



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 4IVJ / pdb_00004ivj
Title : Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains, triple mutant, I222 form
Authors : Lai, Y.-T.; Sawaya, M.R.; Yeates, T.O.
Deposited on : 2013-01-23
Resolution : 7.35 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

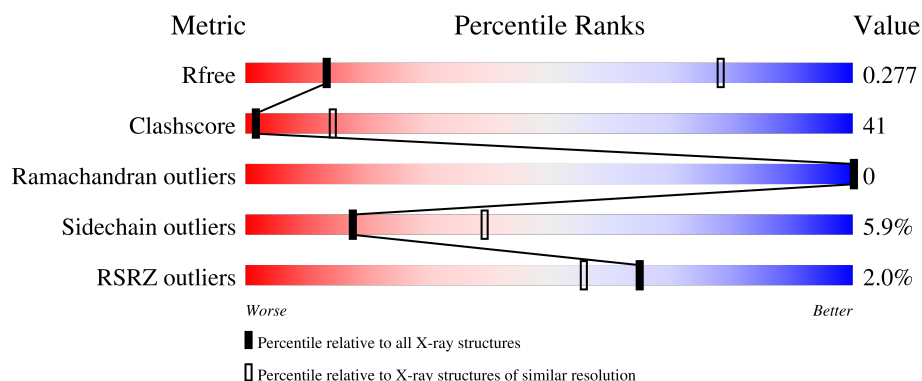
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.35 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	456	
1	B	456	
1	C	456	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10194 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 Non-haem bromoperoxidase BPO-A2, Matrix protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	B	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	C	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	GLN	engineered mutation	UNP P29715
A	118	ALA	LYS	engineered mutation	UNP P29715
A	278	ALA	-	linker	UNP P03485
A	279	GLN	-	linker	UNP P03485
A	280	GLU	-	linker	UNP P03485
A	281	ALA	-	linker	UNP P03485
A	282	GLN	-	linker	UNP P03485
A	283	LYS	-	linker	UNP P03485
A	284	GLN	-	linker	UNP P03485
A	285	LYS	-	linker	UNP P03485
A	448	LEU	-	expression tag	UNP P03485
A	449	GLU	-	expression tag	UNP P03485
A	450	HIS	-	expression tag	UNP P03485
A	451	HIS	-	expression tag	UNP P03485
A	452	HIS	-	expression tag	UNP P03485
A	453	HIS	-	expression tag	UNP P03485
A	454	HIS	-	expression tag	UNP P03485
A	455	HIS	-	expression tag	UNP P03485
B	24	THR	GLN	engineered mutation	UNP P29715
B	118	ALA	LYS	engineered mutation	UNP P29715
B	278	ALA	-	linker	UNP P03485
B	279	GLN	-	linker	UNP P03485
B	280	GLU	-	linker	UNP P03485

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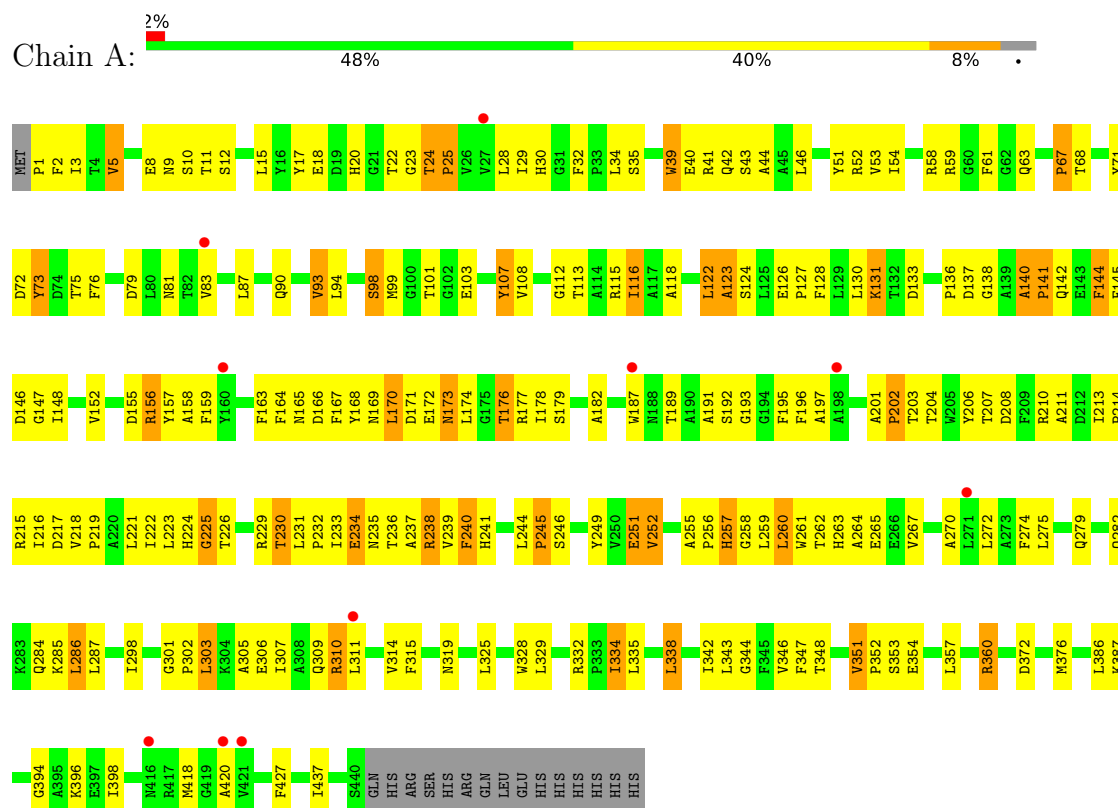
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Chain	Residue	Modelled	Actual	Comment	Reference
B	281	ALA	-	linker	UNP P03485
B	282	GLN	-	linker	UNP P03485
B	283	LYS	-	linker	UNP P03485
B	284	GLN	-	linker	UNP P03485
B	285	LYS	-	linker	UNP P03485
B	448	LEU	-	expression tag	UNP P03485
B	449	GLU	-	expression tag	UNP P03485
B	450	HIS	-	expression tag	UNP P03485
B	451	HIS	-	expression tag	UNP P03485
B	452	HIS	-	expression tag	UNP P03485
B	453	HIS	-	expression tag	UNP P03485
B	454	HIS	-	expression tag	UNP P03485
B	455	HIS	-	expression tag	UNP P03485
C	24	THR	GLN	engineered mutation	UNP P29715
C	118	ALA	LYS	engineered mutation	UNP P29715
C	278	ALA	-	linker	UNP P03485
C	279	GLN	-	linker	UNP P03485
C	280	GLU	-	linker	UNP P03485
C	281	ALA	-	linker	UNP P03485
C	282	GLN	-	linker	UNP P03485
C	283	LYS	-	linker	UNP P03485
C	284	GLN	-	linker	UNP P03485
C	285	LYS	-	linker	UNP P03485
C	448	LEU	-	expression tag	UNP P03485
C	449	GLU	-	expression tag	UNP P03485
C	450	HIS	-	expression tag	UNP P03485
C	451	HIS	-	expression tag	UNP P03485
C	452	HIS	-	expression tag	UNP P03485
C	453	HIS	-	expression tag	UNP P03485
C	454	HIS	-	expression tag	UNP P03485
C	455	HIS	-	expression tag	UNP P03485

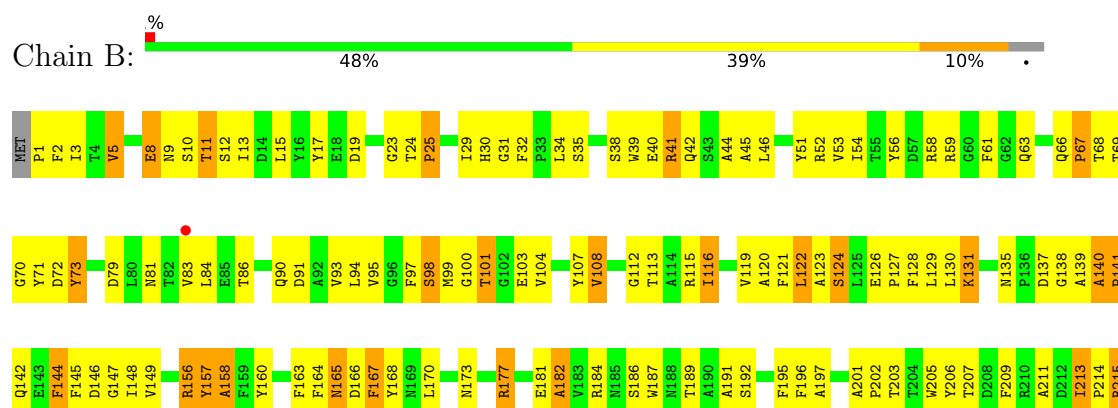
3 Residue-property plots

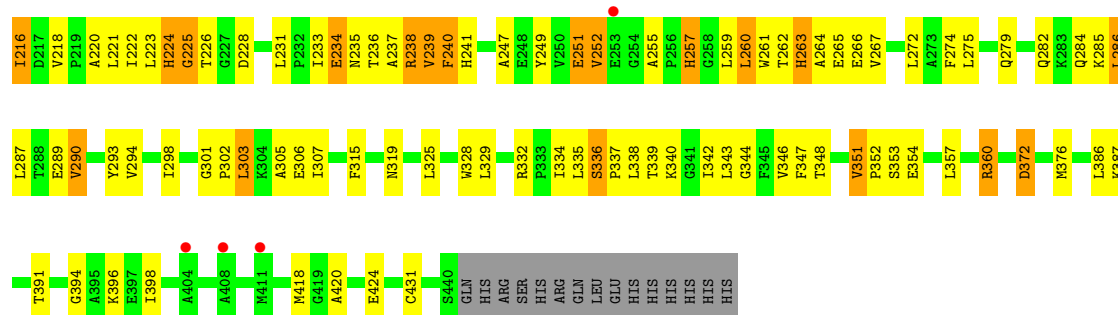
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

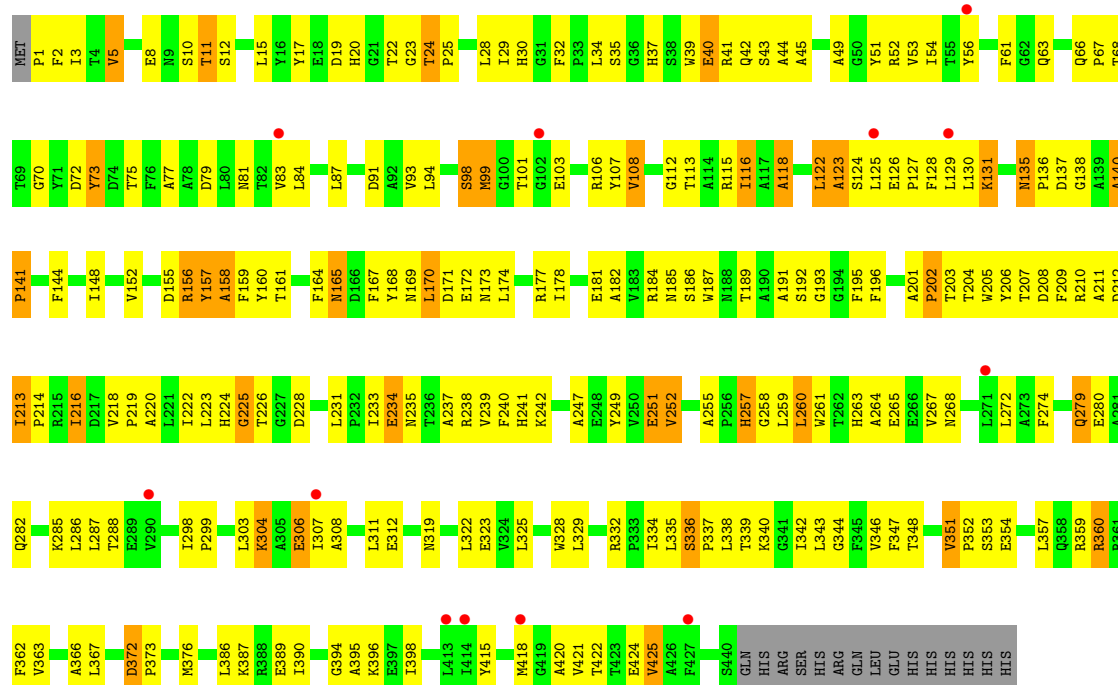


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1





● Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.67Å 160.98Å 167.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.42 – 7.35 28.42 – 7.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.42-7.35) 95.1 (28.42-7.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 7.22Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.276 , 0.288 0.267 , 0.277	Depositor DCC
R_{free} test set	122 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	400.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 289.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	10194	wwPDB-VP
Average B, all atoms (Å ²)	318.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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	1.00	4/3475 (0.1%)	1.72	109/4729 (2.3%)
1	B	0.95	7/3475 (0.2%)	1.64	93/4729 (2.0%)
1	C	0.96	9/3475 (0.3%)	1.62	91/4729 (1.9%)
All	All	0.97	20/10425 (0.2%)	1.66	293/14187 (2.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	ILE	CA-CB	7.83	1.63	1.54
1	A	116	ILE	CA-CB	7.69	1.63	1.54
1	C	116	ILE	CA-CB	7.42	1.62	1.54
1	A	218	VAL	C-N	5.66	1.41	1.33
1	C	336	SER	C-N	5.39	1.41	1.34
1	C	22	THR	CB-OG1	5.38	1.52	1.43
1	C	11	THR	CA-CB	5.35	1.62	1.53
1	C	136	PRO	N-CD	5.35	1.55	1.47
1	B	11	THR	CA-CB	5.30	1.62	1.53
1	B	336	SER	C-N	5.27	1.41	1.34
1	B	112	GLY	N-CA	5.25	1.50	1.45
1	C	56	TYR	N-CA	5.19	1.52	1.45
1	A	22	THR	CB-OG1	5.16	1.52	1.43
1	B	337	PRO	N-CD	5.14	1.54	1.47
1	C	337	PRO	N-CD	5.12	1.54	1.47
1	B	56	TYR	N-CA	5.11	1.52	1.45
1	A	219	PRO	N-CD	5.09	1.54	1.47
1	C	135	ASN	C-N	5.08	1.40	1.34
1	C	112	GLY	N-CA	5.02	1.50	1.45
1	B	86	THR	CA-CB	5.02	1.61	1.53

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	ASP	CA-CB-CG	12.11	124.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	ASP	CA-CB-CG	12.09	124.69	112.60
1	A	79	ASP	CA-CB-CG	11.90	124.50	112.60
1	C	2	PHE	CA-CB-CG	-11.69	102.11	113.80
1	B	2	PHE	CA-CB-CG	-11.67	102.13	113.80
1	A	2	PHE	CA-CB-CG	-11.66	102.14	113.80
1	B	173	ASN	N-CA-C	9.44	125.11	113.50
1	B	146	ASP	CA-C-N	9.03	129.96	119.94
1	B	146	ASP	C-N-CA	9.03	129.96	119.94
1	A	146	ASP	CA-C-N	8.95	129.88	119.94
1	A	146	ASP	C-N-CA	8.95	129.88	119.94
1	A	142	GLN	CG-CD-NE2	-8.92	103.02	116.40
1	B	142	GLN	CG-CD-NE2	-8.91	103.03	116.40
1	A	122	LEU	CA-C-O	-8.61	111.00	120.38
1	B	129	LEU	N-CA-C	-8.53	102.27	114.12
1	A	252	VAL	CA-C-O	8.50	130.60	120.66
1	C	122	LEU	CA-C-O	-8.43	111.19	120.38
1	B	252	VAL	CA-C-O	8.41	130.50	120.66
1	A	225	GLY	O-C-N	8.40	129.56	123.35
1	C	252	VAL	CA-C-O	8.38	130.47	120.66
1	A	232	PRO	CA-C-O	-8.26	112.32	121.32
1	B	207	THR	N-CA-C	-8.21	96.29	109.76
1	B	225	GLY	O-C-N	8.20	129.41	123.35
1	B	116	ILE	N-CA-C	8.07	119.77	107.99
1	A	116	ILE	N-CA-C	8.05	119.74	107.99
1	B	67	PRO	CA-C-O	8.02	133.62	122.31
1	C	225	GLY	O-C-N	8.02	129.28	123.35
1	A	192	SER	CA-C-N	7.97	129.54	120.53
1	A	192	SER	C-N-CA	7.97	129.54	120.53
1	C	168	TYR	CA-C-O	-7.95	110.04	119.35
1	B	168	TYR	CA-C-O	-7.95	110.05	119.35
1	C	116	ILE	N-CA-C	7.94	119.58	107.99
1	A	244	LEU	CA-C-N	7.92	127.84	119.05
1	A	244	LEU	C-N-CA	7.92	127.84	119.05
1	B	192	SER	CA-C-N	7.91	129.47	120.53
1	B	192	SER	C-N-CA	7.91	129.47	120.53
1	A	75	THR	CA-CB-OG1	-7.88	97.78	109.60
1	C	67	PRO	CA-C-O	7.87	133.41	122.31
1	A	67	PRO	CA-C-O	7.87	133.41	122.31
1	A	257	HIS	CA-C-O	7.86	128.88	120.55
1	C	192	SER	CA-C-N	7.86	129.41	120.53
1	C	192	SER	C-N-CA	7.86	129.41	120.53
1	A	168	TYR	CA-C-O	-7.82	110.21	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	425	VAL	N-CA-C	-7.81	103.31	111.58
1	B	239	VAL	CB-CA-C	7.79	122.64	111.65
1	B	145	PHE	CA-CB-CG	-7.68	106.12	113.80
1	A	145	PHE	CA-CB-CG	-7.62	106.18	113.80
1	C	257	HIS	CA-C-O	7.59	128.79	120.82
1	B	257	HIS	CA-C-O	7.52	128.72	120.82
1	C	54	ILE	O-C-N	-7.51	115.29	123.18
1	A	54	ILE	O-C-N	-7.51	115.30	123.18
1	B	54	ILE	O-C-N	-7.45	115.21	123.26
1	B	157	TYR	CA-C-N	7.35	130.72	120.29
1	B	157	TYR	C-N-CA	7.35	130.72	120.29
1	C	157	TYR	CA-C-N	7.33	130.70	120.29
1	C	157	TYR	C-N-CA	7.33	130.70	120.29
1	A	103	GLU	N-CA-CB	7.33	120.64	110.01
1	C	160	TYR	O-C-N	7.27	129.83	122.12
1	C	103	GLU	N-CA-CB	7.25	120.53	110.01
1	B	103	GLU	N-CA-CB	7.18	120.43	110.01
1	B	160	TYR	O-C-N	7.09	129.64	122.12
1	C	8	GLU	CA-C-O	-7.00	112.78	120.33
1	A	218	VAL	CA-C-N	-6.99	112.56	119.76
1	A	218	VAL	C-N-CA	-6.99	112.56	119.76
1	B	8	GLU	CA-C-O	-6.98	112.79	120.33
1	A	75	THR	O-C-N	6.98	129.62	122.09
1	C	22	THR	CA-C-O	-6.84	113.13	121.06
1	A	61	PHE	CA-CB-CG	-6.83	106.97	113.80
1	C	61	PHE	CA-CB-CG	-6.82	106.98	113.80
1	A	22	THR	CA-C-O	-6.78	113.20	121.06
1	A	245	PRO	CA-C-O	6.74	130.38	119.86
1	B	61	PHE	CA-CB-CG	-6.71	107.09	113.80
1	B	23	GLY	N-CA-C	-6.63	101.56	110.97
1	A	23	GLY	N-CA-C	-6.59	101.61	110.97
1	C	23	GLY	N-CA-C	-6.58	101.63	110.97
1	A	5	VAL	N-CA-CB	-6.55	104.54	112.33
1	C	5	VAL	N-CA-CB	-6.48	104.62	112.33
1	C	112	GLY	CA-C-O	6.45	128.51	122.57
1	A	141	PRO	CB-CA-C	6.45	119.50	110.60
1	B	147	GLY	CA-C-O	6.44	127.96	121.00
1	B	5	VAL	N-CA-CB	-6.44	104.67	112.33
1	C	29	ILE	CB-CG1-CD1	6.42	127.29	113.80
1	B	29	ILE	CB-CG1-CD1	6.42	127.28	113.80
1	C	141	PRO	CB-CA-C	6.41	119.45	110.60
1	C	170	LEU	CA-C-O	-6.41	112.85	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ILE	CA-C-O	6.41	127.12	120.39
1	B	141	PRO	CB-CA-C	6.40	119.43	110.60
1	A	29	ILE	CB-CG1-CD1	6.38	127.19	113.80
1	C	22	THR	O-C-N	6.34	130.63	123.27
1	A	213	ILE	CA-C-N	6.33	126.25	119.28
1	A	213	ILE	C-N-CA	6.33	126.25	119.28
1	C	123	ALA	CA-C-N	6.33	129.86	120.87
1	C	123	ALA	C-N-CA	6.33	129.86	120.87
1	A	76	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	54	ILE	CA-C-O	6.31	127.17	120.48
1	A	128	PHE	CA-CB-CG	6.28	120.08	113.80
1	A	101	THR	CA-CB-OG1	-6.28	100.18	109.60
1	A	35	SER	CA-C-O	-6.26	114.23	121.49
1	C	54	ILE	CA-C-O	6.26	127.11	120.48
1	B	131	LYS	CB-CG-CD	-6.25	96.92	111.30
1	A	170	LEU	CA-C-O	-6.25	113.04	120.10
1	A	147	GLY	CA-C-O	6.25	127.74	121.00
1	C	224	HIS	CA-C-N	6.24	127.61	121.62
1	C	224	HIS	C-N-CA	6.24	127.61	121.62
1	B	191	ALA	CA-C-O	6.24	127.15	120.10
1	C	101	THR	CA-CB-OG1	-6.23	100.25	109.60
1	C	35	SER	CA-C-O	-6.23	114.27	121.49
1	A	131	LYS	CB-CG-CD	-6.22	97.00	111.30
1	A	224	HIS	CA-C-N	6.21	127.58	121.62
1	A	224	HIS	C-N-CA	6.21	127.58	121.62
1	B	83	VAL	O-C-N	6.21	128.00	121.91
1	B	101	THR	CA-CB-OG1	-6.21	100.28	109.60
1	C	81	ASN	CA-CB-CG	-6.21	106.39	112.60
1	A	230	THR	CB-CA-C	6.21	120.71	110.90
1	A	22	THR	O-C-N	6.21	130.47	123.27
1	C	191	ALA	CA-C-O	6.20	127.11	120.10
1	B	112	GLY	CA-C-O	6.19	128.27	122.57
1	C	131	LYS	CB-CG-CD	-6.19	97.06	111.30
1	A	230	THR	CA-C-O	-6.18	114.33	120.70
1	B	44	ALA	CA-C-O	-6.18	114.33	120.82
1	B	224	HIS	CA-C-N	6.17	127.54	121.62
1	B	224	HIS	C-N-CA	6.17	127.54	121.62
1	A	191	ALA	CA-C-O	6.16	127.06	120.10
1	B	35	SER	CA-C-O	-6.14	114.36	121.49
1	C	83	VAL	O-C-N	6.13	127.91	121.91
1	A	81	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	83	VAL	O-C-N	6.12	127.90	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	ALA	CA-C-O	-6.09	114.43	120.82
1	B	81	ASN	CA-CB-CG	-6.08	106.52	112.60
1	A	301	GLY	CA-C-N	6.08	125.96	119.28
1	A	301	GLY	C-N-CA	6.08	125.96	119.28
1	C	32	PHE	CA-CB-CG	6.04	119.83	113.80
1	A	32	PHE	CA-CB-CG	6.03	119.83	113.80
1	B	301	GLY	CA-C-N	6.02	125.90	119.28
1	B	301	GLY	C-N-CA	6.02	125.90	119.28
1	B	35	SER	N-CA-CB	-5.99	101.75	111.22
1	B	251	GLU	N-CA-CB	5.97	119.94	110.57
1	A	251	GLU	N-CA-CB	5.94	119.90	110.57
1	B	32	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	35	SER	N-CA-CB	-5.93	101.85	111.22
1	C	124	SER	CB-CA-C	-5.91	99.54	109.65
1	A	241	HIS	N-CA-CB	5.87	119.27	110.22
1	C	241	HIS	N-CA-CB	5.86	119.25	110.22
1	C	22	THR	CA-CB-CG2	5.86	120.47	110.50
1	B	100	GLY	N-CA-C	-5.86	106.49	113.99
1	B	93	VAL	O-C-N	-5.84	117.05	123.18
1	C	40	GLU	CA-C-O	-5.83	114.33	120.63
1	A	22	THR	CA-CB-CG2	5.82	120.40	110.50
1	B	241	HIS	N-CA-CB	5.82	119.18	110.22
1	C	73	TYR	CA-CB-CG	-5.82	103.43	113.90
1	B	73	TYR	CA-CB-CG	-5.79	103.48	113.90
1	A	73	TYR	CA-CB-CG	-5.78	103.49	113.90
1	B	286	LEU	N-CA-C	-5.78	104.98	111.28
1	A	93	VAL	O-C-N	-5.76	117.13	123.18
1	C	336	SER	CA-C-N	-5.75	112.66	119.05
1	C	336	SER	C-N-CA	-5.75	112.66	119.05
1	C	93	VAL	O-C-N	-5.75	117.14	123.18
1	C	251	GLU	N-CA-CB	5.75	119.81	110.43
1	B	63	GLN	CA-CB-CG	-5.74	102.62	114.10
1	C	213	ILE	CB-CA-C	-5.73	108.27	114.35
1	A	12	SER	CA-CB-OG	-5.72	99.65	111.10
1	C	12	SER	CA-CB-OG	-5.72	99.67	111.10
1	A	44	ALA	CA-C-O	-5.69	114.52	120.55
1	C	63	GLN	CA-CB-CG	-5.69	102.72	114.10
1	A	63	GLN	CA-CB-CG	-5.69	102.73	114.10
1	B	12	SER	CA-CB-OG	-5.69	99.73	111.10
1	A	240	PHE	CA-C-N	5.67	128.45	120.28
1	A	240	PHE	C-N-CA	5.67	128.45	120.28
1	B	336	SER	CA-C-N	-5.66	112.77	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	SER	C-N-CA	-5.66	112.77	119.05
1	B	213	ILE	N-CA-C	5.66	121.11	108.88
1	C	240	PHE	CA-C-N	5.65	128.42	120.28
1	C	240	PHE	C-N-CA	5.65	128.42	120.28
1	C	35	SER	N-CA-CB	-5.65	102.30	111.22
1	A	213	ILE	N-CA-C	5.64	121.07	108.88
1	A	123	ALA	CA-C-N	5.63	129.78	120.94
1	A	123	ALA	C-N-CA	5.63	129.78	120.94
1	C	115	ARG	CA-C-N	5.62	130.09	122.90
1	C	115	ARG	C-N-CA	5.62	130.09	122.90
1	B	240	PHE	CA-C-N	5.61	128.36	120.28
1	B	240	PHE	C-N-CA	5.61	128.36	120.28
1	B	115	ARG	CA-C-N	5.61	130.08	122.90
1	B	115	ARG	C-N-CA	5.61	130.08	122.90
1	A	44	ALA	CA-C-N	5.60	128.05	120.44
1	A	44	ALA	C-N-CA	5.60	128.05	120.44
1	A	203	THR	O-C-N	-5.57	115.42	122.27
1	C	53	VAL	CA-CB-CG2	5.57	119.87	110.40
1	A	39	TRP	CB-CA-C	-5.57	102.66	111.17
1	B	182	ALA	N-CA-CB	5.56	118.07	110.01
1	C	203	THR	O-C-N	-5.56	115.43	122.27
1	A	53	VAL	CA-CB-CG2	5.55	119.84	110.40
1	A	124	SER	N-CA-C	5.55	118.33	110.50
1	A	142	GLN	OE1-CD-NE2	5.55	128.15	122.60
1	C	98	SER	CB-CA-C	5.55	121.46	110.42
1	A	98	SER	CB-CA-C	5.54	121.45	110.42
1	A	222	ILE	N-CA-CB	5.54	118.84	111.64
1	A	115	ARG	CA-C-N	5.53	129.98	122.90
1	A	115	ARG	C-N-CA	5.53	129.98	122.90
1	C	124	SER	N-CA-C	5.53	118.47	110.28
1	B	24	THR	O-C-N	5.53	126.22	121.30
1	A	112	GLY	CA-C-O	5.51	128.32	122.59
1	B	252	VAL	CB-CA-C	5.50	118.84	111.19
1	C	252	VAL	CB-CA-C	5.50	118.83	111.19
1	A	193	GLY	CA-C-N	5.49	125.55	120.34
1	A	193	GLY	C-N-CA	5.49	125.55	120.34
1	A	252	VAL	CB-CA-C	5.49	118.81	111.19
1	C	189	THR	O-C-N	5.48	127.71	122.07
1	C	222	ILE	N-CA-CB	5.48	118.76	111.64
1	A	189	THR	O-C-N	5.48	127.71	122.07
1	C	173	ASN	N-CA-C	5.47	120.06	113.17
1	A	173	ASN	N-CA-C	5.46	120.06	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	GLN	OE1-CD-NE2	5.46	128.06	122.60
1	B	222	ILE	N-CA-CB	5.46	118.74	111.64
1	C	24	THR	O-C-N	5.46	126.16	121.30
1	A	146	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	124	SER	CB-CA-C	-5.43	99.55	109.54
1	A	207	THR	N-CA-C	-5.42	102.25	110.28
1	B	166	ASP	CA-C-N	5.42	127.81	120.44
1	B	166	ASP	C-N-CA	5.42	127.81	120.44
1	A	107	TYR	CA-C-O	5.42	126.50	120.82
1	A	24	THR	O-C-N	5.40	126.11	121.30
1	B	145	PHE	O-C-N	5.40	128.31	122.15
1	C	5	VAL	CB-CA-C	5.40	116.45	110.62
1	C	418	MET	N-CA-C	-5.39	106.65	113.18
1	B	144	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	5	VAL	CB-CA-C	5.38	116.43	110.62
1	A	144	PHE	CA-CB-CG	-5.38	108.42	113.80
1	B	146	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	215	ARG	N-CA-C	5.38	117.14	111.28
1	C	207	THR	N-CA-C	-5.36	102.35	110.28
1	C	204	THR	CA-C-O	-5.35	112.26	119.11
1	B	189	THR	O-C-N	5.35	127.58	122.07
1	B	5	VAL	CB-CA-C	5.34	116.39	110.62
1	A	418	MET	N-CA-C	-5.34	106.72	113.18
1	B	25	PRO	N-CA-CB	5.34	108.06	103.36
1	C	25	PRO	N-CA-CB	5.33	108.05	103.36
1	A	145	PHE	O-C-N	5.31	128.21	122.15
1	B	418	MET	N-CA-C	-5.31	106.75	113.18
1	A	176	THR	N-CA-CB	-5.29	101.55	110.49
1	B	115	ARG	CB-CG-CD	-5.28	99.16	111.30
1	C	226	THR	CA-C-O	-5.27	112.89	119.38
1	C	113	THR	CA-CB-CG2	5.27	119.46	110.50
1	B	73	TYR	CA-C-O	-5.27	114.14	120.10
1	A	115	ARG	CB-CG-CD	-5.25	99.22	111.30
1	C	3	ILE	N-CA-CB	5.25	118.95	111.82
1	C	11	THR	N-CA-CB	-5.24	102.77	110.85
1	C	118	ALA	O-C-N	5.24	129.03	123.42
1	A	25	PRO	N-CA-CB	5.23	107.96	103.36
1	C	115	ARG	CB-CG-CD	-5.22	99.29	111.30
1	C	140	ALA	O-C-N	5.21	125.05	121.71
1	A	202	PRO	O-C-N	-5.21	115.87	122.17
1	C	202	PRO	O-C-N	-5.20	115.88	122.17
1	B	11	THR	N-CA-CB	-5.20	102.85	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	ASP	CA-C-N	5.20	125.00	119.28
1	C	372	ASP	C-N-CA	5.20	125.00	119.28
1	A	140	ALA	O-C-N	5.19	125.03	121.71
1	B	113	THR	CA-CB-CG2	5.19	119.33	110.50
1	A	204	THR	CA-C-O	-5.18	112.47	119.11
1	C	251	GLU	CA-C-O	-5.18	114.78	120.43
1	B	140	ALA	O-C-N	5.18	125.02	121.71
1	B	182	ALA	N-CA-C	-5.17	105.53	111.07
1	B	226	THR	CA-C-O	-5.17	113.02	119.38
1	C	11	THR	CA-CB-CG2	5.16	119.26	110.50
1	A	226	THR	CA-C-O	-5.15	113.05	119.38
1	A	118	ALA	O-C-N	5.14	128.92	123.42
1	A	107	TYR	O-C-N	-5.14	116.78	122.07
1	B	11	THR	CA-CB-CG2	5.13	119.22	110.50
1	B	158	ALA	N-CA-C	-5.13	105.77	111.36
1	A	113	THR	CA-CB-CG2	5.12	119.21	110.50
1	B	263	HIS	CB-CA-C	-5.12	102.71	111.46
1	B	252	VAL	N-CA-CB	5.10	118.10	111.67
1	C	193	GLY	CA-C-N	5.10	125.51	120.31
1	C	193	GLY	C-N-CA	5.10	125.51	120.31
1	B	372	ASP	CA-C-N	5.09	124.88	119.28
1	B	372	ASP	C-N-CA	5.09	124.88	119.28
1	B	25	PRO	O-C-N	5.09	128.80	123.10
1	B	8	GLU	N-CA-CB	5.09	118.57	110.84
1	B	167	PHE	N-CA-C	-5.09	105.65	111.14
1	C	158	ALA	N-CA-C	-5.08	105.82	111.36
1	C	25	PRO	O-C-N	5.08	128.79	123.10
1	A	25	PRO	O-C-N	5.08	128.79	123.10
1	B	113	THR	CA-CB-OG1	-5.08	101.98	109.60
1	C	252	VAL	N-CA-CB	5.07	118.05	111.67
1	A	252	VAL	N-CA-CB	5.05	118.03	111.67
1	B	3	ILE	N-CA-CB	5.05	118.68	111.82
1	A	113	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	3	ILE	N-CA-CB	5.04	118.67	111.82
1	C	161	THR	CA-C-N	5.04	125.54	120.00
1	C	161	THR	C-N-CA	5.04	125.54	120.00
1	C	113	THR	CA-CB-OG1	-5.03	102.06	109.60
1	A	122	LEU	O-C-N	5.02	129.21	123.29
1	A	334	ILE	N-CA-C	5.02	115.74	110.62
1	A	251	GLU	CA-C-O	-5.00	114.93	120.38

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	3398	0	3326	251	0
1	B	3398	0	3326	357	0
1	C	3398	0	3326	333	0
All	All	10194	0	9978	831	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 41.

All (831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:CD1	1:B:334:ILE:HB	1.46	1.46
1:B:10:SER:CB	1:C:87:LEU:HD22	1.53	1.39
1:B:303:LEU:HD12	1:B:334:ILE:CB	1.53	1.38
1:C:298:ILE:HD13	1:C:307:ILE:CD1	1.61	1.30
1:B:11:THR:HG22	1:C:17:TYR:CZ	1.65	1.29
1:C:298:ILE:CD1	1:C:307:ILE:HD13	1.66	1.25
1:B:158:ALA:HA	1:C:181:GLU:CD	1.67	1.19
1:B:10:SER:HB3	1:C:87:LEU:HD22	1.30	1.14
1:B:177:ARG:HB3	1:B:262:THR:CG2	1.78	1.13
1:A:233:ILE:HG13	1:A:237:ALA:HB3	1.27	1.12
1:A:178:ILE:HD11	1:A:261:TRP:O	1.47	1.11
1:C:359:ARG:HD2	1:C:415:TYR:CZ	1.85	1.10
1:C:360:ARG:HB2	1:C:363:VAL:HG23	1.35	1.08
1:B:108:VAL:HG11	1:B:216:ILE:HG12	1.14	1.07
1:C:24:THR:CG2	1:C:51:TYR:HD1	1.66	1.07
1:B:99:MET:SD	1:B:205:TRP:NE1	2.29	1.06
1:B:10:SER:HB3	1:C:87:LEU:CD2	1.84	1.06
1:C:24:THR:HG22	1:C:51:TYR:HD1	1.20	1.06
1:B:67:PRO:HA	1:C:20:HIS:HE1	1.20	1.06
1:B:9:ASN:HB2	1:C:19:ASP:CB	1.87	1.05
1:B:177:ARG:HB3	1:B:262:THR:CB	1.87	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HG22	1:B:17:TYR:CZ	1.91	1.05
1:B:9:ASN:CB	1:C:19:ASP:HB3	1.87	1.03
1:B:67:PRO:HA	1:C:20:HIS:CE1	1.94	1.03
1:A:287:LEU:HD13	1:A:315:PHE:HB3	1.42	1.02
1:A:40:GLU:OE1	1:C:156:ARG:HD3	1.57	1.02
1:B:10:SER:CB	1:C:87:LEU:CD2	2.37	1.01
1:C:24:THR:HG22	1:C:51:TYR:CD1	1.94	1.01
1:A:287:LEU:HD13	1:A:315:PHE:CB	1.90	1.00
1:B:177:ARG:HB3	1:B:262:THR:HG22	1.41	1.00
1:A:9:ASN:ND2	1:B:19:ASP:HB3	1.75	1.00
1:A:157:TYR:HB3	1:B:181:GLU:HB3	1.39	1.00
1:B:11:THR:HG22	1:C:17:TYR:CE2	1.95	0.99
1:C:144:PHE:CE2	1:C:148:ILE:HD11	1.97	0.99
1:C:303:LEU:HD22	1:C:334:ILE:HB	1.45	0.99
1:B:108:VAL:HG11	1:B:216:ILE:CG1	1.93	0.98
1:C:24:THR:CG2	1:C:51:TYR:CD1	2.46	0.97
1:B:10:SER:OG	1:C:87:LEU:HD22	1.63	0.97
1:A:157:TYR:HB3	1:B:181:GLU:CB	1.96	0.96
1:B:156:ARG:HD3	1:C:40:GLU:OE1	1.67	0.94
1:A:93:VAL:HG11	1:A:275:LEU:HD21	1.48	0.94
1:C:84:LEU:HD12	1:C:107:TYR:CZ	2.03	0.94
1:A:11:THR:CG2	1:B:17:TYR:CE2	2.51	0.94
1:B:9:ASN:HB2	1:C:19:ASP:HB3	0.96	0.94
1:B:139:ALA:CB	1:B:235:ASN:ND2	2.30	0.94
1:B:263:HIS:HB3	1:B:266:GLU:OE1	1.69	0.93
1:A:260:LEU:HD23	1:A:267:VAL:HG11	1.48	0.93
1:A:303:LEU:HD12	1:A:334:ILE:HB	1.50	0.93
1:A:178:ILE:HD11	1:A:261:TRP:C	1.94	0.93
1:C:360:ARG:HB2	1:C:363:VAL:CG2	1.98	0.93
1:B:108:VAL:CG1	1:B:216:ILE:HG12	1.98	0.93
1:A:260:LEU:O	1:A:264:ALA:HB2	1.69	0.93
1:B:84:LEU:HD12	1:B:107:TYR:CZ	2.03	0.93
1:B:303:LEU:HB2	1:B:334:ILE:CD1	1.98	0.93
1:B:30:HIS:HA	1:B:39:TRP:HE1	1.33	0.92
1:C:359:ARG:HD2	1:C:415:TYR:CE1	2.05	0.91
1:C:233:ILE:O	1:C:237:ALA:HB3	1.69	0.91
1:B:104:VAL:CG1	1:B:121:PHE:CE1	2.53	0.91
1:B:39:TRP:CZ2	1:B:97:PHE:HB3	2.05	0.91
1:B:177:ARG:HB3	1:B:262:THR:HB	1.50	0.91
1:A:127:PRO:CD	1:A:239:VAL:HG13	2.02	0.90
1:B:10:SER:HB2	1:C:19:ASP:OD2	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:CD2	1:C:334:ILE:HB	2.01	0.90
1:C:360:ARG:HG3	1:C:362:PHE:CZ	2.07	0.90
1:B:157:TYR:CD2	1:C:182:ALA:HA	2.06	0.90
1:B:11:THR:CG2	1:C:17:TYR:CE2	2.54	0.90
1:B:51:TYR:HE1	1:B:279:GLN:OE1	1.55	0.89
1:C:41:ARG:HD2	1:C:264:ALA:CB	2.02	0.89
1:A:127:PRO:HD2	1:A:239:VAL:CG1	2.03	0.88
1:B:195:PHE:CG	1:C:40:GLU:HB2	2.08	0.88
1:A:126:GLU:O	1:A:236:THR:HB	1.73	0.88
1:B:139:ALA:HB2	1:B:235:ASN:HD22	1.36	0.87
1:A:11:THR:HG22	1:B:17:TYR:OH	1.74	0.87
1:B:164:PHE:CE1	1:B:186:SER:HB3	2.09	0.87
1:B:233:ILE:HG13	1:B:237:ALA:HB3	1.55	0.87
1:A:233:ILE:HG13	1:A:237:ALA:CB	2.05	0.86
1:A:182:ALA:HB1	1:A:261:TRP:HZ2	1.39	0.86
1:C:129:LEU:CD1	1:C:205:TRP:HB3	2.06	0.86
1:C:303:LEU:HD21	1:C:335:LEU:HG	1.57	0.85
1:A:234:GLU:HA	1:A:238:ARG:HB2	1.58	0.85
1:B:139:ALA:HB2	1:B:235:ASN:ND2	1.89	0.85
1:A:127:PRO:HD2	1:A:239:VAL:HG13	1.58	0.85
1:A:164:PHE:HE2	1:A:187:TRP:HB2	1.40	0.85
1:C:108:VAL:HG11	1:C:216:ILE:HG12	1.59	0.85
1:B:287:LEU:O	1:B:290:VAL:HG12	1.76	0.85
1:C:360:ARG:CB	1:C:363:VAL:HG23	2.06	0.85
1:B:139:ALA:CB	1:B:235:ASN:HD22	1.87	0.84
1:C:129:LEU:HD12	1:C:205:TRP:HB3	1.55	0.84
1:B:39:TRP:HZ2	1:B:97:PHE:HB3	1.38	0.84
1:B:259:LEU:HD23	1:B:259:LEU:H	1.43	0.84
1:C:285:LYS:O	1:C:288:THR:HG22	1.77	0.84
1:C:165:ASN:OD1	1:C:170:LEU:HB2	1.78	0.83
1:C:386:LEU:HD23	1:C:398:ILE:HD11	1.59	0.83
1:B:157:TYR:C	1:C:181:GLU:HB3	2.03	0.83
1:B:303:LEU:HB2	1:B:334:ILE:HD12	1.59	0.83
1:B:158:ALA:HA	1:C:181:GLU:CG	2.08	0.83
1:A:386:LEU:HD23	1:A:398:ILE:HD11	1.59	0.83
1:B:303:LEU:HD12	1:B:334:ILE:CG1	2.09	0.82
1:B:386:LEU:HD23	1:B:398:ILE:HD11	1.59	0.82
1:A:262:THR:HG22	1:A:263:HIS:ND1	1.95	0.82
1:C:298:ILE:HD13	1:C:307:ILE:HD13	0.87	0.82
1:A:8:GLU:OE1	1:A:67:PRO:CB	2.27	0.81
1:C:127:PRO:HB2	1:C:210:ARG:HG2	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:HD21	1:C:335:LEU:CD2	2.10	0.81
1:B:303:LEU:HD12	1:B:334:ILE:HB	0.83	0.81
1:C:128:PHE:HE1	1:C:206:TYR:O	1.63	0.81
1:C:164:PHE:HE2	1:C:187:TRP:HA	1.43	0.81
1:B:164:PHE:CZ	1:B:186:SER:HB3	2.16	0.81
1:C:322:LEU:HD23	1:C:357:LEU:HD12	1.63	0.81
1:A:303:LEU:CD1	1:A:334:ILE:HB	2.11	0.80
1:A:164:PHE:HE2	1:A:187:TRP:CB	1.93	0.80
1:A:51:TYR:CZ	1:A:279:GLN:HG3	2.15	0.80
1:B:195:PHE:CD1	1:C:40:GLU:HB2	2.16	0.80
1:C:303:LEU:HD21	1:C:335:LEU:CG	2.11	0.80
1:A:262:THR:HG22	1:A:263:HIS:CE1	2.17	0.80
1:C:135:ASN:HD21	1:C:137:ASP:HB2	1.44	0.80
1:C:390:ILE:HG22	1:C:390:ILE:O	1.82	0.80
1:B:233:ILE:HD11	1:B:249:TYR:OH	1.83	0.79
1:A:173:ASN:ND2	1:A:177:ARG:HG3	1.96	0.79
1:B:11:THR:CG2	1:C:17:TYR:CZ	2.58	0.79
1:B:177:ARG:CB	1:B:262:THR:HG22	2.12	0.79
1:A:178:ILE:HD13	1:A:261:TRP:CD1	2.18	0.79
1:B:126:GLU:HB3	1:B:127:PRO:HA	1.64	0.79
1:B:164:PHE:HE2	1:B:187:TRP:HA	1.48	0.79
1:C:126:GLU:HB3	1:C:127:PRO:HA	1.64	0.78
1:A:286:LEU:HD11	1:A:427:PHE:CE2	2.19	0.78
1:B:177:ARG:HG3	1:B:263:HIS:CE1	2.18	0.78
1:A:11:THR:HG22	1:B:17:TYR:CE2	2.14	0.77
1:A:360:ARG:HG2	1:A:360:ARG:HH11	1.50	0.77
1:B:128:PHE:HE1	1:B:206:TYR:C	1.92	0.76
1:A:11:THR:CG2	1:B:17:TYR:CZ	2.68	0.76
1:B:360:ARG:HH11	1:B:360:ARG:HG2	1.50	0.76
1:A:287:LEU:CD1	1:A:315:PHE:HB3	2.15	0.76
1:C:360:ARG:CG	1:C:362:PHE:CE1	2.68	0.76
1:C:362:PHE:CE2	1:C:363:VAL:HG22	2.21	0.76
1:C:129:LEU:HB2	1:C:206:TYR:HA	1.68	0.76
1:A:17:TYR:CZ	1:C:11:THR:HG22	2.21	0.75
1:A:234:GLU:HA	1:A:238:ARG:HD2	1.69	0.75
1:A:303:LEU:HD12	1:A:334:ILE:CB	2.17	0.75
1:C:421:VAL:HB	1:C:425:VAL:HG11	1.69	0.75
1:B:234:GLU:HA	1:B:238:ARG:HB2	1.67	0.75
1:C:329:LEU:HD22	1:C:335:LEU:CD1	2.17	0.75
1:A:260:LEU:CD2	1:A:267:VAL:HG11	2.17	0.75
1:B:211:ALA:O	1:B:214:PRO:HD2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG12	1:B:255:ALA:HB2	1.69	0.75
1:A:182:ALA:HB1	1:A:261:TRP:CZ2	2.21	0.75
1:A:259:LEU:H	1:A:259:LEU:HD23	1.50	0.75
1:A:211:ALA:O	1:A:214:PRO:HD2	1.86	0.75
1:C:252:VAL:HG12	1:C:255:ALA:HB2	1.69	0.74
1:C:359:ARG:CD	1:C:415:TYR:CZ	2.69	0.74
1:B:104:VAL:HG12	1:B:121:PHE:CE1	2.22	0.74
1:C:130:LEU:O	1:C:138:GLY:HA3	1.86	0.74
1:B:303:LEU:CG	1:B:334:ILE:HD12	2.18	0.74
1:A:51:TYR:OH	1:A:279:GLN:HG3	1.88	0.74
1:B:104:VAL:HG11	1:B:121:PHE:CE1	2.22	0.74
1:B:177:ARG:CB	1:B:262:THR:CG2	2.64	0.74
1:C:41:ARG:HD2	1:C:264:ALA:HB2	1.70	0.74
1:C:359:ARG:HD2	1:C:415:TYR:CE2	2.23	0.73
1:B:157:TYR:HB3	1:C:181:GLU:HB3	1.68	0.73
1:C:360:ARG:HG3	1:C:362:PHE:CE1	2.23	0.73
1:A:24:THR:HG21	1:A:279:GLN:OE1	1.89	0.73
1:A:131:LYS:HD2	1:A:138:GLY:O	1.88	0.73
1:A:252:VAL:HG12	1:A:255:ALA:HB2	1.69	0.73
1:B:41:ARG:HD2	1:B:264:ALA:HB2	1.71	0.73
1:B:282:GLN:O	1:B:286:LEU:HG	1.88	0.73
1:C:156:ARG:NE	1:C:157:TYR:CZ	2.56	0.73
1:B:344:GLY:O	1:B:348:THR:HG23	1.89	0.73
1:A:177:ARG:HD2	1:A:263:HIS:CE1	2.24	0.73
1:A:344:GLY:O	1:A:348:THR:HG23	1.89	0.73
1:C:211:ALA:O	1:C:214:PRO:HD2	1.88	0.72
1:C:344:GLY:O	1:C:348:THR:HG23	1.89	0.72
1:A:303:LEU:HB2	1:A:334:ILE:HD12	1.70	0.72
1:C:233:ILE:HG13	1:C:237:ALA:CB	2.19	0.72
1:C:164:PHE:CE1	1:C:186:SER:HB3	2.23	0.72
1:B:303:LEU:HD12	1:B:334:ILE:CD1	2.19	0.72
1:A:179:SER:OG	1:C:158:ALA:HB2	1.90	0.71
1:B:221:LEU:HB2	1:B:274:PHE:CE1	2.25	0.71
1:A:41:ARG:CD	1:A:264:ALA:CB	2.67	0.71
1:B:157:TYR:C	1:C:181:GLU:CB	2.63	0.71
1:A:164:PHE:CZ	1:A:187:TRP:HA	2.24	0.71
1:C:233:ILE:O	1:C:237:ALA:CB	2.39	0.71
1:C:421:VAL:HB	1:C:425:VAL:CG1	2.20	0.71
1:A:71:TYR:OH	1:A:197:ALA:HB2	1.90	0.71
1:A:164:PHE:CE2	1:A:187:TRP:HB2	2.25	0.71
1:A:8:GLU:OE1	1:A:67:PRO:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:CB	1:B:334:ILE:HD12	2.20	0.71
1:B:158:ALA:CA	1:C:181:GLU:CD	2.57	0.70
1:A:41:ARG:HD2	1:A:264:ALA:CB	2.22	0.70
1:C:360:ARG:HB3	1:C:362:PHE:CE1	2.26	0.70
1:B:38:SER:HA	1:B:261:TRP:HZ2	1.55	0.70
1:B:39:TRP:CZ2	1:B:97:PHE:CB	2.73	0.70
1:B:177:ARG:CB	1:B:262:THR:HB	2.22	0.70
1:B:156:ARG:CD	1:C:40:GLU:OE1	2.38	0.70
1:C:285:LYS:HG3	1:C:286:LEU:N	2.07	0.70
1:B:157:TYR:HB3	1:C:181:GLU:C	2.16	0.70
1:B:51:TYR:CE1	1:B:279:GLN:OE1	2.44	0.70
1:B:68:THR:OG1	1:C:20:HIS:HB3	1.92	0.69
1:B:158:ALA:N	1:C:181:GLU:HB2	2.07	0.69
1:A:18:GLU:CG	1:A:20:HIS:CE1	2.75	0.69
1:C:165:ASN:ND2	1:C:170:LEU:HD12	2.06	0.69
1:A:71:TYR:CE1	1:A:197:ALA:HA	2.28	0.69
1:B:1:PRO:CB	1:B:17:TYR:CE1	2.75	0.69
1:B:307:ILE:HD11	1:B:335:LEU:HD21	1.75	0.69
1:B:157:TYR:CB	1:C:181:GLU:HB3	2.23	0.69
1:B:158:ALA:N	1:C:181:GLU:CB	2.55	0.69
1:B:303:LEU:HB2	1:B:334:ILE:HD13	1.72	0.69
1:C:329:LEU:CD2	1:C:335:LEU:HD11	2.23	0.69
1:A:234:GLU:HA	1:A:238:ARG:CD	2.23	0.69
1:B:11:THR:HG23	1:C:19:ASP:CG	2.17	0.69
1:B:236:THR:O	1:B:240:PHE:HB2	1.93	0.69
1:C:303:LEU:HD21	1:C:335:LEU:HD23	1.73	0.69
1:A:259:LEU:O	1:A:263:HIS:N	2.25	0.68
1:B:71:TYR:CE1	1:B:197:ALA:HA	2.28	0.68
1:A:18:GLU:CG	1:A:20:HIS:NE2	2.56	0.68
1:A:260:LEU:O	1:A:264:ALA:CB	2.42	0.68
1:C:164:PHE:CZ	1:C:186:SER:HB3	2.28	0.68
1:C:304:LYS:HA	1:C:307:ILE:HD12	1.75	0.68
1:A:259:LEU:O	1:A:263:HIS:CA	2.42	0.68
1:C:137:ASP:CG	1:C:239:VAL:CG2	2.66	0.68
1:C:298:ILE:HG23	1:C:299:PRO:HD2	1.76	0.68
1:A:41:ARG:HD2	1:A:264:ALA:HB2	1.74	0.68
1:A:287:LEU:HD13	1:A:315:PHE:CG	2.29	0.68
1:B:8:GLU:OE2	1:B:13:ILE:HD11	1.94	0.67
1:A:164:PHE:CE2	1:A:187:TRP:HA	2.28	0.67
1:A:221:LEU:HB2	1:A:274:PHE:CD1	2.29	0.67
1:B:135:ASN:HD21	1:B:137:ASP:CB	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ALA:CA	1:B:235:ASN:ND2	2.58	0.67
1:C:164:PHE:CE2	1:C:187:TRP:HA	2.28	0.67
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.77	0.67
1:B:66:GLN:OE1	1:C:37:HIS:CE1	2.48	0.67
1:B:135:ASN:HD21	1:B:137:ASP:HB2	1.58	0.67
1:A:127:PRO:HD3	1:A:239:VAL:HG13	1.76	0.67
1:A:259:LEU:O	1:A:263:HIS:C	2.38	0.67
1:B:259:LEU:H	1:B:259:LEU:CD2	2.08	0.67
1:B:287:LEU:HD13	1:B:315:PHE:CG	2.30	0.67
1:C:303:LEU:HD23	1:C:334:ILE:CG2	2.24	0.67
1:B:139:ALA:HA	1:B:235:ASN:ND2	2.09	0.67
1:C:129:LEU:HD12	1:C:205:TRP:C	2.20	0.67
1:A:158:ALA:HA	1:B:181:GLU:OE2	1.95	0.66
1:A:303:LEU:HD12	1:A:334:ILE:CG1	2.25	0.66
1:C:164:PHE:HE2	1:C:187:TRP:CA	2.08	0.66
1:A:127:PRO:HD2	1:A:239:VAL:HG11	1.76	0.66
1:C:360:ARG:N	1:C:415:TYR:OH	2.27	0.66
1:C:362:PHE:O	1:C:366:ALA:N	2.23	0.66
1:B:71:TYR:OH	1:B:197:ALA:HB2	1.95	0.66
1:B:234:GLU:H	1:B:234:GLU:CD	2.03	0.66
1:B:164:PHE:CE2	1:B:187:TRP:HA	2.30	0.66
1:A:18:GLU:HG3	1:A:20:HIS:CE1	2.29	0.66
1:B:8:GLU:HG3	1:B:67:PRO:HB3	1.77	0.66
1:C:17:TYR:HE2	1:C:19:ASP:OD2	1.79	0.66
1:B:11:THR:HB	1:C:1:PRO:HB3	1.76	0.65
1:C:155:ASP:HB3	1:C:158:ALA:HB3	1.77	0.65
1:A:221:LEU:HB2	1:A:274:PHE:CG	2.31	0.65
1:A:30:HIS:CE1	1:A:34:LEU:O	2.50	0.65
1:B:104:VAL:CG1	1:B:121:PHE:CZ	2.79	0.65
1:B:360:ARG:HG2	1:B:360:ARG:NH1	2.12	0.65
1:B:10:SER:CB	1:C:19:ASP:OD2	2.43	0.65
1:B:195:PHE:HB2	1:C:40:GLU:OE1	1.95	0.65
1:A:163:PHE:O	1:A:167:PHE:HB2	1.97	0.65
1:B:249:TYR:HE1	1:B:251:GLU:HG3	1.62	0.65
1:C:84:LEU:HD12	1:C:107:TYR:CE2	2.31	0.65
1:C:201:ALA:HB3	1:C:202:PRO:HD3	1.76	0.65
1:C:390:ILE:O	1:C:390:ILE:CG2	2.45	0.65
1:A:40:GLU:OE1	1:C:156:ARG:CD	2.42	0.65
1:B:303:LEU:CD1	1:B:334:ILE:CB	2.35	0.65
1:B:336:SER:HB2	1:B:339:THR:CB	2.27	0.65
1:C:144:PHE:HE2	1:C:148:ILE:HD11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ALA:HB2	1:C:425:VAL:HG23	1.78	0.65
1:A:157:TYR:CB	1:B:181:GLU:CB	2.73	0.64
1:A:93:VAL:HG11	1:A:275:LEU:CD2	2.24	0.64
1:B:84:LEU:CD1	1:B:107:TYR:CZ	2.79	0.64
1:B:137:ASP:OD2	1:B:239:VAL:HG11	1.97	0.64
1:B:259:LEU:HD23	1:B:259:LEU:N	2.11	0.64
1:C:233:ILE:O	1:C:237:ALA:N	2.30	0.64
1:A:298:ILE:HD13	1:A:307:ILE:HD12	1.78	0.64
1:B:30:HIS:CE1	1:B:34:LEU:O	2.50	0.64
1:C:329:LEU:CD2	1:C:335:LEU:CD1	2.75	0.64
1:A:1:PRO:HB2	1:A:17:TYR:O	1.98	0.64
1:A:18:GLU:HG2	1:A:20:HIS:NE2	2.13	0.64
1:B:95:VAL:HG22	1:B:120:ALA:HB3	1.80	0.64
1:C:298:ILE:CG2	1:C:299:PRO:HD2	2.27	0.64
1:B:84:LEU:HD12	1:B:107:TYR:CE2	2.32	0.64
1:A:360:ARG:HG2	1:A:360:ARG:NH1	2.12	0.64
1:A:164:PHE:CE2	1:A:187:TRP:CA	2.80	0.64
1:B:1:PRO:HB2	1:B:17:TYR:CE1	2.33	0.64
1:C:259:LEU:O	1:C:263:HIS:N	2.29	0.64
1:B:319:ASN:HA	1:B:352:PRO:HG2	1.80	0.63
1:C:84:LEU:CD1	1:C:107:TYR:CZ	2.79	0.63
1:C:319:ASN:HA	1:C:352:PRO:HG2	1.80	0.63
1:C:178:ILE:HD12	1:C:261:TRP:HD1	1.62	0.63
1:C:359:ARG:CD	1:C:415:TYR:CE1	2.81	0.63
1:A:319:ASN:HA	1:A:352:PRO:HG2	1.80	0.63
1:B:11:THR:HG23	1:C:19:ASP:OD2	1.99	0.63
1:A:262:THR:CG2	1:A:263:HIS:CE1	2.82	0.63
1:A:152:VAL:HG22	1:A:159:PHE:CE1	2.34	0.63
1:A:235:ASN:O	1:A:239:VAL:HG11	1.99	0.62
1:C:127:PRO:HG3	1:C:239:VAL:HG12	1.81	0.62
1:B:73:TYR:OH	1:B:99:MET:HG2	1.99	0.62
1:B:126:GLU:HG3	1:B:209:PHE:CB	2.30	0.62
1:B:11:THR:HB	1:C:1:PRO:CB	2.29	0.62
1:B:335:LEU:HB3	1:B:340:LYS:CG	2.29	0.62
1:A:311:LEU:O	1:A:315:PHE:CG	2.52	0.62
1:C:30:HIS:CE1	1:C:34:LEU:O	2.53	0.61
1:A:18:GLU:HG3	1:A:20:HIS:NE2	2.15	0.61
1:C:137:ASP:CG	1:C:239:VAL:HG21	2.24	0.61
1:A:87:LEU:HD22	1:C:10:SER:CB	2.29	0.61
1:B:119:VAL:HG23	1:B:121:PHE:HE2	1.65	0.61
1:A:9:ASN:HD21	1:B:52:ARG:HE	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HD13	1:A:307:ILE:CD1	2.30	0.61
1:A:8:GLU:OE1	1:A:67:PRO:CA	2.49	0.61
1:B:303:LEU:HD11	1:B:334:ILE:HB	1.70	0.61
1:C:178:ILE:HD12	1:C:261:TRP:CD1	2.36	0.60
1:C:360:ARG:H	1:C:415:TYR:HH	1.49	0.60
1:A:9:ASN:OD1	1:A:10:SER:N	2.35	0.60
1:B:286:LEU:HD13	1:B:424:GLU:CG	2.30	0.60
1:A:17:TYR:CE2	1:C:11:THR:HG22	2.35	0.60
1:B:336:SER:HB2	1:B:339:THR:OG1	2.01	0.60
1:A:152:VAL:HG22	1:A:159:PHE:CD1	2.37	0.60
1:B:135:ASN:ND2	1:B:137:ASP:HB2	2.16	0.60
1:B:157:TYR:HD2	1:C:182:ALA:HA	1.65	0.60
1:C:137:ASP:OD2	1:C:239:VAL:HG13	2.02	0.60
1:B:101:THR:OG1	1:B:124:SER:HA	2.02	0.60
1:B:164:PHE:HE2	1:B:187:TRP:CA	2.13	0.60
1:B:284:GLN:O	1:B:287:LEU:HB2	2.01	0.60
1:B:303:LEU:HD12	1:B:334:ILE:HD12	1.84	0.60
1:B:104:VAL:HG12	1:B:121:PHE:CZ	2.36	0.60
1:A:8:GLU:OE1	1:A:67:PRO:HA	2.00	0.60
1:B:11:THR:HG22	1:C:17:TYR:CE1	2.33	0.60
1:B:72:ASP:OD1	1:B:73:TYR:N	2.35	0.60
1:B:158:ALA:HA	1:C:181:GLU:OE2	1.99	0.60
1:B:99:MET:SD	1:B:205:TRP:CD1	2.94	0.59
1:B:206:TYR:CD2	1:B:206:TYR:O	2.55	0.59
1:C:129:LEU:HD12	1:C:205:TRP:CB	2.29	0.59
1:C:137:ASP:CG	1:C:239:VAL:HG22	2.27	0.59
1:A:259:LEU:HD23	1:A:259:LEU:N	2.17	0.59
1:C:208:ASP:OD1	1:C:210:ARG:HG3	2.03	0.59
1:B:285:LYS:O	1:B:289:GLU:HG3	2.02	0.59
1:C:164:PHE:CZ	1:C:186:SER:C	2.80	0.59
1:C:303:LEU:CD2	1:C:335:LEU:HD23	2.33	0.59
1:B:42:GLN:NE2	1:B:260:LEU:HB3	2.17	0.59
1:B:157:TYR:CB	1:C:181:GLU:C	2.75	0.59
1:C:360:ARG:HD2	1:C:362:PHE:HE1	1.68	0.59
1:A:41:ARG:HD3	1:A:264:ALA:CB	2.33	0.59
1:C:128:PHE:CE1	1:C:206:TYR:O	2.51	0.59
1:C:137:ASP:HB3	1:C:239:VAL:HG21	1.83	0.59
1:C:249:TYR:HE1	1:C:251:GLU:HG3	1.67	0.59
1:C:282:GLN:HA	1:C:285:LYS:HG2	1.84	0.59
1:C:51:TYR:HE1	1:C:279:GLN:OE1	1.86	0.59
1:C:108:VAL:HG11	1:C:216:ILE:CG1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:CG1	1:C:237:ALA:HB3	2.33	0.59
1:B:104:VAL:HG11	1:B:121:PHE:CZ	2.37	0.58
1:B:336:SER:HB2	1:B:339:THR:HB	1.85	0.58
1:B:131:LYS:HD2	1:B:138:GLY:O	2.03	0.58
1:B:41:ARG:HD3	1:B:264:ALA:CB	2.33	0.58
1:B:108:VAL:CG1	1:B:216:ILE:CG1	2.70	0.58
1:A:71:TYR:CZ	1:A:197:ALA:HA	2.39	0.58
1:B:201:ALA:HB3	1:B:202:PRO:HD3	1.85	0.58
1:B:386:LEU:CD2	1:B:398:ILE:HD11	2.32	0.58
1:C:360:ARG:CB	1:C:362:PHE:CE1	2.86	0.58
1:B:68:THR:HA	1:B:196:PHE:CD1	2.38	0.58
1:C:303:LEU:HD11	1:C:332:ARG:HG3	1.85	0.58
1:A:158:ALA:HA	1:B:181:GLU:CD	2.29	0.58
1:B:157:TYR:CZ	1:C:185:ASN:CG	2.82	0.58
1:B:263:HIS:HB3	1:B:266:GLU:CD	2.29	0.58
1:A:259:LEU:H	1:A:259:LEU:CD2	2.14	0.58
1:A:231:LEU:HD12	1:A:257:HIS:HE1	1.69	0.58
1:C:216:ILE:HG22	1:C:218:VAL:H	1.69	0.58
1:C:360:ARG:CD	1:C:362:PHE:CE1	2.87	0.57
1:A:235:ASN:O	1:A:239:VAL:CG1	2.52	0.57
1:B:67:PRO:CA	1:C:20:HIS:CE1	2.79	0.57
1:C:231:LEU:HD12	1:C:257:HIS:HE1	1.69	0.57
1:C:362:PHE:CE2	1:C:363:VAL:CG2	2.86	0.57
1:C:422:THR:O	1:C:425:VAL:HG12	2.03	0.57
1:A:303:LEU:HD12	1:A:334:ILE:HD12	1.85	0.57
1:A:72:ASP:OD1	1:A:73:TYR:N	2.37	0.57
1:B:41:ARG:CD	1:B:264:ALA:CB	2.82	0.57
1:C:137:ASP:OD2	1:C:239:VAL:CG1	2.52	0.57
1:C:360:ARG:CD	1:C:362:PHE:HE1	2.17	0.57
1:A:122:LEU:CD2	1:A:223:LEU:HB3	2.35	0.57
1:B:69:THR:HG22	1:B:70:GLY:N	2.19	0.57
1:B:307:ILE:CD1	1:B:335:LEU:HD21	2.35	0.57
1:A:287:LEU:HD13	1:A:315:PHE:CA	2.34	0.57
1:A:9:ASN:ND2	1:B:19:ASP:CB	2.61	0.57
1:A:164:PHE:HE2	1:A:187:TRP:CA	2.16	0.57
1:A:262:THR:CG2	1:A:263:HIS:ND1	2.67	0.57
1:B:249:TYR:CE1	1:B:251:GLU:HG3	2.40	0.57
1:C:164:PHE:CE2	1:C:187:TRP:CA	2.87	0.57
1:A:286:LEU:HD11	1:A:427:PHE:HE2	1.69	0.57
1:A:386:LEU:CD2	1:A:398:ILE:HD11	2.32	0.57
1:B:126:GLU:HG3	1:B:209:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:CG	1:C:40:GLU:CB	2.85	0.57
1:C:228:ASP:OD2	1:C:257:HIS:HA	2.05	0.56
1:A:259:LEU:O	1:A:263:HIS:HB2	2.05	0.56
1:B:68:THR:HG23	1:C:20:HIS:CD2	2.40	0.56
1:B:119:VAL:HG23	1:B:121:PHE:CE2	2.40	0.56
1:A:157:TYR:CB	1:B:181:GLU:HB2	2.36	0.56
1:B:335:LEU:HD13	1:B:343:LEU:HD12	1.87	0.56
1:C:260:LEU:HA	1:C:267:VAL:HG21	1.87	0.56
1:A:178:ILE:HG22	1:A:179:SER:O	2.06	0.56
1:C:303:LEU:HD23	1:C:334:ILE:HG22	1.86	0.56
1:C:359:ARG:HA	1:C:415:TYR:OH	2.05	0.56
1:A:166:ASP:OD2	1:A:230:THR:OG1	2.22	0.56
1:A:286:LEU:HD11	1:A:427:PHE:CD2	2.40	0.56
1:B:8:GLU:HG2	1:B:13:ILE:HD11	1.86	0.56
1:B:126:GLU:H	1:B:126:GLU:CD	2.13	0.56
1:C:122:LEU:CD2	1:C:223:LEU:HB3	2.34	0.56
1:C:259:LEU:N	1:C:259:LEU:HD23	2.21	0.56
1:A:215:ARG:O	1:A:216:ILE:C	2.45	0.56
1:A:256:PRO:CD	1:A:263:HIS:CE1	2.88	0.56
1:A:137:ASP:O	1:A:235:ASN:ND2	2.39	0.56
1:A:179:SER:CB	1:C:158:ALA:HB2	2.36	0.56
1:C:259:LEU:H	1:C:259:LEU:CD2	2.19	0.56
1:A:234:GLU:CD	1:A:234:GLU:H	2.14	0.56
1:C:386:LEU:CD2	1:C:398:ILE:HD11	2.32	0.56
1:B:231:LEU:HD12	1:B:257:HIS:HE1	1.69	0.56
1:A:163:PHE:CE2	1:A:167:PHE:HD2	2.24	0.56
1:C:131:LYS:HD2	1:C:138:GLY:O	2.06	0.55
1:A:157:TYR:CB	1:B:181:GLU:HB3	2.26	0.55
1:B:228:ASP:OD2	1:B:257:HIS:HA	2.06	0.55
1:B:303:LEU:CB	1:B:334:ILE:CD1	2.77	0.55
1:B:329:LEU:HD22	1:B:335:LEU:CD1	2.36	0.55
1:B:335:LEU:HB3	1:B:340:LYS:HG2	1.88	0.55
1:B:149:VAL:HG21	1:B:203:THR:HG22	1.89	0.55
1:B:289:GLU:O	1:B:293:TYR:HD2	1.89	0.55
1:C:155:ASP:O	1:C:159:PHE:HB3	2.06	0.55
1:B:164:PHE:CZ	1:B:186:SER:CB	2.88	0.55
1:B:95:VAL:HA	1:B:120:ALA:O	2.07	0.55
1:B:177:ARG:CG	1:B:262:THR:HB	2.36	0.55
1:B:260:LEU:HD23	1:B:267:VAL:HG11	1.88	0.55
1:B:287:LEU:HD13	1:B:315:PHE:CD1	2.41	0.55
1:B:126:GLU:HA	1:B:127:PRO:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ARG:HB3	1:C:362:PHE:CD1	2.42	0.55
1:A:163:PHE:O	1:A:167:PHE:CB	2.55	0.55
1:A:260:LEU:HD23	1:A:267:VAL:CG1	2.30	0.55
1:B:94:LEU:HG	1:B:116:ILE:HD12	1.89	0.55
1:B:135:ASN:OD1	1:B:137:ASP:HB2	2.06	0.55
1:C:360:ARG:CG	1:C:362:PHE:CZ	2.85	0.55
1:A:9:ASN:CG	1:A:10:SER:H	2.15	0.54
1:B:187:TRP:NE1	1:C:184:ARG:HH21	2.05	0.54
1:B:336:SER:O	1:B:340:LYS:HG3	2.07	0.54
1:A:256:PRO:HD3	1:A:263:HIS:CE1	2.42	0.54
1:B:164:PHE:CZ	1:B:186:SER:C	2.85	0.54
1:C:359:ARG:HB3	1:C:415:TYR:CE2	2.43	0.54
1:C:42:GLN:NE2	1:C:260:LEU:HB3	2.22	0.54
1:A:223:LEU:CD1	1:A:270:ALA:CB	2.85	0.54
1:B:164:PHE:CE2	1:B:187:TRP:CA	2.89	0.54
1:B:303:LEU:CD1	1:B:334:ILE:HD12	2.38	0.54
1:B:335:LEU:HB3	1:B:340:LYS:HG3	1.88	0.54
1:C:99:MET:HA	1:C:125:LEU:HD11	1.89	0.54
1:A:163:PHE:CE2	1:A:167:PHE:CD2	2.96	0.54
1:A:41:ARG:HB3	1:A:264:ALA:HB1	1.89	0.54
1:B:286:LEU:CD1	1:B:424:GLU:HG2	2.37	0.54
1:C:233:ILE:HG13	1:C:237:ALA:HB3	1.90	0.54
1:C:354:GLU:O	1:C:357:LEU:HG	2.08	0.54
1:A:18:GLU:OE2	1:A:20:HIS:CE1	2.61	0.54
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.90	0.54
1:C:72:ASP:OD1	1:C:73:TYR:N	2.40	0.54
1:A:11:THR:HG21	1:B:17:TYR:CE2	2.41	0.54
1:A:94:LEU:HG	1:A:116:ILE:HD12	1.89	0.54
1:A:131:LYS:HE2	1:A:136:PRO:O	2.08	0.54
1:C:137:ASP:CB	1:C:239:VAL:HG21	2.38	0.54
1:C:164:PHE:HZ	1:C:186:SER:C	2.15	0.54
1:C:94:LEU:HG	1:C:116:ILE:HD12	1.89	0.53
1:C:122:LEU:HD23	1:C:223:LEU:HB3	1.90	0.53
1:B:69:THR:CG2	1:B:70:GLY:N	2.71	0.53
1:B:42:GLN:HE22	1:B:260:LEU:HB3	1.72	0.53
1:C:249:TYR:CE1	1:C:251:GLU:HG3	2.42	0.53
1:C:303:LEU:CD1	1:C:332:ARG:HG3	2.39	0.53
1:B:66:GLN:OE1	1:C:37:HIS:NE2	2.41	0.53
1:C:213:ILE:N	1:C:214:PRO:CD	2.72	0.53
1:C:303:LEU:HB2	1:C:334:ILE:HD12	1.89	0.53
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:O	1:B:346:VAL:HG23	2.08	0.53
1:C:323:GLU:HB2	1:C:357:LEU:HD21	1.91	0.53
1:C:342:ILE:O	1:C:346:VAL:HG23	2.09	0.53
1:A:18:GLU:OE2	1:A:20:HIS:HE1	1.92	0.53
1:A:259:LEU:HD12	1:A:267:VAL:HG22	1.90	0.53
1:A:310:ARG:O	1:A:314:VAL:HG13	2.09	0.53
1:B:9:ASN:ND2	1:C:52:ARG:HG3	2.24	0.53
1:A:249:TYR:CE1	1:A:251:GLU:HG3	2.44	0.53
1:A:342:ILE:O	1:A:346:VAL:HG23	2.08	0.53
1:C:167:PHE:CE1	1:C:258:GLY:CA	2.91	0.53
1:A:25:PRO:HA	1:A:52:ARG:HB3	1.92	0.52
1:B:9:ASN:HD21	1:C:52:ARG:HG3	1.74	0.52
1:B:10:SER:N	1:C:19:ASP:OD2	2.42	0.52
1:C:24:THR:CG2	1:C:51:TYR:CE1	2.92	0.52
1:C:306:GLU:HB3	1:C:328:TRP:CH2	2.44	0.52
1:A:164:PHE:HZ	1:A:187:TRP:HA	1.74	0.52
1:A:233:ILE:HD11	1:A:249:TYR:OH	2.09	0.52
1:B:157:TYR:CD1	1:C:185:ASN:HB2	2.45	0.52
1:B:157:TYR:CE1	1:C:185:ASN:HB2	2.44	0.52
1:B:177:ARG:O	1:B:262:THR:HA	2.09	0.52
1:A:122:LEU:HD23	1:A:223:LEU:HB3	1.91	0.52
1:B:236:THR:O	1:B:240:PHE:CB	2.58	0.52
1:B:360:ARG:HH11	1:B:360:ARG:CG	2.22	0.52
1:C:336:SER:HB2	1:C:339:THR:OG1	2.10	0.52
1:A:182:ALA:HA	1:C:157:TYR:CB	2.40	0.52
1:B:71:TYR:CZ	1:B:197:ALA:HA	2.45	0.52
1:C:259:LEU:HD23	1:C:259:LEU:H	1.73	0.52
1:A:157:TYR:O	1:B:181:GLU:HG2	2.09	0.52
1:B:303:LEU:HD12	1:B:334:ILE:CG2	2.34	0.52
1:A:182:ALA:HA	1:C:157:TYR:CG	2.45	0.52
1:A:360:ARG:HH11	1:A:360:ARG:CG	2.22	0.52
1:B:67:PRO:CA	1:C:20:HIS:HE1	2.07	0.52
1:B:141:PRO:O	1:B:144:PHE:HB3	2.10	0.52
1:B:135:ASN:ND2	1:B:138:GLY:H	2.07	0.51
1:A:24:THR:CG2	1:A:279:GLN:OE1	2.58	0.51
1:B:104:VAL:HG12	1:B:121:PHE:HE1	1.75	0.51
1:B:156:ARG:NE	1:B:157:TYR:CZ	2.79	0.51
1:C:335:LEU:HB3	1:C:340:LYS:HG3	1.92	0.51
1:B:39:TRP:CH2	1:B:97:PHE:HB2	2.45	0.51
1:C:155:ASP:O	1:C:159:PHE:CB	2.59	0.51
1:B:68:THR:HG22	1:B:196:PHE:CG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:TYR:CE1	1:C:185:ASN:CG	2.89	0.51
1:C:165:ASN:CG	1:C:170:LEU:HB2	2.35	0.51
1:B:10:SER:CA	1:C:19:ASP:OD2	2.58	0.51
1:A:141:PRO:O	1:A:144:PHE:HB3	2.10	0.51
1:B:108:VAL:HG11	1:B:216:ILE:HG23	1.93	0.51
1:B:38:SER:HA	1:B:261:TRP:CZ2	2.43	0.51
1:C:165:ASN:O	1:C:169:ASN:N	2.44	0.51
1:A:178:ILE:HD13	1:A:261:TRP:NE1	2.25	0.51
1:A:286:LEU:HD22	1:A:286:LEU:O	2.10	0.51
1:B:157:TYR:HB3	1:C:181:GLU:CB	2.40	0.51
1:A:169:ASN:HA	1:A:229:ARG:NH1	2.25	0.51
1:B:1:PRO:HB2	1:B:17:TYR:CD1	2.46	0.50
1:B:123:ALA:HA	1:B:224:HIS:CE1	2.46	0.50
1:A:155:ASP:O	1:A:159:PHE:HB2	2.11	0.50
1:C:24:THR:HG21	1:C:51:TYR:CE1	2.46	0.50
1:C:118:ALA:HB1	1:C:274:PHE:CZ	2.47	0.50
1:B:11:THR:HB	1:C:1:PRO:CG	2.41	0.50
1:B:104:VAL:CG1	1:B:121:PHE:HE1	2.16	0.50
1:C:216:ILE:CG2	1:C:218:VAL:HG22	2.41	0.50
1:A:303:LEU:CB	1:A:334:ILE:HD12	2.38	0.50
1:B:158:ALA:CA	1:C:181:GLU:CG	2.85	0.50
1:B:290:VAL:O	1:B:294:VAL:HG23	2.12	0.50
1:C:17:TYR:CE2	1:C:19:ASP:OD2	2.61	0.50
1:A:260:LEU:O	1:A:264:ALA:CA	2.60	0.50
1:B:1:PRO:HB3	1:B:17:TYR:CE1	2.45	0.50
1:C:322:LEU:CD2	1:C:357:LEU:HD12	2.39	0.50
1:C:335:LEU:HB2	1:C:340:LYS:HE2	1.94	0.50
1:A:233:ILE:O	1:A:237:ALA:HB3	2.11	0.50
1:B:46:LEU:HD22	1:B:51:TYR:HD2	1.77	0.49
1:B:221:LEU:HB2	1:B:274:PHE:CZ	2.46	0.49
1:A:41:ARG:CD	1:A:264:ALA:HB3	2.42	0.49
1:B:220:ALA:HB3	1:B:247:ALA:HB2	1.94	0.49
1:C:303:LEU:HD23	1:C:334:ILE:HB	1.88	0.49
1:A:68:THR:HA	1:A:196:PHE:CD1	2.47	0.49
1:A:303:LEU:HA	1:A:306:GLU:OE1	2.13	0.49
1:B:84:LEU:HD12	1:B:107:TYR:OH	2.12	0.49
1:C:286:LEU:HD21	1:C:424:GLU:HG3	1.94	0.49
1:A:303:LEU:HD12	1:A:334:ILE:CD1	2.42	0.49
1:B:157:TYR:O	1:C:181:GLU:HG2	2.13	0.49
1:A:178:ILE:CD1	1:A:261:TRP:CD1	2.93	0.49
1:A:182:ALA:CB	1:A:261:TRP:HZ2	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:HIS:CA	1:B:39:TRP:HE1	2.16	0.49
1:B:209:PHE:O	1:B:213:ILE:HG13	2.13	0.49
1:A:127:PRO:HD3	1:A:240:PHE:HB2	1.95	0.49
1:B:221:LEU:HB2	1:B:274:PHE:CD1	2.47	0.49
1:C:135:ASN:ND2	1:C:137:ASP:HB2	2.21	0.49
1:C:303:LEU:CD2	1:C:334:ILE:CB	2.83	0.49
1:A:144:PHE:CZ	1:A:148:ILE:HD11	2.48	0.48
1:A:195:PHE:HB3	1:B:40:GLU:OE1	2.13	0.48
1:A:335:LEU:HD13	1:A:343:LEU:HD12	1.95	0.48
1:B:58:ARG:O	1:B:59:ARG:C	2.56	0.48
1:C:84:LEU:HD12	1:C:107:TYR:OH	2.12	0.48
1:C:259:LEU:O	1:C:263:HIS:HB2	2.13	0.48
1:A:71:TYR:CE2	1:A:196:PHE:HD1	2.32	0.48
1:A:126:GLU:O	1:A:236:THR:CB	2.55	0.48
1:C:70:GLY:O	1:C:75:THR:HG21	2.13	0.48
1:C:335:LEU:O	1:C:340:LYS:HE3	2.13	0.48
1:B:31:GLY:HA3	1:B:98:SER:HB3	1.95	0.48
1:B:164:PHE:HZ	1:B:186:SER:C	2.21	0.48
1:B:233:ILE:HG23	1:B:238:ARG:HD2	1.94	0.48
1:A:177:ARG:HD2	1:A:262:THR:HG22	1.94	0.48
1:B:164:PHE:CE1	1:B:186:SER:CB	2.91	0.48
1:A:9:ASN:ND2	1:B:52:ARG:HE	2.10	0.48
1:A:41:ARG:HD3	1:A:264:ALA:HB3	1.96	0.48
1:A:354:GLU:O	1:A:357:LEU:HG	2.13	0.48
1:B:135:ASN:CG	1:B:137:ASP:HB2	2.38	0.48
1:A:195:PHE:CB	1:B:40:GLU:OE1	2.62	0.48
1:B:144:PHE:CZ	1:B:148:ILE:HD11	2.48	0.48
1:B:177:ARG:C	1:B:262:THR:HG22	2.38	0.48
1:C:249:TYR:HE1	1:C:251:GLU:CG	2.26	0.48
1:A:156:ARG:NE	1:A:157:TYR:CZ	2.81	0.48
1:A:208:ASP:OD1	1:A:210:ARG:HG3	2.12	0.48
1:B:354:GLU:O	1:B:357:LEU:HG	2.13	0.48
1:B:123:ALA:HA	1:B:224:HIS:ND1	2.29	0.48
1:B:157:TYR:CB	1:C:181:GLU:CB	2.91	0.48
1:B:303:LEU:HA	1:B:306:GLU:OE1	2.13	0.48
1:C:17:TYR:HE2	1:C:19:ASP:CG	2.21	0.48
1:C:127:PRO:HG3	1:C:239:VAL:CG1	2.42	0.48
1:C:164:PHE:CZ	1:C:186:SER:CB	2.96	0.48
1:A:256:PRO:HD2	1:A:263:HIS:CE1	2.47	0.48
1:B:201:ALA:N	1:B:202:PRO:CD	2.77	0.48
1:A:24:THR:OG1	1:A:279:GLN:OE1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASP:CG	1:C:257:HIS:HA	2.39	0.47
1:A:171:ASP:OD1	1:A:172:GLU:N	2.46	0.47
1:B:122:LEU:CD2	1:B:223:LEU:HB3	2.44	0.47
1:C:234:GLU:HG2	1:C:235:ASN:N	2.30	0.47
1:C:303:LEU:HD23	1:C:334:ILE:CB	2.43	0.47
1:B:31:GLY:CA	1:B:98:SER:HB3	2.44	0.47
1:C:167:PHE:CE1	1:C:258:GLY:HA2	2.50	0.47
1:B:11:THR:HG23	1:C:17:TYR:CE2	2.44	0.47
1:A:287:LEU:HB3	1:A:315:PHE:CD2	2.49	0.47
1:B:31:GLY:HA3	1:B:98:SER:CB	2.45	0.47
1:B:234:GLU:HA	1:B:238:ARG:CB	2.42	0.47
1:B:10:SER:HB3	1:C:87:LEU:HD21	1.89	0.47
1:B:157:TYR:HB3	1:C:181:GLU:O	2.14	0.47
1:B:157:TYR:CE1	1:C:185:ASN:CB	2.98	0.47
1:A:223:LEU:HD12	1:A:270:ALA:HB1	1.97	0.47
1:A:171:ASP:OD1	1:A:172:GLU:HG3	2.14	0.47
1:B:25:PRO:HA	1:B:52:ARG:HB3	1.97	0.47
1:B:41:ARG:CD	1:B:264:ALA:HB2	2.37	0.47
1:C:77:ALA:HB2	1:C:106:ARG:HG3	1.96	0.47
1:C:171:ASP:OD1	1:C:172:GLU:HG3	2.14	0.47
1:B:260:LEU:CD2	1:B:267:VAL:HG11	2.45	0.46
1:A:223:LEU:HD11	1:A:270:ALA:CB	2.45	0.46
1:C:220:ALA:HB3	1:C:247:ALA:HB2	1.98	0.46
1:A:249:TYR:CE1	1:A:251:GLU:CG	2.98	0.46
1:A:249:TYR:HE1	1:A:251:GLU:HG3	1.79	0.46
1:A:259:LEU:O	1:A:263:HIS:CB	2.63	0.46
1:B:119:VAL:CG2	1:B:121:PHE:CE2	2.99	0.46
1:C:167:PHE:CE1	1:C:258:GLY:HA3	2.51	0.46
1:A:39:TRP:CE3	1:A:42:GLN:HG2	2.51	0.46
1:A:43:SER:HB2	1:C:195:PHE:CZ	2.51	0.46
1:B:228:ASP:CG	1:B:257:HIS:HA	2.40	0.46
1:B:260:LEU:HA	1:B:267:VAL:HG21	1.98	0.46
1:C:126:GLU:CB	1:C:127:PRO:HA	2.37	0.46
1:B:156:ARG:HG3	1:B:157:TYR:CE2	2.51	0.46
1:C:45:ALA:HB2	1:C:268:ASN:ND2	2.31	0.46
1:C:68:THR:HA	1:C:196:PHE:CD1	2.51	0.46
1:C:298:ILE:HD13	1:C:307:ILE:HD12	1.81	0.46
1:A:329:LEU:HD11	1:A:347:PHE:HD2	1.81	0.46
1:B:121:PHE:N	1:B:121:PHE:CD2	2.83	0.46
1:B:303:LEU:CD1	1:B:334:ILE:CG2	2.94	0.46
1:C:148:ILE:O	1:C:152:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:HG12	1:C:237:ALA:HB3	1.97	0.46
1:A:245:PRO:HG2	1:A:246:SER:H	1.81	0.46
1:C:329:LEU:HD22	1:C:335:LEU:HD11	1.92	0.46
1:A:173:ASN:HD22	1:A:177:ARG:HG3	1.74	0.46
1:A:275:LEU:O	1:A:279:GLN:HG2	2.16	0.46
1:B:303:LEU:HG	1:B:334:ILE:HD12	1.94	0.46
1:B:319:ASN:CA	1:B:352:PRO:HG2	2.46	0.46
1:C:68:THR:HG22	1:C:196:PHE:CG	2.51	0.46
1:A:234:GLU:CA	1:A:238:ARG:HB2	2.40	0.45
1:B:101:THR:HB	1:B:124:SER:HB3	1.98	0.45
1:B:249:TYR:CE1	1:B:251:GLU:CG	2.99	0.45
1:C:70:GLY:O	1:C:75:THR:HB	2.15	0.45
1:C:329:LEU:HD23	1:C:335:LEU:HD11	1.98	0.45
1:A:30:HIS:ND1	1:A:34:LEU:O	2.49	0.45
1:A:265:GLU:OE1	1:A:265:GLU:HA	2.17	0.45
1:C:394:GLY:O	1:C:398:ILE:HG23	2.16	0.45
1:B:108:VAL:HG11	1:B:216:ILE:CG2	2.45	0.45
1:B:329:LEU:HD11	1:B:347:PHE:HD2	1.81	0.45
1:C:238:ARG:NH1	1:C:242:LYS:NZ	2.65	0.45
1:C:249:TYR:CE1	1:C:251:GLU:CG	3.00	0.45
1:B:394:GLY:O	1:B:398:ILE:HG23	2.17	0.45
1:C:329:LEU:HD11	1:C:347:PHE:HD2	1.81	0.45
1:A:394:GLY:O	1:A:398:ILE:HG23	2.16	0.45
1:A:223:LEU:CD1	1:A:270:ALA:HB1	2.47	0.45
1:A:258:GLY:O	1:A:262:THR:HB	2.17	0.45
1:C:218:VAL:O	1:C:219:PRO:C	2.60	0.45
1:C:259:LEU:N	1:C:259:LEU:CD2	2.79	0.45
1:C:372:ASP:HA	1:C:373:PRO:HD3	1.86	0.45
1:B:71:TYR:CE2	1:B:196:PHE:HD1	2.35	0.45
1:B:263:HIS:O	1:B:264:ALA:C	2.59	0.45
1:A:319:ASN:CA	1:A:352:PRO:HG2	2.46	0.45
1:B:135:ASN:ND2	1:B:137:ASP:N	2.64	0.45
1:B:10:SER:O	1:C:17:TYR:OH	2.35	0.45
1:B:263:HIS:C	1:B:265:GLU:N	2.73	0.45
1:B:249:TYR:HE1	1:B:251:GLU:CG	2.28	0.44
1:B:286:LEU:CD1	1:B:424:GLU:CG	2.93	0.44
1:C:360:ARG:HB2	1:C:363:VAL:HG21	1.91	0.44
1:B:156:ARG:H	1:B:156:ARG:HG2	1.55	0.44
1:B:290:VAL:HG23	1:B:431:CYS:SG	2.57	0.44
1:C:98:SER:HA	1:C:123:ALA:O	2.18	0.44
1:C:118:ALA:HB1	1:C:274:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:HIS:CE1	1:C:66:GLN:O	2.70	0.44
1:C:144:PHE:CE2	1:C:148:ILE:CD1	2.86	0.44
1:C:363:VAL:HG12	1:C:367:LEU:HD12	2.00	0.44
1:C:421:VAL:HB	1:C:425:VAL:HG13	1.98	0.44
1:A:182:ALA:HA	1:C:157:TYR:CD2	2.53	0.44
1:C:233:ILE:HG13	1:C:237:ALA:HB2	1.99	0.44
1:C:237:ALA:HB1	1:C:249:TYR:OH	2.18	0.44
1:C:49:ALA:CB	1:C:272:LEU:HD22	2.48	0.44
1:C:156:ARG:NE	1:C:157:TYR:OH	2.36	0.44
1:A:195:PHE:CD2	1:B:40:GLU:HB2	2.52	0.44
1:C:339:THR:HG22	1:C:343:LEU:CD1	2.46	0.44
1:B:30:HIS:ND1	1:B:34:LEU:O	2.49	0.44
1:B:104:VAL:HB	1:B:121:PHE:CE1	2.53	0.44
1:B:286:LEU:HD13	1:B:424:GLU:HG3	2.00	0.44
1:C:177:ARG:CD	1:C:263:HIS:CE1	3.01	0.44
1:C:319:ASN:CA	1:C:352:PRO:HG2	2.46	0.44
1:A:90:GLN:HE21	1:A:90:GLN:HB3	1.59	0.43
1:A:98:SER:HA	1:A:123:ALA:O	2.18	0.43
1:A:249:TYR:HE1	1:A:251:GLU:CG	2.31	0.43
1:C:155:ASP:CB	1:C:158:ALA:HB3	2.46	0.43
1:A:176:THR:HG22	1:A:177:ARG:N	2.33	0.43
1:C:303:LEU:O	1:C:307:ILE:HG13	2.18	0.43
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.81	0.43
1:C:49:ALA:CB	1:C:272:LEU:CD2	2.96	0.43
1:A:239:VAL:HG13	1:A:240:PHE:N	2.33	0.43
1:C:225:GLY:HA2	1:C:255:ALA:HB3	2.00	0.43
1:A:225:GLY:HA2	1:A:255:ALA:HB3	2.00	0.43
1:B:135:ASN:HD21	1:B:137:ASP:CA	2.31	0.43
1:B:156:ARG:HD3	1:C:40:GLU:CD	2.38	0.43
1:C:265:GLU:OE1	1:C:265:GLU:HA	2.18	0.43
1:B:329:LEU:CD2	1:B:335:LEU:HD11	2.48	0.43
1:A:68:THR:HG22	1:A:196:PHE:CG	2.53	0.43
1:A:68:THR:HG22	1:A:196:PHE:CB	2.49	0.43
1:B:139:ALA:HB1	1:B:235:ASN:ND2	2.30	0.43
1:B:177:ARG:HA	1:B:177:ARG:HD3	1.57	0.43
1:A:178:ILE:HG22	1:A:179:SER:N	2.33	0.43
1:A:178:ILE:CG2	1:A:179:SER:N	2.81	0.43
1:C:127:PRO:CG	1:C:239:VAL:HG12	2.48	0.43
1:C:322:LEU:HB3	1:C:357:LEU:CD1	2.49	0.43
1:A:10:SER:OG	1:B:19:ASP:OD2	2.37	0.42
1:A:140:ALA:HB1	1:A:141:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HD22	1:C:174:LEU:HD13	2.01	0.42
1:A:170:LEU:HD22	1:A:174:LEU:HD13	2.01	0.42
1:B:71:TYR:CE1	1:B:197:ALA:CB	3.01	0.42
1:B:328:TRP:O	1:B:332:ARG:HG2	2.20	0.42
1:C:41:ARG:CD	1:C:264:ALA:CB	2.88	0.42
1:C:335:LEU:HD13	1:C:343:LEU:HD12	2.01	0.42
1:A:58:ARG:O	1:A:59:ARG:C	2.62	0.42
1:B:126:GLU:HG3	1:B:209:PHE:CG	2.54	0.42
1:C:171:ASP:OD1	1:C:172:GLU:N	2.47	0.42
1:C:238:ARG:NH1	1:C:242:LYS:HZ1	2.17	0.42
1:B:329:LEU:CD2	1:B:335:LEU:CD1	2.98	0.42
1:C:140:ALA:HB1	1:C:141:PRO:HD2	2.01	0.42
1:C:322:LEU:HB3	1:C:357:LEU:HD12	2.01	0.42
1:A:39:TRP:HE3	1:A:42:GLN:HG2	1.83	0.42
1:B:122:LEU:HD22	1:B:223:LEU:HD22	2.01	0.42
1:B:163:PHE:O	1:B:167:PHE:HB2	2.20	0.42
1:C:329:LEU:HD11	1:C:347:PHE:CD2	2.54	0.42
1:B:225:GLY:HA2	1:B:255:ALA:HB3	2.00	0.42
1:B:287:LEU:HD22	1:B:315:PHE:CE1	2.55	0.42
1:B:329:LEU:HD11	1:B:347:PHE:CD2	2.54	0.42
1:A:71:TYR:CE1	1:A:197:ALA:CB	3.03	0.42
1:A:223:LEU:CD1	1:A:270:ALA:HB3	2.50	0.42
1:B:289:GLU:O	1:B:293:TYR:CD2	2.72	0.42
1:C:201:ALA:N	1:C:202:PRO:CD	2.82	0.42
1:B:122:LEU:HA	1:B:223:LEU:O	2.20	0.42
1:C:328:TRP:O	1:C:332:ARG:HG2	2.19	0.42
1:B:104:VAL:CB	1:B:121:PHE:CE1	3.02	0.41
1:B:195:PHE:CD2	1:C:40:GLU:CB	3.03	0.41
1:B:220:ALA:HB3	1:B:247:ALA:CB	2.51	0.41
1:B:302:PRO:O	1:B:305:ALA:HB3	2.19	0.41
1:B:372:ASP:O	1:B:376:MET:HG3	2.20	0.41
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.80	0.41
1:C:307:ILE:HG22	1:C:311:LEU:CD1	2.50	0.41
1:A:157:TYR:CD2	1:B:182:ALA:HA	2.55	0.41
1:A:201:ALA:N	1:A:202:PRO:CD	2.83	0.41
1:A:302:PRO:O	1:A:305:ALA:HB3	2.19	0.41
1:A:329:LEU:HD11	1:A:347:PHE:CD2	2.54	0.41
1:B:9:ASN:HB3	1:C:52:ARG:HH21	1.85	0.41
1:B:71:TYR:CE1	1:B:197:ALA:CA	3.01	0.41
1:B:231:LEU:HD12	1:B:257:HIS:CE1	2.54	0.41
1:C:70:GLY:O	1:C:75:THR:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:LYS:NZ	1:C:420:ALA:O	2.53	0.41
1:A:20:HIS:CG	1:C:68:THR:HG23	2.55	0.41
1:B:8:GLU:HG2	1:B:13:ILE:CG1	2.50	0.41
1:C:260:LEU:O	1:C:264:ALA:CA	2.69	0.41
1:A:338:LEU:HD13	1:A:437:ILE:HD13	2.01	0.41
1:A:347:PHE:O	1:A:351:VAL:HB	2.20	0.41
1:B:9:ASN:HD21	1:C:20:HIS:C	2.27	0.41
1:B:39:TRP:CZ2	1:B:97:PHE:HB2	2.55	0.41
1:B:177:ARG:HG3	1:B:262:THR:HB	2.02	0.41
1:C:128:PHE:CE2	1:C:130:LEU:HB3	2.55	0.41
1:A:236:THR:HA	1:A:239:VAL:HG12	2.01	0.41
1:B:140:ALA:HB1	1:B:141:PRO:HD2	2.01	0.41
1:A:9:ASN:CG	1:A:10:SER:N	2.77	0.41
1:A:156:ARG:H	1:A:156:ARG:HG2	1.57	0.41
1:B:40:GLU:OE2	1:B:261:TRP:HH2	2.04	0.41
1:B:234:GLU:O	1:B:239:VAL:HG23	2.20	0.41
1:B:347:PHE:O	1:B:351:VAL:HB	2.21	0.41
1:C:165:ASN:CG	1:C:170:LEU:HD12	2.43	0.41
1:A:178:ILE:HD13	1:A:261:TRP:CG	2.56	0.41
1:A:187:TRP:CE2	1:B:184:ARG:NH2	2.85	0.41
1:B:195:PHE:CZ	1:C:43:SER:HB2	2.56	0.41
1:B:387:LYS:NZ	1:B:420:ALA:O	2.53	0.41
1:B:424:GLU:CD	1:B:424:GLU:H	2.29	0.41
1:A:28:LEU:HB3	1:A:39:TRP:CE2	2.56	0.41
1:B:5:VAL:HG11	1:B:15:LEU:CD1	2.51	0.41
1:B:45:ALA:HB1	1:B:272:LEU:HD11	2.01	0.41
1:B:216:ILE:HG22	1:B:218:VAL:HG22	2.01	0.41
1:B:263:HIS:O	1:B:266:GLU:N	2.54	0.41
1:B:335:LEU:HB2	1:B:340:LYS:HE2	2.02	0.41
1:C:5:VAL:HG11	1:C:15:LEU:CD1	2.51	0.41
1:C:233:ILE:O	1:C:237:ALA:CA	2.68	0.41
1:C:323:GLU:N	1:C:357:LEU:HD11	2.36	0.41
1:C:347:PHE:O	1:C:351:VAL:HB	2.20	0.41
1:A:5:VAL:HG11	1:A:15:LEU:CD1	2.51	0.41
1:A:42:GLN:N	1:A:42:GLN:CD	2.79	0.41
1:A:252:VAL:CG1	1:A:255:ALA:HB2	2.46	0.41
1:A:328:TRP:O	1:A:332:ARG:HG2	2.20	0.41
1:A:387:LYS:NZ	1:A:420:ALA:O	2.53	0.41
1:B:165:ASN:OD1	1:B:170:LEU:HB2	2.20	0.41
1:B:335:LEU:CB	1:B:340:LYS:HG2	2.50	0.41
1:C:17:TYR:CE2	1:C:19:ASP:CG	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:HIS:ND1	1:C:34:LEU:O	2.54	0.41
1:C:225:GLY:CA	1:C:255:ALA:HB3	2.51	0.41
1:C:372:ASP:O	1:C:376:MET:HG3	2.20	0.41
1:C:422:THR:C	1:C:425:VAL:HG12	2.46	0.41
1:A:372:ASP:O	1:A:376:MET:HG3	2.20	0.41
1:B:46:LEU:HD21	1:B:275:LEU:CD1	2.51	0.41
1:B:260:LEU:H	1:B:260:LEU:HG	1.52	0.41
1:B:265:GLU:HA	1:B:265:GLU:OE1	2.20	0.41
1:B:298:ILE:HD13	1:B:307:ILE:HD13	2.03	0.41
1:B:19:ASP:HA	1:B:53:VAL:O	2.21	0.40
1:B:263:HIS:N	1:B:263:HIS:ND1	2.68	0.40
1:C:106:ARG:NH2	1:C:209:PHE:CE1	2.89	0.40
1:A:225:GLY:CA	1:A:255:ALA:HB3	2.51	0.40
1:A:305:ALA:O	1:A:309:GLN:HG2	2.22	0.40
1:B:319:ASN:HA	1:B:352:PRO:CG	2.49	0.40
1:C:28:LEU:HB3	1:C:39:TRP:CE2	2.56	0.40
1:C:129:LEU:HD12	1:C:205:TRP:O	2.21	0.40
1:C:209:PHE:O	1:C:212:ASP:HB2	2.22	0.40
1:C:308:ALA:O	1:C:312:GLU:CD	2.65	0.40
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.82	0.40
1:A:236:THR:CA	1:A:239:VAL:HG12	2.52	0.40
1:B:90:GLN:HB2	1:B:391:THR:HG21	2.03	0.40
1:B:225:GLY:CA	1:B:255:ALA:HB3	2.51	0.40
1:C:299:PRO:HG2	1:C:334:ILE:CG2	2.51	0.40
1:A:46:LEU:HD23	1:A:272:LEU:HD21	2.04	0.40
1:B:158:ALA:HA	1:C:181:GLU:HG2	1.97	0.40
1:B:195:PHE:HZ	1:C:43:SER:HB2	1.86	0.40
1:C:70:GLY:O	1:C:75:THR:CB	2.70	0.40
1:C:223:LEU:C	1:C:223:LEU:HD23	2.46	0.40
1:C:424:GLU:H	1:C:424:GLU:CD	2.29	0.40
1:A:107:TYR:CD1	1:A:107:TYR:C	2.99	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	438/456 (96%)	427 (98%)	11 (2%)	0	100	100
1	B	438/456 (96%)	428 (98%)	10 (2%)	0	100	100
1	C	438/456 (96%)	427 (98%)	11 (2%)	0	100	100
All	All	1314/1368 (96%)	1282 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	354/370 (96%)	333 (94%)	21 (6%)	18	39
1	B	354/370 (96%)	332 (94%)	22 (6%)	16	38
1	C	354/370 (96%)	334 (94%)	20 (6%)	19	40
All	All	1062/1110 (96%)	999 (94%)	63 (6%)	18	39

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	MET
1	A	108	VAL
1	A	133	ASP
1	A	156	ARG
1	A	165	ASN
1	A	217	ASP
1	A	234	GLU
1	A	238	ARG
1	A	260	LEU
1	A	282	GLN
1	A	284	GLN
1	A	285	LYS
1	A	286	LEU

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	310	ARG
1	A	325	LEU
1	A	338	LEU
1	A	351	VAL
1	A	353	SER
1	A	360	ARG
1	A	396	LYS
1	B	41	ARG
1	B	91	ASP
1	B	98	SER
1	B	108	VAL
1	B	122	LEU
1	B	124	SER
1	B	156	ARG
1	B	165	ASN
1	B	177	ARG
1	B	215	ARG
1	B	216	ILE
1	B	234	GLU
1	B	238	ARG
1	B	260	LEU
1	B	290	VAL
1	B	303	LEU
1	B	325	LEU
1	B	338	LEU
1	B	351	VAL
1	B	353	SER
1	B	360	ARG
1	B	396	LYS
1	C	91	ASP
1	C	99	MET
1	C	108	VAL
1	C	156	ARG
1	C	165	ASN
1	C	216	ILE
1	C	234	GLU
1	C	260	LEU
1	C	279	GLN
1	C	280	GLU
1	C	287	LEU
1	C	304	LYS

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Mol	Chain	Res	Type
1	C	306	GLU
1	C	325	LEU
1	C	338	LEU
1	C	351	VAL
1	C	353	SER
1	C	360	ARG
1	C	389	GLU
1	C	396	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	90	GLN
1	A	135	ASN
1	A	173	ASN
1	A	188	ASN
1	B	9	ASN
1	B	42	GLN
1	B	90	GLN
1	B	135	ASN
1	B	173	ASN
1	B	188	ASN
1	B	235	ASN
1	B	279	GLN
1	C	135	ASN
1	C	173	ASN
1	C	188	ASN
1	C	268	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 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

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	440/456 (96%)	-0.16	10 (2%) 61 53	184, 286, 365, 403	0
1	B	440/456 (96%)	-0.29	5 (1%) 78 66	268, 397, 443, 467	0
1	C	440/456 (96%)	-0.13	12 (2%) 56 48	165, 260, 336, 373	0
All	All	1320/1368 (96%)	-0.19	27 (2%) 65 56	165, 306, 426, 467	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	125	LEU	7.1
1	B	83	VAL	5.1
1	A	421	VAL	4.5
1	B	408	ALA	4.1
1	A	198	ALA	3.8
1	C	427	PHE	3.5
1	A	83	VAL	3.4
1	C	414	ILE	3.3
1	A	27	VAL	3.1
1	B	404	ALA	3.0
1	C	129	LEU	2.9
1	B	411	MET	2.8
1	A	420	ALA	2.8
1	C	271	LEU	2.7
1	C	102	GLY	2.7
1	A	311	LEU	2.6
1	C	83	VAL	2.6
1	A	271	LEU	2.4
1	C	307	ILE	2.4
1	C	413	LEU	2.3
1	A	187	TRP	2.2
1	B	253	GLU	2.1
1	C	56	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	418	MET	2.1
1	C	290	VAL	2.1
1	A	160	TYR	2.0
1	A	416	ASN	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.