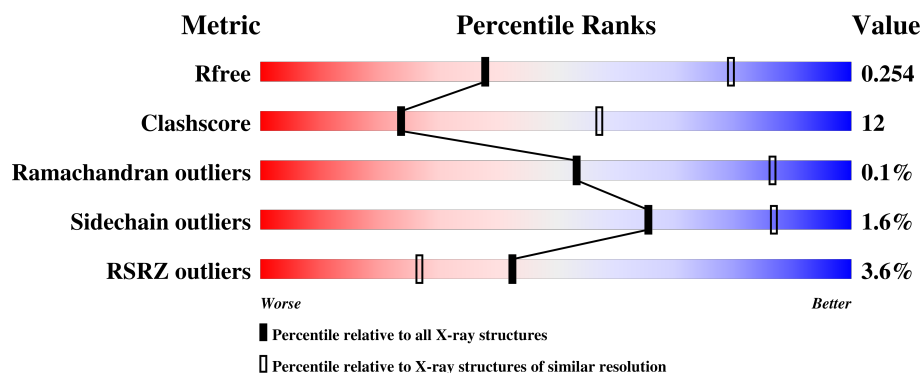
1 Overall quality at a glance

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}	111664	1235 (3.20-3.16)
Clashscore	122126	1362 (3.20-3.16)
Ramachandran outliers	120053	1340 (3.20-3.16)
Sidechain outliers	120020	1339 (3.20-3.16)
RSRZ outliers	108989	1193 (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. 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	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> </div>
1	B	796	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>6%</div> </div> </div>
1	C	796	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>7%</div> </div> </div>
1	D	796	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>8%</div> </div> </div>

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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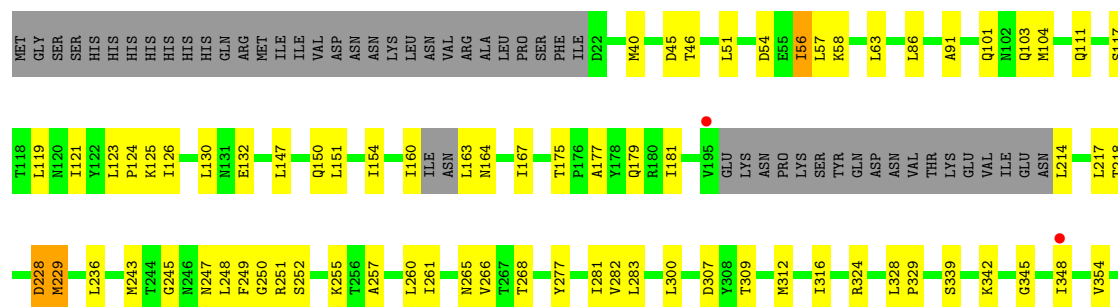
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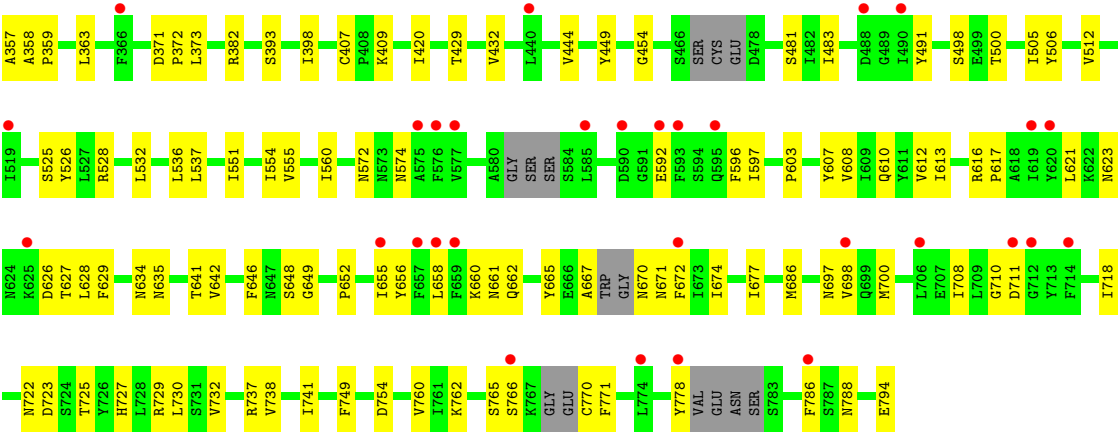
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP A0A290WPI2
C	-1	HIS	-	expression tag	UNP A0A290WPI2
C	0	HIS	-	expression tag	UNP A0A290WPI2
C	1	HIS	-	expression tag	UNP A0A290WPI2
C	?	-	TRP	deletion	UNP A0A290WPI2
C	?	-	LYS	deletion	UNP A0A290WPI2
C	?	-	GLU	deletion	UNP 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





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 49.84 – 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
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.218 , 0.259 0.215 , 0.254	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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

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	0.59	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(°)	Ideal(°)
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

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%)	53	86
1	B	736/796 (92%)	693 (94%)	43 (6%)	0	100	100
1	C	729/796 (92%)	682 (94%)	46 (6%)	1 (0%)	53	86
1	D	715/796 (90%)	673 (94%)	41 (6%)	1 (0%)	53	86
All	All	2920/3184 (92%)	2739 (94%)	178 (6%)	3 (0%)	53	86

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%)	670 (98%)	10 (2%)	67	88
1	B	678/718 (94%)	667 (98%)	11 (2%)	65	87
1	C	663/718 (92%)	650 (98%)	13 (2%)	58	83
1	D	658/718 (92%)	650 (99%)	8 (1%)	74	90
All	All	2679/2872 (93%)	2637 (98%)	42 (2%)	65	87

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 [i](#)

There are no carbohydrates 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	752/796 (94%)	-0.02	16 (2%) 63 48	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.