



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:12 PM EDT

PDB ID : 4M64 / pdb_00004m64
Title : 3D crystal structure of Na⁺/melibiose symporter of Salmonella typhimurium
Authors : Ethayathulla, A.S.; Guan, L.
Deposited on : 2013-08-08
Resolution : 3.35 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:

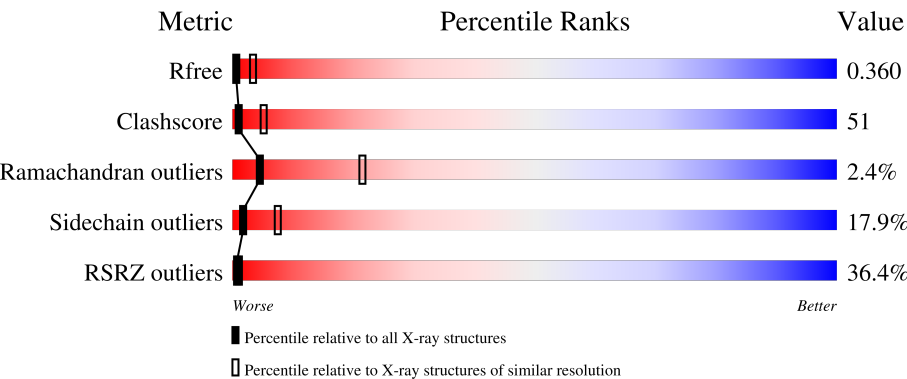
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	486	29% 29%50%12%•8%
1	B	486	40% 36%42%10%12%
1	C	486	26% 28%44%16%•11%
1	D	486	32% 32%38%8%•21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12982 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 Melibiose carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3442	2295	540	585	22			
1	B	426	Total	C	N	O	S	0	0	0
			3258	2176	503	558	21			
1	C	431	Total	C	N	O	S	0	0	0
			3352	2242	520	568	22			
1	D	382	Total	C	N	O	S	0	0	0
			2930	1965	449	497	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	LEU	engineered mutation	UNP P30878
A	477	HIS	-	expression tag	UNP P30878
A	478	HIS	-	expression tag	UNP P30878
A	479	HIS	-	expression tag	UNP P30878
A	480	HIS	-	expression tag	UNP P30878
A	481	HIS	-	expression tag	UNP P30878
A	482	HIS	-	expression tag	UNP P30878
A	483	HIS	-	expression tag	UNP P30878
A	484	HIS	-	expression tag	UNP P30878
A	485	HIS	-	expression tag	UNP P30878
A	486	HIS	-	expression tag	UNP P30878
B	5	MET	LEU	engineered mutation	UNP P30878
B	477	HIS	-	expression tag	UNP P30878
B	478	HIS	-	expression tag	UNP P30878
B	479	HIS	-	expression tag	UNP P30878
B	480	HIS	-	expression tag	UNP P30878
B	481	HIS	-	expression tag	UNP P30878
B	482	HIS	-	expression tag	UNP P30878
B	483	HIS	-	expression tag	UNP P30878
B	484	HIS	-	expression tag	UNP P30878
B	485	HIS	-	expression tag	UNP P30878

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Chain	Residue	Modelled	Actual	Comment	Reference
B	486	HIS	-	expression tag	UNP P30878
C	5	MET	LEU	engineered mutation	UNP P30878
C	477	HIS	-	expression tag	UNP P30878
C	478	HIS	-	expression tag	UNP P30878
C	479	HIS	-	expression tag	UNP P30878
C	480	HIS	-	expression tag	UNP P30878
C	481	HIS	-	expression tag	UNP P30878
C	482	HIS	-	expression tag	UNP P30878
C	483	HIS	-	expression tag	UNP P30878
C	484	HIS	-	expression tag	UNP P30878
C	485	HIS	-	expression tag	UNP P30878
C	486	HIS	-	expression tag	UNP P30878
D	5	MET	LEU	engineered mutation	UNP P30878
D	477	HIS	-	expression tag	UNP P30878
D	478	HIS	-	expression tag	UNP P30878
D	479	HIS	-	expression tag	UNP P30878
D	480	HIS	-	expression tag	UNP P30878
D	481	HIS	-	expression tag	UNP P30878
D	482	HIS	-	expression tag	UNP P30878
D	483	HIS	-	expression tag	UNP P30878
D	484	HIS	-	expression tag	UNP P30878
D	485	HIS	-	expression tag	UNP P30878
D	486	HIS	-	expression tag	UNP P30878

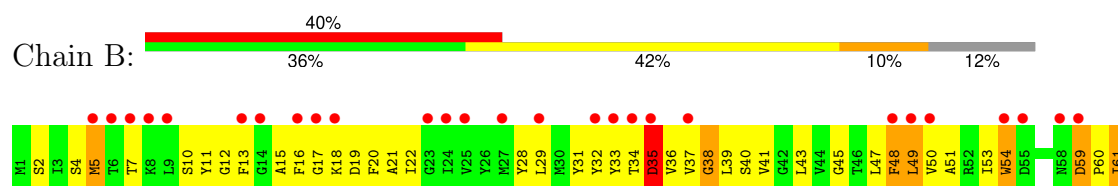
3 Residue-property plots

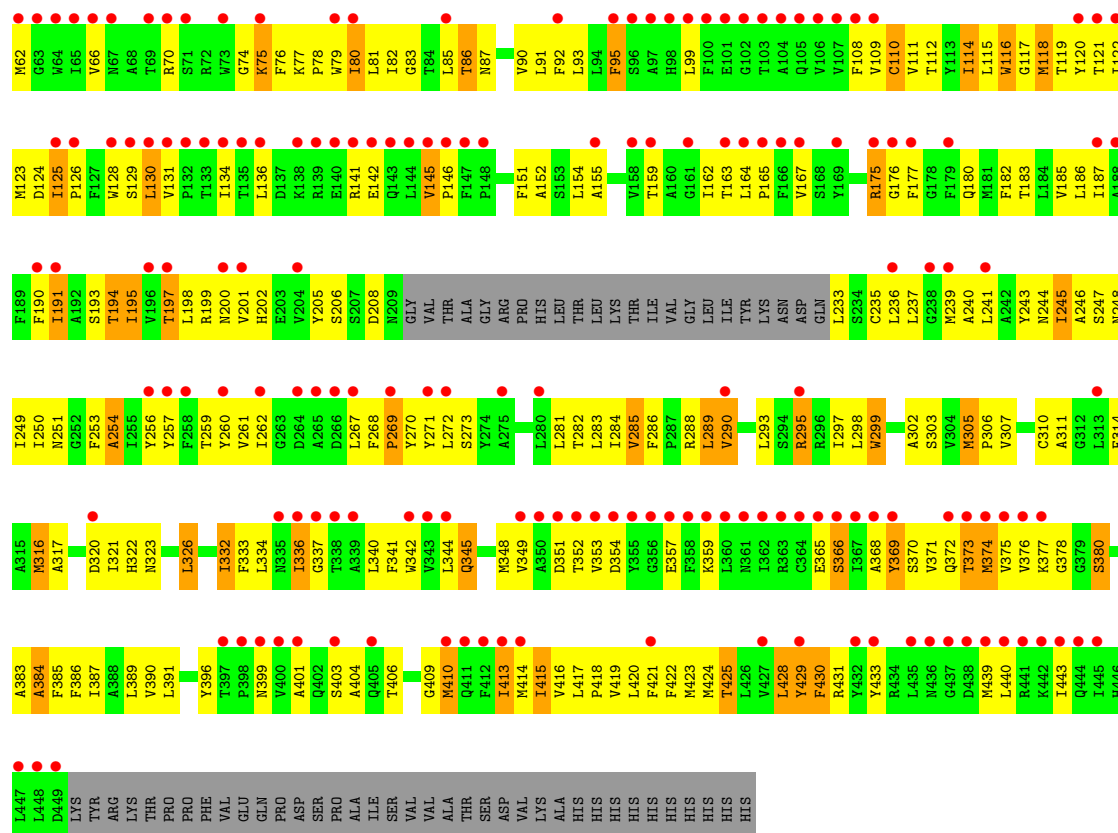
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

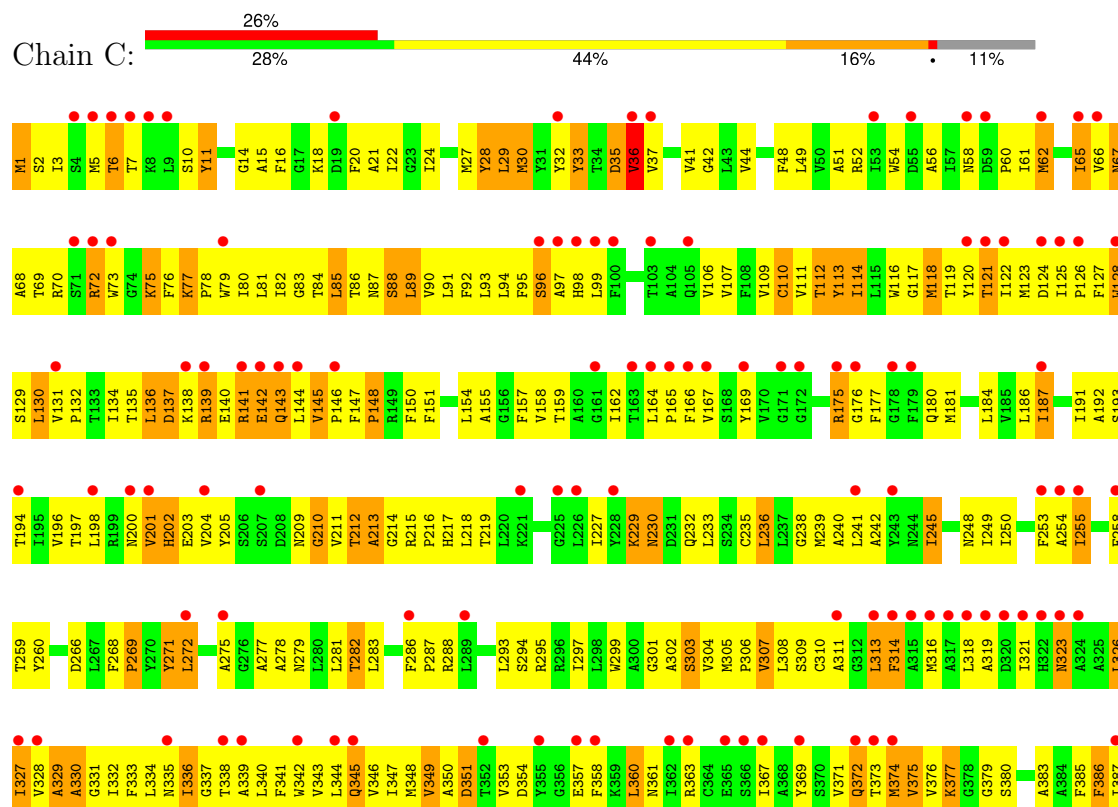


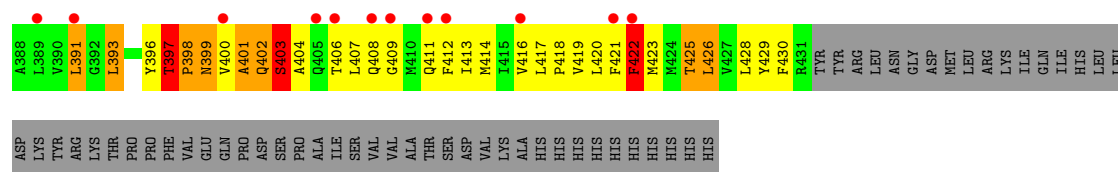
• Molecule 1: Melibiose carrier protein



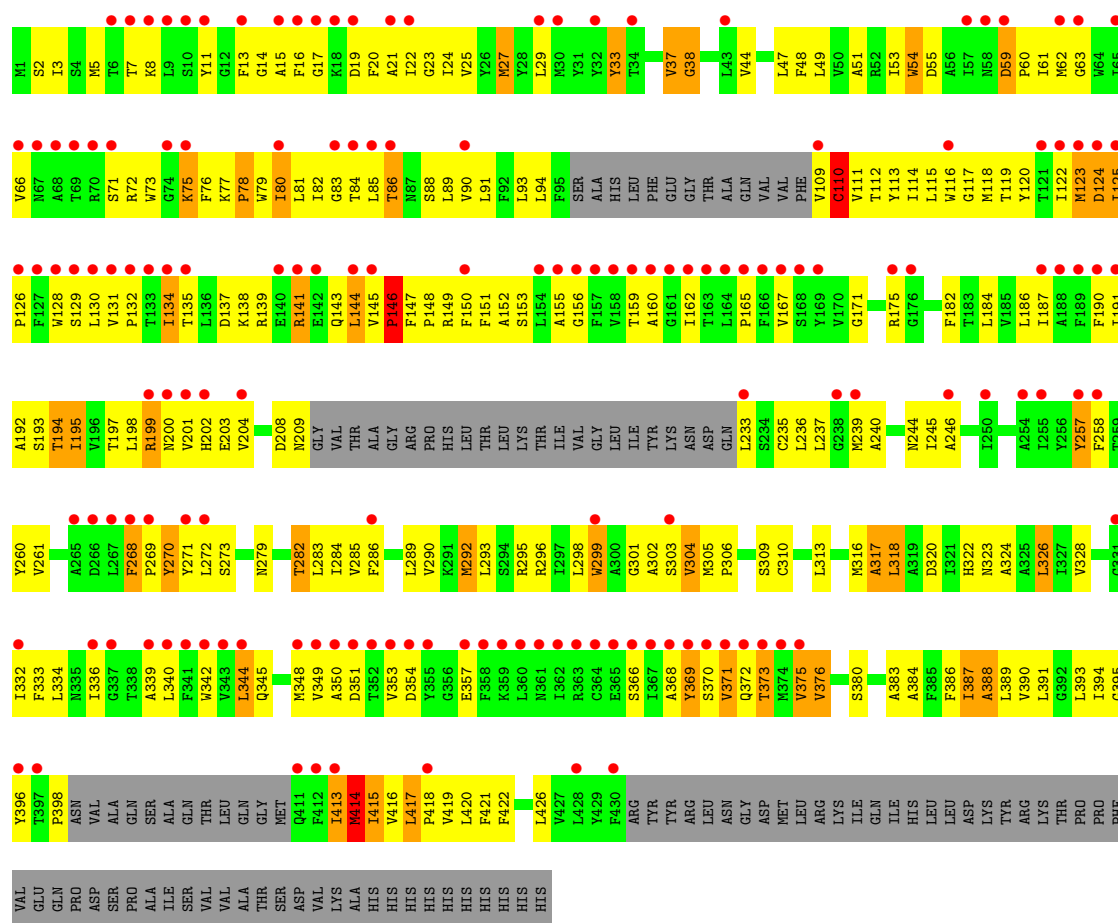


● Molecule 1: Melibiose carrier protein





● Molecule 1: Melibiose carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	127.21Å 127.21Å 206.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.64 – 3.35 38.64 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.64-3.35) 99.4 (38.64-3.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	47.41 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.312 , 0.359 0.311 , 0.360	Depositor DCC
R_{free} test set	2712 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	94.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.039 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3433e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.90	2/3530 (0.1%)	1.26	29/4813 (0.6%)
1	B	0.87	2/3342 (0.1%)	1.17	12/4561 (0.3%)
1	C	0.93	3/3440 (0.1%)	1.32	28/4689 (0.6%)
1	D	0.84	0/3004	1.15	13/4097 (0.3%)
All	All	0.89	7/13316 (0.1%)	1.23	82/18160 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	C	0	4
1	D	0	1
All	All	0	10

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	SER	CA-C	7.62	1.63	1.52
1	C	112	THR	CA-C	-5.88	1.44	1.52
1	A	231	ASP	C-O	5.49	1.28	1.23
1	B	116	TRP	CA-C	-5.27	1.46	1.52
1	B	118	MET	N-CA	-5.26	1.39	1.46
1	C	336	ILE	CA-C	5.07	1.59	1.52
1	A	364	CYS	CA-C	5.05	1.58	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	375	VAL	N-CA-C	10.36	120.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	VAL	N-CA-C	10.06	120.88	110.62
1	D	373	THR	N-CA-C	9.09	121.27	111.36
1	C	402	GLN	N-CA-C	9.07	121.25	111.36
1	C	210	GLY	N-CA-C	-8.87	101.91	112.64
1	B	373	THR	N-CA-C	8.85	120.61	110.97
1	B	116	TRP	N-CA-C	-8.44	102.02	111.14
1	C	65	ILE	N-CA-C	8.26	119.06	110.72
1	C	245	ILE	N-CA-CB	8.08	119.48	110.51
1	B	332	ILE	N-CA-C	8.06	118.15	110.42
1	C	425	THR	N-CA-C	8.03	119.72	110.97
1	C	245	ILE	CB-CA-C	-7.99	101.66	111.88
1	C	213	ALA	N-CA-C	-7.76	99.09	110.42
1	C	349	VAL	N-CA-C	7.68	117.75	110.30
1	C	202	HIS	N-CA-C	7.38	120.20	111.71
1	B	110	CYS	N-CA-C	7.04	118.60	111.07
1	D	318	LEU	N-CA-C	6.92	118.48	111.07
1	C	403	SER	N-CA-C	6.84	120.84	112.23
1	A	90	VAL	CB-CA-C	-6.64	103.20	111.70
1	A	127	PHE	N-CA-C	6.61	118.37	111.03
1	B	399	ASN	N-CA-C	6.59	119.25	111.02
1	C	145	VAL	CB-CA-C	-6.53	107.43	114.35
1	A	289	LEU	N-CA-C	6.50	118.24	111.03
1	A	349	VAL	N-CA-C	6.43	116.58	110.53
1	A	425	THR	N-CA-C	6.38	117.93	110.97
1	A	82	ILE	N-CA-C	-6.34	104.75	113.00
1	D	44	VAL	N-CA-C	6.12	116.82	111.56
1	A	303	SER	N-CA-C	-6.09	104.72	111.36
1	C	69	THR	N-CA-C	6.03	118.75	111.40
1	C	113	TYR	N-CA-C	-5.89	105.18	112.90
1	C	89	LEU	N-CA-C	-5.89	104.05	111.11
1	A	232	GLN	N-CA-C	5.86	117.75	111.36
1	D	54	TRP	CB-CA-C	-5.79	101.79	110.88
1	A	376	VAL	N-CA-CB	5.75	117.28	110.55
1	C	96	SER	N-CA-C	5.72	117.85	108.52
1	D	376	VAL	N-CA-C	5.71	117.13	110.62
1	A	429	TYR	N-CA-C	5.70	119.22	112.72
1	C	377	LYS	N-CA-C	-5.70	104.97	111.07
1	C	303	SER	N-CA-C	-5.69	104.98	111.07
1	D	82	ILE	N-CA-C	-5.68	104.79	110.30
1	B	285	VAL	N-CA-C	-5.68	106.68	111.56
1	B	378	GLY	N-CA-C	-5.65	105.54	112.77
1	C	336	ILE	N-CA-C	5.64	117.05	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ALA	N-CA-C	5.62	119.86	112.89
1	C	107	VAL	N-CA-C	5.58	115.67	110.42
1	C	330	ALA	N-CA-C	5.57	118.42	110.24
1	C	307	VAL	CB-CA-C	-5.55	104.78	111.88
1	D	414	MET	N-CA-C	-5.54	104.46	111.11
1	D	388	ALA	N-CA-C	-5.54	105.32	111.36
1	A	260	TYR	N-CA-C	5.51	119.70	109.56
1	A	320	ASP	N-CA-C	5.49	118.69	111.28
1	A	196	VAL	N-CA-C	-5.48	105.16	110.42
1	A	270	TYR	N-CA-C	5.47	117.95	111.33
1	C	200	ASN	N-CA-C	5.45	119.45	111.34
1	D	110	CYS	N-CA-C	5.43	116.89	110.97
1	D	417	LEU	CA-C-N	-5.40	113.05	119.05
1	D	417	LEU	C-N-CA	-5.40	113.05	119.05
1	A	366	SER	N-CA-C	5.39	117.27	109.07
1	A	54	TRP	N-CA-C	5.39	117.57	111.11
1	C	404	ALA	N-CA-C	5.36	116.81	110.97
1	A	75	LYS	N-CA-C	5.35	116.98	108.79
1	A	403	SER	N-CA-C	5.33	118.25	111.69
1	C	75	LYS	N-CA-C	5.33	116.38	108.86
1	A	98	HIS	N-CA-C	5.31	118.09	111.24
1	A	65	ILE	CB-CA-C	-5.30	105.09	112.04
1	A	319	ALA	N-CA-C	5.29	116.86	111.14
1	A	339	ALA	CB-CA-C	-5.26	110.08	117.23
1	B	334	LEU	CA-C-N	-5.22	112.47	121.66
1	B	334	LEU	C-N-CA	-5.22	112.47	121.66
1	C	397	THR	CA-C-N	-5.21	114.58	119.90
1	C	397	THR	C-N-CA	-5.21	114.58	119.90
1	C	36	VAL	N-CA-CB	5.20	116.47	110.49
1	D	373	THR	CB-CA-C	-5.19	102.03	110.85
1	A	89	LEU	N-CA-C	-5.17	105.34	110.97
1	A	135	THR	N-CA-CB	5.14	117.53	109.97
1	C	266	ASP	N-CA-C	-5.12	106.89	113.23
1	A	162	ILE	CB-CA-C	-5.07	106.60	111.06
1	A	170	VAL	N-CA-C	5.07	115.22	110.30
1	A	340	LEU	N-CA-C	5.06	117.72	110.68
1	B	290	VAL	CB-CA-C	-5.06	105.69	110.65
1	A	399	ASN	N-CA-C	5.04	121.54	110.80
1	B	443	ILE	N-CA-C	5.03	115.25	110.42

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ILE	Peptide
1	B	254	ALA	Peptide
1	B	38	GLY	Peptide
1	B	429	TYR	Peptide
1	B	74	GLY	Peptide
1	C	201	VAL	Peptide
1	C	329	ALA	Peptide
1	C	399	ASN	Peptide
1	C	68	ALA	Peptide
1	D	146	PRO	Peptide

5.2 Too-close contacts [i](#)

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	3442	0	3479	359	0
1	B	3258	0	3249	310	0
1	C	3352	0	3433	373	0
1	D	2930	0	2965	299	0
All	All	12982	0	13126	1332	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 51.

All (1332) 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:299:TRP:CB	1:D:344:LEU:HD13	1.63	1.26
1:D:86:THR:CG2	1:D:115:LEU:HG	1.65	1.26
1:C:75:LYS:HG3	1:C:205:TYR:CB	1.77	1.15
1:D:299:TRP:HB2	1:D:344:LEU:CD1	1.77	1.15
1:C:128:TRP:CH2	1:C:373:THR:HG21	1.83	1.13
1:A:3:ILE:HG23	1:A:203:GLU:HG3	1.28	1.11
1:B:93:LEU:HD13	1:B:112:THR:HG21	1.32	1.11
1:D:86:THR:HG21	1:D:115:LEU:HG	1.24	1.09
1:C:250:ILE:O	1:C:254:ALA:HB2	1.52	1.07
1:C:93:LEU:CD2	1:C:112:THR:HB	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HG23	1:A:191:ILE:HG13	1.36	1.06
1:B:352:THR:HA	1:B:433:TYR:OH	1.55	1.06
1:B:306:PRO:HG2	1:B:422:PHE:CD2	1.90	1.05
1:A:24:ILE:HD12	1:A:186:LEU:HD13	1.38	1.05
1:D:75:LYS:HE3	1:D:76:PHE:H	1.18	1.05
1:D:80:ILE:HG22	1:D:126:PRO:HB2	1.32	1.05
1:B:141:ARG:NH1	1:B:354:ASP:HB2	1.72	1.04
1:A:183:THR:HG22	1:A:187:ILE:HD12	1.36	1.04
1:C:175:ARG:HG3	1:C:175:ARG:HH11	1.22	1.03
1:D:353:VAL:HG12	1:D:357:GLU:CB	1.88	1.03
1:D:75:LYS:HG3	1:D:202:HIS:HA	1.38	1.02
1:A:58:ASN:CG	1:A:121:THR:HG21	1.83	1.02
1:A:417:LEU:HD23	1:A:418:PRO:HD3	1.37	1.01
1:D:75:LYS:HE3	1:D:76:PHE:N	1.76	1.01
1:D:302:ALA:HA	1:D:305:MET:SD	2.01	1.01
1:D:349:VAL:O	1:D:353:VAL:HG23	1.63	0.99
1:B:352:THR:HA	1:B:433:TYR:CZ	1.97	0.99
1:D:313:LEU:HD12	1:D:313:LEU:O	1.63	0.98
1:C:397:THR:OG1	1:C:398:PRO:HD2	1.61	0.98
1:B:306:PRO:HG2	1:B:422:PHE:CE2	1.99	0.97
1:C:282:THR:HG21	1:C:337:GLY:O	1.63	0.97
1:A:3:ILE:HG23	1:A:203:GLU:CG	1.94	0.97
1:D:79:TRP:CE3	1:D:126:PRO:HB3	1.98	0.97
1:D:137:ASP:O	1:D:138:LYS:HG3	1.61	0.97
1:D:141:ARG:O	1:D:141:ARG:HG2	1.63	0.97
1:C:142:GLU:O	1:C:146:PRO:HG3	1.65	0.96
1:B:141:ARG:HH12	1:B:354:ASP:HB2	1.27	0.96
1:C:106:VAL:O	1:C:110:CYS:HB2	1.65	0.96
1:B:77:LYS:HA	1:B:201:VAL:HG11	1.45	0.96
1:B:414:MET:O	1:B:418:PRO:HD2	1.67	0.95
1:D:299:TRP:O	1:D:303:SER:HB2	1.67	0.95
1:D:310:CYS:O	1:D:310:CYS:SG	2.25	0.94
1:C:128:TRP:CZ2	1:C:373:THR:HG21	2.02	0.94
1:A:105:GLN:HE21	1:A:105:GLN:N	1.65	0.94
1:D:296:ARG:HA	1:D:344:LEU:HD11	1.45	0.94
1:C:11:TYR:CE2	1:C:130:LEU:HB3	2.03	0.94
1:A:417:LEU:HD23	1:A:418:PRO:CD	1.98	0.93
1:A:283:LEU:O	1:A:287:PRO:HG2	1.69	0.93
1:C:139:ARG:HD2	1:C:139:ARG:N	1.82	0.93
1:C:82:ILE:O	1:C:86:THR:HG23	1.69	0.93
1:A:1:MET:SD	1:A:3:ILE:HB	2.08	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:VAL:HG11	1:B:295:ARG:HG2	1.50	0.93
1:A:3:ILE:CG2	1:A:203:GLU:HG3	1.98	0.92
1:A:7:THR:HG23	1:A:201:VAL:HG13	1.46	0.92
1:D:86:THR:HG22	1:D:90:VAL:CG2	1.99	0.91
1:B:47:LEU:O	1:B:50:VAL:HG12	1.70	0.91
1:C:24:ILE:HD12	1:C:186:LEU:HD13	1.49	0.91
1:C:139:ARG:HH22	1:C:358:PHE:HB2	1.35	0.91
1:B:302:ALA:HA	1:B:305:MET:SD	2.09	0.91
1:A:77:LYS:HG3	1:A:201:VAL:HB	1.53	0.91
1:B:320:ASP:HB2	1:B:323:ASN:CB	2.01	0.91
1:C:78:PRO:HA	1:C:81:LEU:HD23	1.52	0.91
1:C:387:ILE:HG23	1:C:417:LEU:HD11	1.54	0.90
1:C:75:LYS:HG2	1:C:76:PHE:H	1.37	0.90
1:B:112:THR:O	1:B:115:LEU:HB3	1.70	0.89
1:D:236:LEU:HD22	1:D:348:MET:HB3	1.51	0.89
1:C:7:THR:O	1:C:11:TYR:HB2	1.73	0.88
1:D:150:PHE:HD1	1:D:283:LEU:CD2	1.86	0.88
1:B:62:MET:CE	1:B:122:ILE:HD11	2.03	0.88
1:C:93:LEU:HD21	1:C:112:THR:HB	1.54	0.88
1:B:32:TYR:O	1:B:32:TYR:CD1	2.27	0.88
1:D:236:LEU:HD23	1:D:349:VAL:HG23	1.56	0.88
1:B:32:TYR:O	1:B:32:TYR:HD1	1.56	0.87
1:C:21:ALA:HA	1:C:186:LEU:HD11	1.56	0.87
1:A:241:LEU:HD23	1:A:379:GLY:HA3	1.55	0.87
1:D:86:THR:HG21	1:D:115:LEU:CG	2.04	0.87
1:B:352:THR:HA	1:B:433:TYR:CE2	2.10	0.86
1:D:86:THR:HG22	1:D:90:VAL:HG21	1.56	0.86
1:A:261:VAL:HG21	1:A:328:VAL:HG23	1.57	0.86
1:A:397:THR:CG2	1:A:398:PRO:HD2	2.06	0.86
1:C:215:ARG:N	1:C:216:PRO:HD2	1.91	0.86
1:D:414:MET:O	1:D:418:PRO:HD2	1.75	0.86
1:C:75:LYS:CG	1:C:205:TYR:CB	2.53	0.85
1:A:417:LEU:CD2	1:A:418:PRO:HD3	2.05	0.85
1:B:254:ALA:O	1:B:257:TYR:HB3	1.74	0.85
1:C:212:THR:O	1:C:213:ALA:C	2.18	0.85
1:D:301:GLY:O	1:D:305:MET:HG3	1.77	0.85
1:C:287:PRO:HG3	1:C:340:LEU:HD22	1.59	0.85
1:A:250:ILE:O	1:A:254:ALA:HB2	1.77	0.85
1:B:32:TYR:CD1	1:B:176:GLY:HA2	2.12	0.85
1:B:62:MET:HE2	1:B:122:ILE:HD11	1.58	0.84
1:A:87:ASN:HB2	1:A:119:THR:HG21	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:TRP:CE3	1:B:429:TYR:CE2	2.65	0.84
1:B:245:ILE:HG21	1:B:421:PHE:CD2	2.13	0.84
1:B:77:LYS:HD3	1:B:201:VAL:HB	1.60	0.84
1:A:76:PHE:O	1:A:80:ILE:HG23	1.78	0.84
1:A:344:LEU:O	1:A:348:MET:HG2	1.78	0.84
1:A:3:ILE:HG22	1:A:203:GLU:HB3	1.58	0.84
1:C:3:ILE:HG22	1:C:204:VAL:HG22	1.58	0.84
1:D:296:ARG:HG3	1:D:344:LEU:HD21	1.60	0.83
1:A:202:HIS:O	1:A:203:GLU:OE1	1.97	0.83
1:D:299:TRP:CB	1:D:344:LEU:CD1	2.45	0.83
1:D:244:ASN:CB	1:D:376:VAL:HG11	2.08	0.83
1:C:240:ALA:HB3	1:C:376:VAL:HG21	1.58	0.83
1:C:387:ILE:HG23	1:C:417:LEU:CD1	2.08	0.83
1:A:58:ASN:ND2	1:A:121:THR:HG21	1.93	0.82
1:A:325:ALA:O	1:A:328:VAL:HG12	1.80	0.82
1:C:175:ARG:HD2	1:C:175:ARG:O	1.80	0.82
1:C:239:MET:HG2	1:C:425:THR:HA	1.62	0.82
1:A:86:THR:HG22	1:A:119:THR:OG1	1.80	0.81
1:A:167:VAL:HG23	1:A:182:PHE:CE2	2.14	0.81
1:B:307:VAL:O	1:B:311:ALA:HB2	1.80	0.81
1:A:189:PHE:O	1:A:192:ALA:HB3	1.80	0.81
1:C:15:ALA:HB2	1:C:127:PHE:CE2	2.15	0.81
1:C:140:GLU:HG2	1:C:143:GLN:HB2	1.60	0.81
1:B:35:ASP:HA	1:B:38:GLY:HA2	1.63	0.80
1:B:39:LEU:HD22	1:B:41:VAL:HG23	1.63	0.80
1:C:387:ILE:CG2	1:C:417:LEU:HD21	2.12	0.80
1:D:125:ILE:HG23	1:D:369:TYR:CD1	2.16	0.80
1:B:87:ASN:HB2	1:B:119:THR:HG21	1.63	0.80
1:D:386:PHE:O	1:D:390:VAL:HG22	1.82	0.80
1:C:387:ILE:O	1:C:391:LEU:HD23	1.81	0.79
1:D:244:ASN:HB3	1:D:376:VAL:HG11	1.64	0.79
1:D:384:ALA:O	1:D:387:ILE:HG13	1.82	0.79
1:C:240:ALA:CB	1:C:376:VAL:HG21	2.12	0.79
1:C:58:ASN:CG	1:C:121:THR:HG21	2.08	0.79
1:A:62:MET:HE2	1:A:122:ILE:HB	1.62	0.79
1:C:85:LEU:HD11	1:C:194:THR:OG1	1.82	0.79
1:C:144:LEU:O	1:C:148:PRO:HD2	1.82	0.79
1:D:129:SER:HB3	1:D:369:TYR:OH	1.83	0.79
1:A:15:ALA:HB2	1:A:127:PHE:CZ	2.16	0.78
1:C:139:ARG:NH2	1:C:358:PHE:HB2	1.97	0.78
1:C:283:LEU:O	1:C:287:PRO:CD	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:TRP:HB2	1:D:344:LEU:HD13	0.82	0.78
1:C:307:VAL:O	1:C:310:CYS:HB3	1.83	0.78
1:C:77:LYS:HA	1:C:80:ILE:HG12	1.64	0.78
1:B:320:ASP:HB2	1:B:323:ASN:HB2	1.66	0.78
1:A:78:PRO:HA	1:A:81:LEU:HB3	1.66	0.78
1:C:93:LEU:CD2	1:C:112:THR:CB	2.62	0.78
1:D:150:PHE:CD1	1:D:283:LEU:HD23	2.18	0.78
1:C:139:ARG:N	1:C:139:ARG:CD	2.46	0.77
1:C:250:ILE:O	1:C:254:ALA:CB	2.30	0.77
1:A:8:LYS:HA	1:A:11:TYR:HB2	1.65	0.77
1:D:3:ILE:O	1:D:7:THR:HG23	1.84	0.77
1:A:141:ARG:HG3	1:A:142:GLU:N	1.98	0.77
1:D:25:VAL:O	1:D:29:LEU:HG	1.85	0.77
1:A:270:TYR:O	1:A:274:TYR:HB2	1.83	0.77
1:D:387:ILE:HD13	1:D:414:MET:HE1	1.67	0.77
1:A:15:ALA:HB2	1:A:127:PHE:HZ	1.49	0.76
1:C:236:LEU:HD13	1:C:349:VAL:HA	1.65	0.76
1:A:257:TYR:O	1:A:261:VAL:HG12	1.85	0.76
1:B:320:ASP:HB2	1:B:323:ASN:HB3	1.65	0.76
1:A:183:THR:HG22	1:A:187:ILE:CD1	2.15	0.76
1:C:142:GLU:O	1:C:146:PRO:CG	2.33	0.76
1:A:128:TRP:CD1	1:A:369:TYR:HE1	2.02	0.76
1:C:308:LEU:O	1:C:309:SER:C	2.29	0.76
1:B:122:ILE:O	1:B:126:PRO:HD2	1.86	0.76
1:D:150:PHE:HD1	1:D:283:LEU:HD23	1.47	0.76
1:A:90:VAL:HG21	1:A:116:TRP:HB2	1.69	0.75
1:B:75:LYS:O	1:B:78:PRO:HD2	1.87	0.75
1:B:163:THR:HG22	1:B:182:PHE:CZ	2.22	0.75
1:B:299:TRP:CD1	1:B:344:LEU:HB2	2.22	0.75
1:C:387:ILE:HG21	1:C:417:LEU:HD21	1.68	0.75
1:C:387:ILE:HD12	1:C:417:LEU:HD21	1.68	0.74
1:C:78:PRO:HA	1:C:81:LEU:CD2	2.15	0.74
1:C:88:SER:O	1:C:92:PHE:HB2	1.86	0.74
1:B:316:MET:HE3	1:B:316:MET:O	1.87	0.74
1:C:75:LYS:HD2	1:C:202:HIS:O	1.88	0.74
1:D:129:SER:CB	1:D:369:TYR:OH	2.35	0.74
1:D:245:ILE:HG12	1:D:376:VAL:HG23	1.68	0.74
1:A:149:ARG:CB	1:A:283:LEU:HD21	2.18	0.74
1:C:95:PHE:O	1:C:180:GLN:HG2	1.87	0.73
1:C:397:THR:OG1	1:C:398:PRO:CD	2.35	0.73
1:D:125:ILE:HG23	1:D:369:TYR:CE1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:O	1:A:11:TYR:HB2	1.88	0.73
1:B:39:LEU:HD23	1:B:39:LEU:O	1.87	0.73
1:C:33:TYR:O	1:C:33:TYR:CD1	2.42	0.73
1:C:282:THR:HG23	1:C:286:PHE:CD1	2.22	0.73
1:C:143:GLN:HA	1:C:295:ARG:HH21	1.54	0.73
1:C:162:ILE:C	1:C:165:PRO:HD2	2.13	0.73
1:C:236:LEU:HA	1:C:239:MET:HE3	1.69	0.73
1:A:92:PHE:CD1	1:A:187:ILE:HD13	2.23	0.73
1:C:283:LEU:O	1:C:287:PRO:HD2	1.88	0.73
1:B:417:LEU:O	1:B:421:PHE:N	2.21	0.72
1:C:44:VAL:O	1:C:48:PHE:N	2.22	0.72
1:D:246:ALA:HB1	1:D:422:PHE:CE1	2.24	0.72
1:A:28:TYR:CZ	1:A:179:PHE:HB2	2.25	0.72
1:A:268:PHE:N	1:A:269:PRO:HD3	2.05	0.72
1:C:1:MET:HE1	1:C:204:VAL:HG13	1.71	0.72
1:A:80:ILE:HG22	1:A:126:PRO:HB3	1.71	0.72
1:D:75:LYS:O	1:D:78:PRO:HD2	1.90	0.72
1:C:211:VAL:HG12	1:C:212:THR:H	1.53	0.72
1:A:286:PHE:HA	1:A:289:LEU:HD12	1.70	0.72
1:B:299:TRP:CE3	1:B:429:TYR:CD2	2.78	0.72
1:C:3:ILE:HG22	1:C:204:VAL:CG2	2.19	0.72
1:D:244:ASN:HD22	1:D:376:VAL:HG11	1.54	0.72
1:D:86:THR:CG2	1:D:115:LEU:CG	2.57	0.71
1:A:3:ILE:CG2	1:A:203:GLU:CG	2.63	0.71
1:B:244:ASN:ND2	1:B:376:VAL:HG11	2.04	0.71
1:A:215:ARG:N	1:A:216:PRO:HD2	2.04	0.71
1:C:316:MET:O	1:C:319:ALA:HB3	1.89	0.71
1:B:77:LYS:HB2	1:B:201:VAL:HG12	1.71	0.71
1:D:138:LYS:HD2	1:D:138:LYS:O	1.91	0.71
1:D:380:SER:HA	1:D:383:ALA:HB3	1.72	0.71
1:B:10:SER:O	1:B:13:PHE:HB2	1.91	0.71
1:C:145:VAL:N	1:C:146:PRO:HD2	2.06	0.71
1:D:86:THR:HG22	1:D:90:VAL:HG23	1.71	0.71
1:B:77:LYS:HA	1:B:201:VAL:CG1	2.21	0.71
1:B:298:LEU:HD12	1:B:340:LEU:HD22	1.73	0.71
1:A:18:LYS:HZ3	1:A:127:PHE:HB2	1.56	0.71
1:D:353:VAL:CG1	1:D:357:GLU:CB	2.68	0.71
1:A:249:ILE:O	1:A:253:PHE:HB2	1.91	0.70
1:A:282:THR:HG23	1:A:286:PHE:CD1	2.26	0.70
1:A:397:THR:HG23	1:A:398:PRO:HD2	1.72	0.70
1:B:320:ASP:CB	1:B:323:ASN:HB2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:THR:N	1:B:374:MET:HE2	2.06	0.70
1:D:271:TYR:CD1	1:D:332:ILE:HD11	2.24	0.70
1:C:56:ALA:O	1:C:374:MET:HE3	1.90	0.70
1:C:391:LEU:HD13	1:C:413:ILE:HD13	1.73	0.70
1:C:30:MET:O	1:C:33:TYR:HB3	1.92	0.70
1:C:128:TRP:CE2	1:C:346:VAL:HG11	2.26	0.70
1:B:142:GLU:HA	1:B:145:VAL:HG23	1.74	0.70
1:D:125:ILE:CG2	1:D:369:TYR:CE1	2.74	0.70
1:A:61:ILE:O	1:A:65:ILE:HG12	1.92	0.70
1:C:143:GLN:O	1:C:147:PHE:CD1	2.44	0.70
1:B:77:LYS:HB2	1:B:201:VAL:CG1	2.21	0.69
1:B:131:VAL:O	1:B:134:ILE:HG12	1.92	0.69
1:A:397:THR:HG22	1:A:398:PRO:HD2	1.74	0.69
1:B:141:ARG:NH1	1:B:354:ASP:CB	2.52	0.69
1:C:334:LEU:HD23	1:C:334:LEU:O	1.92	0.69
1:D:153:SER:CB	1:D:283:LEU:HD22	2.22	0.69
1:A:77:LYS:HG3	1:A:201:VAL:CB	2.20	0.69
1:B:374:MET:HE2	1:B:374:MET:H	1.57	0.69
1:C:301:GLY:O	1:C:305:MET:N	2.25	0.69
1:A:187:ILE:HG23	1:A:191:ILE:CG1	2.19	0.69
1:D:246:ALA:HB1	1:D:422:PHE:CZ	2.27	0.69
1:A:67:ASN:HB3	1:A:217:HIS:CD2	2.28	0.69
1:C:128:TRP:CE3	1:C:346:VAL:HG21	2.27	0.69
1:C:175:ARG:O	1:C:177:PHE:N	2.25	0.69
1:D:391:LEU:HD22	1:D:413:ILE:HD12	1.75	0.69
1:A:127:PHE:CD1	1:A:127:PHE:C	2.70	0.69
1:B:51:ALA:HA	1:B:54:TRP:CE3	2.27	0.69
1:A:243:TYR:CE1	1:A:341:PHE:HD2	2.11	0.68
1:C:240:ALA:HB3	1:C:376:VAL:CG2	2.23	0.68
1:C:77:LYS:HB2	1:C:201:VAL:HG21	1.76	0.68
1:D:77:LYS:O	1:D:81:LEU:CB	2.42	0.68
1:D:380:SER:O	1:D:384:ALA:N	2.26	0.68
1:B:376:VAL:HG23	1:B:377:LYS:HG3	1.75	0.68
1:C:116:TRP:O	1:C:117:GLY:C	2.32	0.68
1:A:283:LEU:O	1:A:287:PRO:CG	2.41	0.68
1:C:90:VAL:HG11	1:C:116:TRP:N	2.09	0.68
1:C:241:LEU:HD23	1:C:376:VAL:O	1.94	0.68
1:A:346:VAL:HG12	1:A:369:TYR:CE1	2.29	0.68
1:B:122:ILE:HG23	1:B:126:PRO:HG2	1.74	0.68
1:C:27:MET:SD	1:C:159:THR:HG22	2.34	0.68
1:D:59:ASP:CG	1:D:60:PRO:HD3	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:PHE:HD1	1:D:150:PHE:HD2	1.42	0.68
1:A:95:PHE:O	1:A:180:GLN:CG	2.42	0.68
1:B:320:ASP:CB	1:B:323:ASN:CB	2.72	0.68
1:C:93:LEU:HD23	1:C:112:THR:CB	2.23	0.68
1:D:75:LYS:HD2	1:D:201:VAL:HG12	1.75	0.68
1:A:51:ALA:HA	1:A:54:TRP:CG	2.29	0.68
1:A:58:ASN:CG	1:A:121:THR:CG2	2.63	0.68
1:A:124:ASP:O	1:A:128:TRP:NE1	2.27	0.68
1:D:83:GLY:HA3	1:D:122:ILE:HD11	1.74	0.68
1:D:147:PHE:CD1	1:D:150:PHE:HD2	2.12	0.68
1:A:21:ALA:HA	1:A:186:LEU:HD11	1.74	0.68
1:A:119:THR:HA	1:A:122:ILE:HG22	1.74	0.67
1:B:295:ARG:HB3	1:B:344:LEU:HD11	1.76	0.67
1:B:414:MET:O	1:B:417:LEU:HB2	1.94	0.67
1:C:33:TYR:CD1	1:C:33:TYR:C	2.72	0.67
1:D:75:LYS:CE	1:D:76:PHE:H	2.02	0.67
1:D:415:ILE:O	1:D:418:PRO:HG2	1.94	0.67
1:B:77:LYS:CA	1:B:201:VAL:HG11	2.21	0.67
1:B:99:LEU:HD11	1:B:177:PHE:HB2	1.76	0.67
1:C:347:ILE:HA	1:C:369:TYR:OH	1.94	0.67
1:A:32:TYR:O	1:A:36:VAL:HG23	1.93	0.67
1:A:92:PHE:CE1	1:A:187:ILE:HD13	2.29	0.67
1:D:296:ARG:CG	1:D:344:LEU:HD21	2.24	0.67
1:C:347:ILE:HD13	1:C:369:TYR:OH	1.94	0.67
1:A:28:TYR:CE1	1:A:179:PHE:HB2	2.30	0.67
1:C:32:TYR:HA	1:C:35:ASP:HB2	1.75	0.67
1:C:72:ARG:HD3	1:D:109:VAL:HG13	1.74	0.67
1:C:346:VAL:HG12	1:C:369:TYR:CD2	2.30	0.67
1:B:244:ASN:HB3	1:B:376:VAL:HB	1.76	0.67
1:A:192:ALA:HA	1:A:195:ILE:HG22	1.77	0.67
1:B:244:ASN:HD22	1:B:376:VAL:CB	2.07	0.67
1:D:77:LYS:O	1:D:77:LYS:HD3	1.95	0.67
1:A:149:ARG:HB3	1:A:283:LEU:HD21	1.77	0.67
1:B:352:THR:CA	1:B:433:TYR:OH	2.39	0.67
1:C:128:TRP:CZ3	1:C:346:VAL:HG21	2.30	0.67
1:D:77:LYS:O	1:D:81:LEU:HB3	1.95	0.67
1:B:86:THR:HG21	1:B:115:LEU:HD11	1.77	0.67
1:D:122:ILE:O	1:D:126:PRO:HD2	1.95	0.67
1:A:278:ALA:HB1	1:A:336:ILE:HG22	1.77	0.66
1:D:244:ASN:HD22	1:D:376:VAL:CG1	2.07	0.66
1:D:391:LEU:HB2	1:D:413:ILE:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ILE:O	1:C:84:THR:HG23	1.95	0.66
1:B:417:LEU:O	1:B:421:PHE:HB2	1.95	0.66
1:D:236:LEU:CD2	1:D:348:MET:HB3	2.22	0.66
1:B:353:VAL:HG21	1:B:366:SER:HB3	1.77	0.66
1:C:211:VAL:HG12	1:C:212:THR:N	2.10	0.66
1:C:215:ARG:N	1:C:216:PRO:CD	2.59	0.66
1:D:86:THR:CG2	1:D:90:VAL:CG2	2.72	0.66
1:B:125:ILE:HD11	1:B:369:TYR:CG	2.31	0.66
1:D:75:LYS:CD	1:D:201:VAL:HG12	2.26	0.66
1:A:321:ILE:H	1:A:321:ILE:HD12	1.60	0.65
1:C:76:PHE:O	1:C:79:TRP:HB3	1.96	0.65
1:C:175:ARG:HH11	1:C:175:ARG:CG	2.05	0.65
1:A:177:PHE:O	1:A:180:GLN:HB3	1.96	0.65
1:B:4:SER:HB2	1:B:134:ILE:HG21	1.79	0.65
1:B:351:ASP:C	1:B:433:TYR:HE2	2.04	0.65
1:D:296:ARG:O	1:D:299:TRP:HB3	1.96	0.65
1:B:77:LYS:O	1:B:81:LEU:HB3	1.97	0.65
1:C:282:THR:HB	1:C:336:ILE:O	1.96	0.65
1:C:342:TRP:O	1:C:346:VAL:HG23	1.97	0.65
1:C:85:LEU:CD1	1:C:194:THR:OG1	2.45	0.65
1:C:176:GLY:O	1:C:180:GLN:N	2.30	0.65
1:D:413:ILE:O	1:D:416:VAL:HG12	1.97	0.65
1:B:85:LEU:HD11	1:B:194:THR:HG21	1.79	0.65
1:A:374:MET:SD	1:A:375:VAL:HG23	2.36	0.64
1:B:125:ILE:HG22	1:B:126:PRO:HD3	1.79	0.64
1:D:292:MET:O	1:D:293:LEU:HG	1.97	0.64
1:B:268:PHE:N	1:B:269:PRO:CD	2.60	0.64
1:B:114:ILE:O	1:B:118:MET:N	2.30	0.64
1:B:117:GLY:O	1:B:118:MET:C	2.40	0.64
1:B:187:ILE:O	1:B:191:ILE:N	2.30	0.64
1:D:240:ALA:HA	1:D:345:GLN:OE1	1.98	0.64
1:D:244:ASN:HB3	1:D:376:VAL:CG1	2.26	0.64
1:A:93:LEU:HD13	1:A:112:THR:HB	1.79	0.64
1:B:19:ASP:HA	1:B:22:ILE:HG22	1.80	0.64
1:D:306:PRO:HG2	1:D:422:PHE:CD2	2.32	0.64
1:B:241:LEU:HD22	1:B:375:VAL:HG21	1.79	0.64
1:C:75:LYS:HB2	1:C:205:TYR:CB	2.28	0.64
1:C:91:LEU:HD13	1:C:116:TRP:HZ3	1.63	0.64
1:D:366:SER:HB2	1:D:369:TYR:CD2	2.33	0.64
1:C:371:VAL:O	1:C:375:VAL:HG22	1.98	0.64
1:D:75:LYS:HE3	1:D:76:PHE:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ASP:HA	1:D:354:ASP:HB2	1.80	0.64
1:A:78:PRO:O	1:A:82:ILE:HG12	1.97	0.64
1:C:96:SER:OG	1:D:198:LEU:HD13	1.98	0.64
1:C:229:LYS:HG2	1:C:233:LEU:HB2	1.80	0.64
1:C:299:TRP:O	1:C:302:ALA:HB3	1.97	0.64
1:B:383:ALA:O	1:B:386:PHE:N	2.30	0.64
1:C:82:ILE:O	1:C:86:THR:CG2	2.46	0.64
1:C:304:VAL:O	1:C:307:VAL:HB	1.96	0.64
1:C:387:ILE:HD12	1:C:417:LEU:CD2	2.28	0.64
1:D:7:THR:HG22	1:D:200:ASN:O	1.98	0.64
1:B:21:ALA:HB1	1:B:87:ASN:HD21	1.63	0.63
1:A:98:HIS:CD2	1:A:99:LEU:HB2	2.33	0.63
1:C:242:ALA:HA	1:C:245:ILE:HG12	1.79	0.63
1:B:391:LEU:HA	1:B:413:ILE:HG21	1.81	0.63
1:C:14:GLY:O	1:C:18:LYS:N	2.24	0.63
1:C:142:GLU:O	1:C:295:ARG:CZ	2.46	0.63
1:D:83:GLY:HA3	1:D:122:ILE:CD1	2.27	0.63
1:D:167:VAL:O	1:D:171:GLY:N	2.31	0.63
1:A:91:LEU:HG	1:A:183:THR:HG23	1.79	0.63
1:A:236:LEU:HD11	1:A:348:MET:HB3	1.80	0.63
1:A:245:ILE:CG2	1:A:417:LEU:HD21	2.28	0.63
1:A:438:ASP:O	1:A:441:ARG:N	2.31	0.63
1:B:306:PRO:CG	1:B:422:PHE:CE2	2.77	0.63
1:C:109:VAL:O	1:C:113:TYR:HB2	1.98	0.63
1:D:86:THR:HG23	1:D:115:LEU:HG	1.71	0.63
1:D:366:SER:HB2	1:D:369:TYR:HD2	1.64	0.63
1:B:124:ASP:HB2	1:B:373:THR:HG23	1.81	0.63
1:D:313:LEU:O	1:D:313:LEU:CD1	2.44	0.63
1:C:87:ASN:O	1:C:90:VAL:HG22	1.99	0.63
1:D:282:THR:HA	1:D:285:VAL:HG22	1.80	0.63
1:B:32:TYR:CE1	1:B:176:GLY:HA2	2.34	0.63
1:C:128:TRP:CD2	1:C:346:VAL:HG11	2.33	0.63
1:D:77:LYS:N	1:D:78:PRO:CD	2.62	0.63
1:D:353:VAL:O	1:D:357:GLU:N	2.29	0.63
1:A:212:THR:HG22	1:A:212:THR:O	1.98	0.63
1:A:250:ILE:O	1:A:254:ALA:CB	2.46	0.63
1:C:128:TRP:CH2	1:C:373:THR:CG2	2.74	0.63
1:D:115:LEU:O	1:D:118:MET:HB3	1.97	0.62
1:B:16:PHE:HB2	1:B:151:PHE:CD2	2.34	0.62
1:C:93:LEU:HD23	1:C:112:THR:OG1	1.99	0.62
1:D:391:LEU:HB2	1:D:413:ILE:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:LEU:HD23	1:C:334:LEU:HD11	1.82	0.62
1:C:387:ILE:CG2	1:C:417:LEU:CD2	2.77	0.62
1:C:77:LYS:HE2	1:C:197:THR:O	1.99	0.62
1:C:91:LEU:HD13	1:C:116:TRP:CZ3	2.34	0.62
1:C:129:SER:C	1:C:132:PRO:HD2	2.25	0.62
1:C:346:VAL:HG12	1:C:369:TYR:CE2	2.33	0.62
1:A:243:TYR:CZ	1:A:341:PHE:HD2	2.17	0.62
1:D:15:ALA:HB1	1:D:152:ALA:HB2	1.81	0.62
1:D:305:MET:HB2	1:D:306:PRO:HD3	1.81	0.62
1:A:342:TRP:O	1:A:346:VAL:HG23	1.98	0.62
1:D:340:LEU:HG	1:D:340:LEU:O	2.00	0.62
1:D:59:ASP:OD1	1:D:59:ASP:N	2.33	0.62
1:D:20:PHE:CD2	1:D:186:LEU:HA	2.35	0.62
1:B:268:PHE:N	1:B:269:PRO:HD2	2.15	0.61
1:C:51:ALA:O	1:C:54:TRP:HB2	2.00	0.61
1:C:143:GLN:O	1:C:147:PHE:CE1	2.53	0.61
1:D:20:PHE:HD2	1:D:186:LEU:HA	1.65	0.61
1:B:86:THR:HG21	1:B:115:LEU:CD1	2.30	0.61
1:D:5:MET:SD	1:D:144:LEU:HD22	2.40	0.61
1:A:349:VAL:HG21	1:A:372:GLN:CB	2.30	0.61
1:B:374:MET:H	1:B:374:MET:CE	2.12	0.61
1:C:164:LEU:O	1:C:167:VAL:HG12	1.99	0.61
1:D:47:LEU:HD13	1:D:113:TYR:OH	2.00	0.61
1:D:156:GLY:O	1:D:160:ALA:CB	2.48	0.61
1:D:194:THR:O	1:D:198:LEU:HG	1.99	0.61
1:B:117:GLY:O	1:B:120:TYR:N	2.31	0.61
1:B:142:GLU:HA	1:B:145:VAL:CG2	2.31	0.61
1:D:86:THR:HG21	1:D:115:LEU:CD1	2.30	0.61
1:C:87:ASN:CG	1:C:119:THR:HG21	2.26	0.61
1:D:76:PHE:O	1:D:80:ILE:HG23	2.00	0.61
1:A:8:LYS:HD2	1:A:134:ILE:HD13	1.82	0.61
1:A:236:LEU:O	1:A:236:LEU:HD23	2.01	0.61
1:B:112:THR:O	1:B:115:LEU:CB	2.48	0.61
1:C:310:CYS:O	1:C:311:ALA:C	2.44	0.61
1:C:340:LEU:O	1:C:340:LEU:HG	2.01	0.61
1:B:51:ALA:HA	1:B:54:TRP:CD2	2.35	0.61
1:C:87:ASN:ND2	1:C:119:THR:HG21	2.15	0.61
1:A:58:ASN:ND2	1:A:121:THR:CG2	2.62	0.61
1:B:380:SER:O	1:B:383:ALA:HB3	2.01	0.61
1:C:56:ALA:O	1:C:60:PRO:HD2	2.01	0.61
1:A:18:LYS:NZ	1:A:127:PHE:HB2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:HB1	1:A:376:VAL:HG11	1.82	0.61
1:B:417:LEU:O	1:B:421:PHE:CB	2.49	0.61
1:C:14:GLY:O	1:C:18:LYS:HG3	2.01	0.61
1:C:353:VAL:O	1:C:357:GLU:N	2.32	0.61
1:A:73:TRP:CZ2	1:B:109:VAL:HB	2.34	0.60
1:B:21:ALA:HB1	1:B:87:ASN:ND2	2.16	0.60
1:A:91:LEU:HD13	1:A:116:TRP:HZ3	1.65	0.60
1:D:80:ILE:HG13	1:D:81:LEU:N	2.14	0.60
1:A:5:MET:CG	1:A:135:THR:HG23	2.32	0.60
1:D:86:THR:CG2	1:D:90:VAL:HG23	2.32	0.60
1:B:80:ILE:HG13	1:B:81:LEU:N	2.16	0.60
1:B:115:LEU:HA	1:B:118:MET:HB2	1.82	0.60
1:A:105:GLN:HE21	1:A:105:GLN:CA	2.15	0.60
1:B:99:LEU:HD22	1:B:180:GLN:CD	2.27	0.60
1:A:219:THR:CG2	1:A:360:LEU:HD11	2.32	0.60
1:B:78:PRO:O	1:B:82:ILE:HG12	2.01	0.60
1:D:14:GLY:HA2	1:D:193:SER:OG	2.00	0.60
1:A:24:ILE:CD1	1:A:186:LEU:HD13	2.24	0.60
1:C:175:ARG:HG3	1:C:175:ARG:NH1	2.01	0.60
1:C:323:ASN:O	1:C:323:ASN:ND2	2.32	0.60
1:C:380:SER:O	1:C:383:ALA:HB3	2.02	0.60
1:D:156:GLY:O	1:D:160:ALA:HB2	2.02	0.60
1:B:163:THR:CG2	1:B:182:PHE:CZ	2.85	0.59
1:B:246:ALA:HB1	1:B:422:PHE:CE1	2.37	0.59
1:B:62:MET:HE2	1:B:122:ILE:CD1	2.30	0.59
1:B:387:ILE:HG21	1:B:414:MET:SD	2.42	0.59
1:B:244:ASN:HD22	1:B:376:VAL:CG1	2.15	0.59
1:C:51:ALA:HA	1:C:54:TRP:CG	2.36	0.59
1:C:321:ILE:HB	1:C:326:LEU:HD13	1.84	0.59
1:D:62:MET:SD	1:D:122:ILE:HG22	2.42	0.59
1:A:77:LYS:CG	1:A:201:VAL:HB	2.31	0.59
1:A:138:LYS:HG3	1:A:139:ARG:HG2	1.84	0.59
1:C:3:ILE:CG2	1:C:204:VAL:HG22	2.32	0.59
1:C:323:ASN:ND2	1:C:323:ASN:C	2.59	0.59
1:B:244:ASN:HD22	1:B:376:VAL:HB	1.68	0.59
1:C:143:GLN:HA	1:C:295:ARG:NH2	2.18	0.59
1:B:110:CYS:O	1:B:114:ILE:HG13	2.02	0.59
1:B:285:VAL:O	1:B:288:ARG:HB2	2.02	0.59
1:D:290:VAL:CG1	1:D:298:LEU:HD22	2.32	0.59
1:B:342:TRP:HA	1:B:345:GLN:HG3	1.85	0.59
1:C:343:VAL:O	1:C:347:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:TRP:HB3	1:D:344:LEU:CD1	2.31	0.59
1:D:391:LEU:HB2	1:D:413:ILE:CG1	2.33	0.59
1:A:233:LEU:O	1:A:237:LEU:HG	2.02	0.59
1:C:391:LEU:HD13	1:C:413:ILE:HG21	1.83	0.59
1:D:77:LYS:HB3	1:D:78:PRO:HD3	1.85	0.59
1:B:141:ARG:NH1	1:B:351:ASP:HA	2.17	0.59
1:B:239:MET:HE1	1:B:429:TYR:CD1	2.36	0.59
1:B:340:LEU:HD23	1:B:340:LEU:O	2.03	0.59
1:C:386:PHE:CD1	1:C:386:PHE:C	2.81	0.59
1:A:384:ALA:O	1:A:387:ILE:HG13	2.03	0.58
1:C:88:SER:O	1:C:92:PHE:CB	2.50	0.58
1:A:232:GLN:HB2	1:A:352:THR:CG2	2.33	0.58
1:C:91:LEU:HD12	1:C:94:LEU:HD23	1.85	0.58
1:D:75:LYS:HE3	1:D:76:PHE:CB	2.34	0.58
1:A:95:PHE:O	1:A:180:GLN:HG3	2.02	0.58
1:B:195:ILE:HA	1:B:198:LEU:HD12	1.85	0.58
1:C:387:ILE:HG21	1:C:417:LEU:CD2	2.32	0.58
1:D:33:TYR:HD1	1:D:33:TYR:O	1.87	0.58
1:A:195:ILE:HG23	1:A:196:VAL:N	2.19	0.58
1:B:34:THR:CG2	1:B:43:LEU:HG	2.33	0.58
1:C:75:LYS:CB	1:C:205:TYR:CB	2.81	0.58
1:B:77:LYS:CA	1:B:201:VAL:CG1	2.81	0.58
1:D:150:PHE:CD1	1:D:283:LEU:CD2	2.75	0.58
1:D:86:THR:CG2	1:D:90:VAL:HG21	2.31	0.58
1:D:162:ILE:HG13	1:D:165:PRO:HG2	1.85	0.57
1:D:236:LEU:HD21	1:D:345:GLN:O	2.04	0.57
1:A:239:MET:HB2	1:A:425:THR:HA	1.87	0.57
1:C:140:GLU:HG2	1:C:143:GLN:CB	2.34	0.57
1:D:244:ASN:ND2	1:D:376:VAL:HG11	2.17	0.57
1:D:290:VAL:HG21	1:D:295:ARG:CZ	2.34	0.57
1:A:118:MET:O	1:A:121:THR:HG23	2.04	0.57
1:B:17:GLY:HA3	1:B:190:PHE:HD1	1.69	0.57
1:B:187:ILE:O	1:B:191:ILE:HB	2.03	0.57
1:B:430:PHE:O	1:B:431:ARG:C	2.47	0.57
1:C:242:ALA:HB1	1:C:422:PHE:HA	1.85	0.57
1:A:313:LEU:HA	1:A:316:MET:HG2	1.87	0.57
1:B:272:LEU:HA	1:B:332:ILE:HD13	1.86	0.57
1:D:271:TYR:CD1	1:D:332:ILE:CD1	2.88	0.57
1:A:187:ILE:O	1:A:191:ILE:N	2.32	0.57
1:C:399:ASN:OD1	1:C:399:ASN:N	2.38	0.57
1:A:75:LYS:HG2	1:A:76:PHE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:O	1:B:53:ILE:HG13	2.05	0.57
1:B:374:MET:HE2	1:B:374:MET:N	2.19	0.57
1:C:342:TRP:O	1:C:345:GLN:HB2	2.05	0.57
1:C:372:GLN:O	1:C:376:VAL:CG2	2.53	0.57
1:C:374:MET:CE	1:C:375:VAL:HG12	2.35	0.57
1:D:290:VAL:HG13	1:D:298:LEU:HD22	1.86	0.57
1:A:73:TRP:HZ2	1:B:109:VAL:HB	1.70	0.57
1:B:180:GLN:HA	1:B:183:THR:HG22	1.87	0.57
1:C:62:MET:CE	1:C:122:ILE:HD12	2.34	0.57
1:C:235:CYS:O	1:C:428:LEU:HD21	2.05	0.57
1:A:332:ILE:O	1:A:335:ASN:N	2.36	0.57
1:B:239:MET:SD	1:B:428:LEU:HB3	2.45	0.57
1:C:275:ALA:HB1	1:C:335:ASN:ND2	2.20	0.57
1:A:30:MET:O	1:A:33:TYR:HB3	2.03	0.57
1:A:282:THR:CB	1:A:337:GLY:HA2	2.35	0.57
1:B:80:ILE:HG21	1:B:130:LEU:HD13	1.87	0.57
1:C:72:ARG:HG2	1:C:73:TRP:O	2.05	0.57
1:A:232:GLN:HB2	1:A:352:THR:HG21	1.86	0.56
1:A:349:VAL:HG21	1:A:372:GLN:HB2	1.86	0.56
1:C:138:LYS:C	1:C:139:ARG:CD	2.77	0.56
1:C:141:ARG:HH21	1:C:351:ASP:CG	2.13	0.56
1:D:33:TYR:HE2	1:D:94:LEU:HD21	1.69	0.56
1:D:279:ASN:HA	1:D:282:THR:HG22	1.87	0.56
1:C:140:GLU:O	1:C:143:GLN:HB2	2.06	0.56
1:A:84:THR:HB	1:A:194:THR:HB	1.87	0.56
1:A:164:LEU:O	1:A:167:VAL:HG12	2.05	0.56
1:A:368:ALA:O	1:A:371:VAL:HG22	2.03	0.56
1:B:401:ALA:HB3	1:B:406:THR:HA	1.87	0.56
1:C:275:ALA:HB1	1:C:335:ASN:HD22	1.70	0.56
1:D:79:TRP:CE3	1:D:126:PRO:CB	2.81	0.56
1:A:92:PHE:HD1	1:A:187:ILE:CD1	2.18	0.56
1:B:18:LYS:HZ3	1:B:123:MET:HA	1.70	0.56
1:A:212:THR:O	1:A:213:ALA:HB3	2.04	0.56
1:B:39:LEU:O	1:B:40:SER:HB3	2.04	0.56
1:B:267:LEU:C	1:B:269:PRO:HD2	2.31	0.56
1:C:202:HIS:O	1:C:202:HIS:ND1	2.38	0.56
1:C:302:ALA:O	1:C:306:PRO:HD2	2.05	0.56
1:D:125:ILE:CG2	1:D:369:TYR:CD1	2.87	0.56
1:C:83:GLY:HA2	1:C:122:ILE:HG23	1.87	0.56
1:A:220:LEU:O	1:A:224:VAL:HG23	2.06	0.56
1:B:93:LEU:HD13	1:B:112:THR:CG2	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:O	1:B:126:PRO:CD	2.54	0.56
1:B:194:THR:O	1:B:198:LEU:HG	2.06	0.56
1:B:293:LEU:HD21	1:C:321:ILE:HG12	1.88	0.56
1:A:127:PHE:C	1:A:127:PHE:HD1	2.13	0.56
1:A:147:PHE:O	1:A:149:ARG:N	2.39	0.56
1:D:90:VAL:CG1	1:D:116:TRP:HB2	2.36	0.56
1:A:236:LEU:HD11	1:A:348:MET:C	2.31	0.56
1:A:243:TYR:HE2	1:A:342:TRP:HA	1.70	0.56
1:C:209:ASN:O	1:C:211:VAL:O	2.24	0.56
1:C:416:VAL:O	1:C:419:VAL:HB	2.06	0.56
1:D:124:ASP:HB2	1:D:373:THR:CG2	2.36	0.56
1:A:146:PRO:HB3	1:A:343:VAL:HG11	1.87	0.55
1:B:17:GLY:CA	1:B:190:PHE:HD1	2.19	0.55
1:C:110:CYS:O	1:C:111:VAL:C	2.47	0.55
1:D:29:LEU:HD22	1:D:33:TYR:CZ	2.41	0.55
1:D:124:ASP:HB2	1:D:373:THR:HG21	1.87	0.55
1:D:112:THR:O	1:D:115:LEU:HB3	2.06	0.55
1:A:92:PHE:HD1	1:A:187:ILE:HD13	1.71	0.55
1:A:147:PHE:CZ	1:A:288:ARG:HG2	2.41	0.55
1:C:217:HIS:NE2	1:C:218:LEU:HG	2.22	0.55
1:D:236:LEU:HA	1:D:239:MET:HE3	1.88	0.55
1:C:242:ALA:CB	1:C:422:PHE:HA	2.37	0.55
1:A:215:ARG:N	1:A:216:PRO:CD	2.70	0.55
1:A:219:THR:HG21	1:A:360:LEU:HD11	1.89	0.55
1:B:7:THR:O	1:B:11:TYR:N	2.37	0.55
1:C:143:GLN:O	1:C:147:PHE:HD1	1.90	0.55
1:C:282:THR:OG1	1:C:337:GLY:HA2	2.07	0.55
1:D:48:PHE:CD1	1:D:51:ALA:HB3	2.41	0.55
1:A:11:TYR:CE2	1:A:130:LEU:HB3	2.42	0.55
1:A:25:VAL:HG11	1:A:116:TRP:HH2	1.71	0.55
1:A:125:ILE:CG2	1:A:126:PRO:HD3	2.37	0.55
1:A:294:SER:O	1:A:297:ILE:HG12	2.06	0.55
1:D:77:LYS:O	1:D:81:LEU:HB2	2.05	0.55
1:D:387:ILE:CG2	1:D:414:MET:SD	2.94	0.55
1:D:391:LEU:HD22	1:D:413:ILE:CD1	2.37	0.55
1:A:250:ILE:O	1:A:254:ALA:N	2.40	0.55
1:B:86:THR:CG2	1:B:115:LEU:HG	2.37	0.55
1:C:241:LEU:HA	1:C:376:VAL:HG13	1.88	0.55
1:D:75:LYS:CE	1:D:76:PHE:HB2	2.36	0.55
1:D:387:ILE:HG22	1:D:417:LEU:HD12	1.87	0.55
1:A:236:LEU:HD13	1:A:349:VAL:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TRP:O	1:A:303:SER:N	2.39	0.55
1:C:140:GLU:O	1:C:143:GLN:N	2.40	0.55
1:D:415:ILE:HA	1:D:418:PRO:CG	2.37	0.55
1:C:175:ARG:CG	1:C:175:ARG:NH1	2.69	0.55
1:D:75:LYS:C	1:D:77:LYS:H	2.12	0.55
1:D:391:LEU:HB2	1:D:413:ILE:HD12	1.89	0.55
1:C:75:LYS:HG2	1:C:76:PHE:N	2.13	0.55
1:C:77:LYS:N	1:C:78:PRO:HD2	2.21	0.55
1:D:62:MET:O	1:D:79:TRP:HZ2	1.90	0.55
1:C:282:THR:CG2	1:C:282:THR:O	2.55	0.54
1:D:125:ILE:HB	1:D:126:PRO:HD3	1.89	0.54
1:A:51:ALA:O	1:A:54:TRP:HB2	2.07	0.54
1:C:119:THR:HA	1:C:122:ILE:HG22	1.90	0.54
1:B:48:PHE:O	1:B:51:ALA:HB3	2.07	0.54
1:B:163:THR:HG22	1:B:182:PHE:HZ	1.72	0.54
1:B:245:ILE:HG21	1:B:421:PHE:CE2	2.43	0.54
1:C:419:VAL:HA	1:C:422:PHE:HB3	1.90	0.54
1:A:13:PHE:CZ	1:A:192:ALA:HB1	2.43	0.54
1:D:110:CYS:O	1:D:111:VAL:C	2.50	0.54
1:A:149:ARG:HB2	1:A:283:LEU:HD21	1.90	0.54
1:B:244:ASN:HD22	1:B:376:VAL:HG11	1.68	0.54
1:C:232:GLN:HG2	1:C:232:GLN:O	2.08	0.54
1:C:233:LEU:O	1:C:236:LEU:N	2.31	0.54
1:D:16:PHE:HB2	1:D:151:PHE:CD2	2.42	0.54
1:D:245:ILE:HG12	1:D:376:VAL:CG2	2.36	0.54
1:D:324:ALA:O	1:D:328:VAL:HG23	2.08	0.54
1:C:72:ARG:HG2	1:C:73:TRP:N	2.19	0.54
1:C:139:ARG:HH22	1:C:358:PHE:CB	2.15	0.54
1:C:287:PRO:HG3	1:C:340:LEU:CD2	2.35	0.54
1:D:270:TYR:CD1	1:D:270:TYR:C	2.85	0.54
1:D:420:LEU:HD23	1:D:420:LEU:O	2.08	0.54
1:A:8:LYS:HA	1:A:11:TYR:CB	2.34	0.54
1:A:125:ILE:HG23	1:A:126:PRO:HD3	1.89	0.54
1:B:32:TYR:CE1	1:B:176:GLY:CA	2.90	0.54
1:B:285:VAL:HG12	1:B:289:LEU:HD13	1.90	0.54
1:C:387:ILE:HD12	1:C:417:LEU:CG	2.38	0.54
1:A:59:ASP:HB3	1:A:374:MET:HG2	1.89	0.54
1:C:122:ILE:O	1:C:126:PRO:HG2	2.07	0.54
1:D:11:TYR:CD1	1:D:130:LEU:HD22	2.43	0.54
1:C:123:MET:O	1:C:126:PRO:HD2	2.08	0.53
1:D:124:ASP:OD2	1:D:373:THR:CG2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:HB1	1:A:376:VAL:CG1	2.38	0.53
1:C:110:CYS:O	1:C:114:ILE:HG12	2.08	0.53
1:C:162:ILE:O	1:C:165:PRO:HD2	2.08	0.53
1:D:125:ILE:HG22	1:D:369:TYR:CE1	2.43	0.53
1:A:236:LEU:CD2	1:A:372:GLN:NE2	2.71	0.53
1:C:310:CYS:SG	1:C:416:VAL:HA	2.49	0.53
1:A:81:LEU:CD1	1:A:85:LEU:HD12	2.39	0.53
1:B:15:ALA:HB1	1:B:152:ALA:HB2	1.89	0.53
1:C:177:PHE:O	1:C:180:GLN:HB2	2.08	0.53
1:C:387:ILE:HG23	1:C:417:LEU:HD21	1.90	0.53
1:A:67:ASN:OD1	1:A:220:LEU:HD23	2.08	0.53
1:B:322:HIS:O	1:B:326:LEU:N	2.33	0.53
1:D:285:VAL:O	1:D:289:LEU:HG	2.08	0.53
1:B:286:PHE:O	1:B:290:VAL:HG23	2.08	0.53
1:B:351:ASP:O	1:B:433:TYR:HE2	1.92	0.53
1:C:139:ARG:O	1:C:140:GLU:CB	2.54	0.53
1:C:391:LEU:CD1	1:C:413:ILE:HD13	2.37	0.53
1:A:295:ARG:O	1:A:298:LEU:HB3	2.09	0.53
1:C:240:ALA:O	1:C:241:LEU:C	2.50	0.53
1:D:135:THR:HB	1:D:141:ARG:HG3	1.89	0.53
1:B:39:LEU:HD22	1:B:41:VAL:CG2	2.38	0.53
1:C:360:LEU:HD22	1:C:361:ASN:OD1	2.07	0.53
1:D:77:LYS:HD3	1:D:77:LYS:C	2.34	0.53
1:A:7:THR:HG23	1:A:201:VAL:CG1	2.30	0.53
1:A:18:LYS:O	1:A:22:ILE:HG22	2.09	0.53
1:A:67:ASN:HB3	1:A:217:HIS:HD2	1.71	0.53
1:A:285:VAL:O	1:A:289:LEU:HG	2.08	0.53
1:C:175:ARG:C	1:C:177:PHE:N	2.67	0.53
1:D:349:VAL:HG11	1:D:366:SER:HB3	1.91	0.53
1:B:233:LEU:HG	1:B:368:ALA:HB3	1.90	0.53
1:B:384:ALA:O	1:B:387:ILE:HG13	2.09	0.53
1:C:1:MET:SD	1:C:3:ILE:HB	2.49	0.53
1:C:98:HIS:O	1:C:99:LEU:C	2.52	0.53
1:C:127:PHE:C	1:C:127:PHE:CD1	2.88	0.53
1:D:19:ASP:HA	1:D:22:ILE:HG22	1.91	0.53
1:D:111:VAL:HG23	1:D:112:THR:N	2.24	0.53
1:D:268:PHE:N	1:D:269:PRO:CD	2.72	0.52
1:A:352:THR:HA	1:A:355:TYR:CE2	2.44	0.52
1:C:229:LYS:HD2	1:C:229:LYS:O	2.09	0.52
1:D:153:SER:CB	1:D:283:LEU:CD2	2.86	0.52
1:A:59:ASP:CB	1:A:374:MET:HG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:CB	1:B:60:PRO:HD3	2.40	0.52
1:C:78:PRO:O	1:C:81:LEU:HG	2.10	0.52
1:C:79:TRP:CZ2	1:C:125:ILE:HG23	2.44	0.52
1:D:128:TRP:HD1	1:D:129:SER:N	2.08	0.52
1:D:153:SER:HB2	1:D:283:LEU:CD2	2.38	0.52
1:B:440:LEU:HD12	1:B:440:LEU:N	2.25	0.52
1:C:124:ASP:OD2	1:C:128:TRP:CZ2	2.63	0.52
1:C:146:PRO:HG3	1:C:295:ARG:NH1	2.24	0.52
1:C:387:ILE:HG23	1:C:417:LEU:CD2	2.38	0.52
1:A:75:LYS:O	1:A:78:PRO:HD2	2.10	0.52
1:B:81:LEU:HD21	1:B:198:LEU:HD23	1.91	0.52
1:B:83:GLY:O	1:B:86:THR:OG1	2.28	0.52
1:C:62:MET:HE3	1:C:122:ILE:HD12	1.90	0.52
1:C:138:LYS:HA	1:C:139:ARG:HD3	1.90	0.52
1:D:120:TYR:HA	1:D:123:MET:HB2	1.90	0.52
1:A:3:ILE:CG2	1:A:203:GLU:HB3	2.36	0.52
1:A:76:PHE:HB3	1:A:130:LEU:HD22	1.91	0.52
1:B:33:TYR:HB2	1:B:43:LEU:HD21	1.92	0.52
1:C:235:CYS:O	1:C:428:LEU:CD2	2.58	0.52
1:C:239:MET:HE1	1:C:429:TYR:HD2	1.73	0.52
1:D:138:LYS:HE3	1:D:139:ARG:HG3	1.90	0.52
1:C:144:LEU:O	1:C:148:PRO:CD	2.54	0.52
1:C:192:ALA:O	1:C:196:VAL:HG23	2.09	0.52
1:D:59:ASP:CG	1:D:60:PRO:CD	2.82	0.52
1:D:301:GLY:C	1:D:305:MET:HG3	2.35	0.52
1:A:11:TYR:CZ	1:A:130:LEU:HD23	2.44	0.52
1:A:90:VAL:HG21	1:A:116:TRP:CB	2.40	0.52
1:A:183:THR:CG2	1:A:187:ILE:HD12	2.26	0.52
1:D:370:SER:O	1:D:372:GLN:N	2.42	0.52
1:A:125:ILE:O	1:A:129:SER:HB3	2.09	0.52
1:A:346:VAL:CG1	1:A:369:TYR:CE1	2.91	0.52
1:B:243:TYR:O	1:B:247:SER:N	2.38	0.52
1:C:32:TYR:O	1:C:36:VAL:N	2.42	0.52
1:C:56:ALA:HA	1:C:374:MET:HE3	1.91	0.52
1:A:87:ASN:CB	1:A:119:THR:HG21	2.36	0.51
1:C:78:PRO:HD3	1:C:202:HIS:CD2	2.45	0.51
1:A:13:PHE:CD2	1:A:196:VAL:HG21	2.45	0.51
1:A:91:LEU:HD13	1:A:116:TRP:CZ3	2.44	0.51
1:A:241:LEU:O	1:A:245:ILE:HG13	2.11	0.51
1:A:271:TYR:OH	1:A:329:ALA:HA	2.10	0.51
1:B:28:TYR:CE2	1:B:32:TYR:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:LEU:CD1	1:C:94:LEU:HD23	2.39	0.51
1:C:397:THR:HG1	1:C:398:PRO:HD2	1.71	0.51
1:D:396:TYR:O	1:D:398:PRO:HD3	2.10	0.51
1:A:150:PHE:O	1:A:150:PHE:CD1	2.64	0.51
1:B:77:LYS:CD	1:B:201:VAL:HB	2.35	0.51
1:D:384:ALA:O	1:D:387:ILE:CG1	2.55	0.51
1:B:81:LEU:CD2	1:B:198:LEU:HD23	2.40	0.51
1:D:79:TRP:CZ3	1:D:126:PRO:HB3	2.42	0.51
1:A:3:ILE:HG22	1:A:203:GLU:CB	2.35	0.51
1:A:25:VAL:HG23	1:A:26:TYR:N	2.25	0.51
1:A:212:THR:C	1:A:214:GLY:H	2.19	0.51
1:C:323:ASN:HA	1:C:327:ILE:HG12	1.91	0.51
1:D:8:LYS:HD2	1:D:134:ILE:HG21	1.92	0.51
1:B:342:TRP:O	1:B:345:GLN:HB2	2.10	0.51
1:C:7:THR:HA	1:C:201:VAL:HB	1.93	0.51
1:C:123:MET:C	1:C:126:PRO:HD2	2.35	0.51
1:C:349:VAL:HG11	1:C:369:TYR:HA	1.93	0.51
1:C:383:ALA:O	1:C:387:ILE:HB	2.10	0.51
1:D:387:ILE:HG21	1:D:414:MET:SD	2.51	0.51
1:A:73:TRP:HZ2	1:B:109:VAL:CB	2.23	0.51
1:A:208:ASP:OD1	1:A:208:ASP:C	2.54	0.51
1:C:216:PRO:HA	1:C:219:THR:HG1	1.75	0.51
1:B:36:VAL:HG13	1:B:37:VAL:H	1.76	0.51
1:B:77:LYS:HB2	1:B:201:VAL:CB	2.40	0.51
1:B:370:SER:O	1:B:374:MET:HE1	2.11	0.51
1:C:58:ASN:CG	1:C:121:THR:CG2	2.82	0.51
1:A:353:VAL:O	1:A:357:GLU:N	2.34	0.51
1:C:125:ILE:HG22	1:C:126:PRO:HD3	1.93	0.51
1:D:122:ILE:O	1:D:126:PRO:CD	2.59	0.51
1:A:58:ASN:CB	1:A:121:THR:HG21	2.40	0.50
1:A:230:ASN:OD1	1:A:230:ASN:N	2.41	0.50
1:B:373:THR:O	1:B:376:VAL:HG13	2.11	0.50
1:C:11:TYR:CZ	1:C:130:LEU:HB3	2.45	0.50
1:C:421:PHE:C	1:C:423:MET:H	2.19	0.50
1:A:61:ILE:HA	1:A:64:TRP:HB3	1.93	0.50
1:A:272:LEU:HA	1:A:275:ALA:HB3	1.92	0.50
1:A:296:ARG:O	1:A:299:TRP:HB3	2.12	0.50
1:B:17:GLY:CA	1:B:190:PHE:CD1	2.94	0.50
1:B:34:THR:O	1:B:36:VAL:N	2.44	0.50
1:C:99:LEU:HD12	1:C:177:PHE:HB2	1.93	0.50
1:C:399:ASN:O	1:C:401:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:O	1:A:134:ILE:HG12	2.11	0.50
1:A:238:GLY:HA3	1:A:424:MET:SD	2.51	0.50
1:B:413:ILE:HD13	1:B:413:ILE:H	1.77	0.50
1:C:41:VAL:HG13	1:C:42:GLY:H	1.76	0.50
1:A:195:ILE:HG23	1:A:196:VAL:H	1.75	0.50
1:B:77:LYS:CB	1:B:201:VAL:CG1	2.90	0.50
1:B:299:TRP:CD2	1:B:429:TYR:CE2	3.00	0.50
1:C:66:VAL:HG12	1:C:67:ASN:N	2.27	0.50
1:A:282:THR:CG2	1:A:282:THR:O	2.58	0.50
1:A:351:ASP:HA	1:A:354:ASP:CB	2.42	0.50
1:A:355:TYR:HA	1:A:358:PHE:HB2	1.94	0.50
1:B:159:THR:HG22	1:B:159:THR:O	2.10	0.50
1:B:239:MET:HE3	1:B:425:THR:O	2.11	0.50
1:C:351:ASP:O	1:C:354:ASP:N	2.44	0.50
1:D:117:GLY:O	1:D:118:MET:C	2.53	0.50
1:D:153:SER:HB2	1:D:283:LEU:HD21	1.93	0.50
1:A:92:PHE:CD1	1:A:187:ILE:CD1	2.93	0.50
1:A:378:GLY:O	1:A:380:SER:N	2.45	0.50
1:B:32:TYR:CD1	1:B:32:TYR:C	2.85	0.50
1:D:304:VAL:O	1:D:305:MET:C	2.55	0.50
1:A:380:SER:O	1:A:383:ALA:HB3	2.12	0.50
1:B:83:GLY:O	1:B:119:THR:OG1	2.27	0.50
1:B:182:PHE:O	1:B:185:VAL:HG12	2.12	0.50
1:C:139:ARG:HD2	1:C:139:ARG:H	1.71	0.50
1:D:197:THR:O	1:D:201:VAL:HG23	2.12	0.50
1:A:240:ALA:CB	1:A:376:VAL:CG1	2.90	0.50
1:A:332:ILE:O	1:A:335:ASN:CB	2.60	0.50
1:B:124:ASP:HB2	1:B:373:THR:CG2	2.42	0.50
1:A:290:VAL:HG23	1:A:290:VAL:O	2.12	0.49
1:A:390:VAL:HG12	1:A:413:ILE:HG23	1.94	0.49
1:B:237:LEU:HA	1:B:372:GLN:HE21	1.76	0.49
1:B:391:LEU:HB2	1:B:413:ILE:HD12	1.93	0.49
1:C:349:VAL:CG1	1:C:369:TYR:HA	2.42	0.49
1:B:76:PHE:HA	1:B:79:TRP:CB	2.42	0.49
1:B:241:LEU:O	1:B:245:ILE:HG13	2.12	0.49
1:B:383:ALA:O	1:B:385:PHE:N	2.45	0.49
1:D:77:LYS:CE	1:D:81:LEU:HD22	2.42	0.49
1:A:322:HIS:O	1:A:323:ASN:HB2	2.12	0.49
1:C:272:LEU:HA	1:C:275:ALA:HB3	1.94	0.49
1:D:88:SER:HB2	1:D:190:PHE:CD2	2.46	0.49
1:B:130:LEU:O	1:B:134:ILE:HD11	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:TYR:CE2	1:C:127:PHE:HA	2.47	0.49
1:C:16:PHE:O	1:C:20:PHE:HB2	2.11	0.49
1:D:17:GLY:HA3	1:D:190:PHE:HD1	1.78	0.49
1:D:85:LEU:HD21	1:D:194:THR:HG21	1.94	0.49
1:A:20:PHE:O	1:A:24:ILE:HG13	2.12	0.49
1:A:236:LEU:HD11	1:A:348:MET:CB	2.42	0.49
1:B:17:GLY:HA3	1:B:190:PHE:CD1	2.48	0.49
1:C:236:LEU:HD11	1:C:348:MET:HB3	1.94	0.49
1:D:416:VAL:O	1:D:420:LEU:HB2	2.13	0.49
1:A:148:PRO:C	1:A:150:PHE:H	2.21	0.49
1:A:242:ALA:HA	1:A:245:ILE:HD12	1.94	0.49
1:B:244:ASN:ND2	1:B:376:VAL:CG1	2.71	0.49
1:B:387:ILE:HG22	1:B:417:LEU:HD22	1.95	0.49
1:C:122:ILE:O	1:C:126:PRO:CG	2.61	0.49
1:A:11:TYR:CE2	1:A:127:PHE:HA	2.48	0.49
1:A:133:THR:O	1:A:134:ILE:O	2.31	0.49
1:A:397:THR:HG22	1:A:398:PRO:CD	2.42	0.49
1:A:413:ILE:O	1:A:416:VAL:HG12	2.12	0.49
1:B:59:ASP:HB2	1:B:60:PRO:HD3	1.95	0.49
1:B:77:LYS:CB	1:B:78:PRO:HD3	2.42	0.49
1:C:79:TRP:CD1	1:C:122:ILE:HG13	2.47	0.49
1:C:129:SER:O	1:C:132:PRO:HD2	2.13	0.49
1:C:157:PHE:CE1	1:C:277:ALA:HB1	2.48	0.49
1:C:349:VAL:HG13	1:C:350:ALA:N	2.27	0.49
1:C:374:MET:HE1	1:C:375:VAL:HG12	1.94	0.49
1:D:332:ILE:C	1:D:334:LEU:H	2.19	0.49
1:D:396:TYR:C	1:D:398:PRO:HD3	2.37	0.49
1:A:120:TYR:OH	1:A:377:LYS:NZ	2.46	0.49
1:A:216:PRO:O	1:A:219:THR:HB	2.13	0.49
1:B:34:THR:HG23	1:B:43:LEU:HG	1.94	0.49
1:B:77:LYS:HB2	1:B:201:VAL:HB	1.94	0.49
1:C:33:TYR:HA	1:C:36:VAL:CG1	2.43	0.49
1:D:2:SER:O	1:D:5:MET:N	2.44	0.49
1:A:29:LEU:O	1:A:32:TYR:N	2.43	0.49
1:B:415:ILE:C	1:B:417:LEU:N	2.70	0.49
1:C:10:SER:HB2	1:C:196:VAL:HG12	1.94	0.49
1:C:125:ILE:HA	1:C:128:TRP:HE1	1.76	0.49
1:D:75:LYS:HG3	1:D:202:HIS:CA	2.27	0.49
1:C:351:ASP:O	1:C:354:ASP:HB2	2.13	0.49
1:D:23:GLY:O	1:D:27:MET:HG2	2.13	0.49
1:A:11:TYR:CE1	1:A:130:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:HD21	1:A:118:MET:HA	1.77	0.48
1:A:128:TRP:O	1:A:369:TYR:OH	2.23	0.48
1:A:243:TYR:OH	1:A:341:PHE:HB3	2.13	0.48
1:A:271:TYR:O	1:A:275:ALA:N	2.44	0.48
1:B:145:VAL:N	1:B:146:PRO:CD	2.76	0.48
1:D:51:ALA:HA	1:D:54:TRP:CD2	2.48	0.48
1:A:222:THR:O	1:A:226:LEU:N	2.38	0.48
1:B:80:ILE:HD13	1:B:130:LEU:HD13	1.95	0.48
1:A:76:PHE:CE2	1:A:126:PRO:HA	2.48	0.48
1:A:321:ILE:HD12	1:A:321:ILE:N	2.25	0.48
1:C:110:CYS:O	1:C:112:THR:N	2.46	0.48
1:C:230:ASN:C	1:C:230:ASN:HD22	2.22	0.48
1:C:240:ALA:HB1	1:C:376:VAL:HG21	1.92	0.48
1:A:37:VAL:HG13	1:A:38:GLY:N	2.29	0.48
1:A:203:GLU:O	1:A:206:SER:N	2.46	0.48
1:C:78:PRO:O	1:C:82:ILE:HG12	2.13	0.48
1:C:97:ALA:HA	1:D:199:ARG:HB3	1.95	0.48
1:D:76:PHE:HB3	1:D:80:ILE:HG23	1.95	0.48
1:D:236:LEU:CD2	1:D:349:VAL:HG23	2.37	0.48
1:D:387:ILE:HA	1:D:390:VAL:HG22	1.96	0.48
1:A:4:SER:OG	1:A:134:ILE:HA	2.12	0.48
1:A:227:ILE:O	1:A:227:ILE:HD12	2.14	0.48
1:A:268:PHE:N	1:A:269:PRO:CD	2.74	0.48
1:B:349:VAL:O	1:B:352:THR:HG22	2.13	0.48
1:C:211:VAL:CG1	1:C:212:THR:H	2.23	0.48
1:D:146:PRO:O	1:D:149:ARG:HB2	2.13	0.48
1:D:306:PRO:O	1:D:309:SER:N	2.46	0.48
1:A:5:MET:HG3	1:A:135:THR:HG23	1.95	0.48
1:A:22:ILE:O	1:A:22:ILE:HG13	2.13	0.48
1:A:187:ILE:CG2	1:A:191:ILE:HG13	2.25	0.48
1:B:121:THR:HG22	1:B:374:MET:HB3	1.95	0.48
1:C:236:LEU:O	1:C:236:LEU:HD23	2.12	0.48
1:D:80:ILE:CG1	1:D:81:LEU:N	2.77	0.48
1:D:417:LEU:O	1:D:421:PHE:N	2.47	0.48
1:A:419:VAL:HA	1:A:422:PHE:HB2	1.94	0.48
1:D:3:ILE:HG21	1:D:203:GLU:HG3	1.95	0.48
1:D:415:ILE:HA	1:D:418:PRO:HG2	1.96	0.48
1:A:286:PHE:N	1:A:287:PRO:CD	2.76	0.48
1:B:352:THR:CA	1:B:433:TYR:CE2	2.89	0.48
1:B:354:ASP:O	1:B:359:LYS:N	2.47	0.48
1:C:15:ALA:HB2	1:C:127:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLY:O	1:C:120:TYR:HB3	2.14	0.48
1:C:191:ILE:HA	1:C:194:THR:HG22	1.95	0.48
1:C:216:PRO:HA	1:C:219:THR:OG1	2.14	0.48
1:C:260:TYR:CG	1:C:260:TYR:O	2.66	0.48
1:C:310:CYS:HG	1:C:314:PHE:HD2	1.61	0.48
1:D:286:PHE:CE2	1:D:339:ALA:CB	2.97	0.48
1:A:182:PHE:O	1:A:185:VAL:HB	2.14	0.48
1:B:36:VAL:HG13	1:B:37:VAL:N	2.28	0.48
1:D:350:ALA:O	1:D:354:ASP:HB2	2.14	0.48
1:A:92:PHE:HE1	1:A:187:ILE:HG21	1.79	0.48
1:C:214:GLY:O	1:C:217:HIS:ND1	2.45	0.48
1:D:75:LYS:HD3	1:D:201:VAL:HG12	1.96	0.48
1:A:122:ILE:O	1:A:126:PRO:HG2	2.14	0.47
1:A:145:VAL:CG1	1:A:146:PRO:HD3	2.43	0.47
1:B:383:ALA:C	1:B:385:PHE:N	2.71	0.47
1:D:21:ALA:O	1:D:25:VAL:HB	2.14	0.47
1:A:282:THR:HB	1:A:336:ILE:O	2.14	0.47
1:C:84:THR:OG1	1:C:85:LEU:HD13	2.14	0.47
1:D:125:ILE:H	1:D:126:PRO:HD2	1.79	0.47
1:A:191:ILE:HA	1:A:194:THR:HG22	1.95	0.47
1:A:240:ALA:O	1:A:241:LEU:C	2.56	0.47
1:A:245:ILE:CG2	1:A:417:LEU:CD2	2.92	0.47
1:A:309:SER:HB3	1:A:334:LEU:HD22	1.96	0.47
1:C:56:ALA:CA	1:C:374:MET:HE3	2.44	0.47
1:C:245:ILE:O	1:C:249:ILE:HD13	2.14	0.47
1:A:59:ASP:HA	1:A:62:MET:HB2	1.97	0.47
1:A:105:GLN:O	1:A:106:VAL:C	2.56	0.47
1:D:233:LEU:CB	1:D:368:ALA:HB3	2.44	0.47
1:A:25:VAL:HG11	1:A:116:TRP:CH2	2.49	0.47
1:A:377:LYS:O	1:A:378:GLY:C	2.58	0.47
1:B:81:LEU:HD21	1:B:198:LEU:CD2	2.44	0.47
1:B:162:ILE:O	1:B:162:ILE:HG22	2.14	0.47
1:B:333:PHE:CE1	1:B:336:ILE:HD12	2.50	0.47
1:C:56:ALA:C	1:C:374:MET:HE3	2.40	0.47
1:C:313:LEU:HB2	1:C:331:GLY:HA3	1.97	0.47
1:B:124:ASP:CG	1:B:373:THR:HG23	2.39	0.47
1:C:80:ILE:CD1	1:C:126:PRO:HB3	2.44	0.47
1:D:244:ASN:CB	1:D:376:VAL:HG21	2.45	0.47
1:D:369:TYR:O	1:D:372:GLN:HG2	2.14	0.47
1:A:3:ILE:CG2	1:A:203:GLU:CB	2.93	0.47
1:B:29:LEU:HD23	1:B:33:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:CG1	1:B:116:TRP:HB2	2.45	0.47
1:B:108:PHE:CD1	1:B:108:PHE:N	2.83	0.47
1:B:128:TRP:HD1	1:B:129:SER:N	2.12	0.47
1:B:282:THR:O	1:B:286:PHE:CD2	2.68	0.47
1:B:413:ILE:C	1:B:415:ILE:N	2.72	0.47
1:C:239:MET:HA	1:C:425:THR:OG1	2.15	0.47
1:C:422:PHE:CG	1:C:422:PHE:O	2.68	0.47
1:D:83:GLY:O	1:D:119:THR:HB	2.14	0.47
1:A:37:VAL:CG1	1:A:38:GLY:N	2.77	0.47
1:A:304:VAL:O	1:A:308:LEU:N	2.47	0.47
1:A:332:ILE:O	1:A:335:ASN:HB2	2.15	0.47
1:B:240:ALA:HA	1:B:345:GLN:HE22	1.80	0.47
1:B:245:ILE:CG2	1:B:421:PHE:CD2	2.94	0.47
1:D:320:ASP:OD1	1:D:320:ASP:N	2.48	0.47
1:A:240:ALA:HB2	1:A:372:GLN:HE21	1.80	0.47
1:C:211:VAL:CG1	1:C:212:THR:N	2.78	0.47
1:C:272:LEU:HG	1:C:275:ALA:HB3	1.95	0.47
1:D:124:ASP:CB	1:D:373:THR:HG21	2.45	0.47
1:A:16:PHE:O	1:A:20:PHE:HB2	2.14	0.47
1:A:86:THR:HG22	1:A:119:THR:HG1	1.80	0.47
1:B:141:ARG:HH12	1:B:351:ASP:HA	1.80	0.47
1:C:209:ASN:O	1:C:210:GLY:C	2.55	0.47
1:D:90:VAL:HG12	1:D:90:VAL:O	2.15	0.47
1:A:291:LYS:HD2	1:A:291:LYS:O	2.14	0.46
1:B:236:LEU:HD13	1:B:348:MET:HG2	1.97	0.46
1:C:14:GLY:HA2	1:C:193:SER:OG	2.14	0.46
1:D:119:THR:HA	1:D:122:ILE:HG13	1.96	0.46
1:A:68:ALA:O	1:A:71:SER:O	2.32	0.46
1:A:128:TRP:CD1	1:A:369:TYR:CE1	2.93	0.46
1:A:376:VAL:HG23	1:A:377:LYS:HG3	1.97	0.46
1:A:388:ALA:O	1:A:392:GLY:HA3	2.15	0.46
1:C:166:PHE:HA	1:C:169:TYR:CD2	2.50	0.46
1:D:184:LEU:O	1:D:187:ILE:HG13	2.14	0.46
1:A:240:ALA:CB	1:A:376:VAL:HG12	2.45	0.46
1:A:257:TYR:OH	1:A:327:ILE:O	2.34	0.46
1:C:268:PHE:N	1:C:269:PRO:HD3	2.30	0.46
1:D:47:LEU:HD13	1:D:113:TYR:CZ	2.51	0.46
1:D:420:LEU:HD22	1:D:421:PHE:CE1	2.51	0.46
1:A:8:LYS:O	1:A:12:GLY:N	2.44	0.46
1:B:81:LEU:HD11	1:B:198:LEU:CD2	2.46	0.46
1:B:136:LEU:HD23	1:B:136:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:THR:CA	1:B:374:MET:HE2	2.44	0.46
1:B:383:ALA:O	1:B:384:ALA:C	2.58	0.46
1:C:20:PHE:HD1	1:C:155:ALA:HB1	1.79	0.46
1:C:294:SER:O	1:C:297:ILE:HG13	2.16	0.46
1:D:239:MET:SD	1:D:299:TRP:HH2	2.38	0.46
1:A:111:VAL:HG12	1:A:112:THR:N	2.31	0.46
1:A:239:MET:CB	1:A:425:THR:HA	2.46	0.46
1:A:304:VAL:O	1:A:307:VAL:HB	2.15	0.46
1:B:76:PHE:HA	1:B:79:TRP:HB2	1.98	0.46
1:B:233:LEU:HG	1:B:368:ALA:CB	2.46	0.46
1:B:271:TYR:C	1:B:273:SER:H	2.22	0.46
1:B:303:SER:HA	1:B:341:PHE:CZ	2.50	0.46
1:B:341:PHE:CE2	1:B:425:THR:HG21	2.50	0.46
1:C:77:LYS:CB	1:C:201:VAL:CG2	2.94	0.46
1:C:387:ILE:HD12	1:C:417:LEU:HG	1.97	0.46
1:D:380:SER:CA	1:D:383:ALA:HB3	2.45	0.46
1:D:387:ILE:HA	1:D:390:VAL:CG2	2.46	0.46
1:A:282:THR:HB	1:A:337:GLY:HA2	1.97	0.46
1:C:142:GLU:H	1:C:142:GLU:HG2	1.54	0.46
1:C:426:LEU:O	1:C:430:PHE:N	2.36	0.46
1:D:80:ILE:O	1:D:84:THR:HG23	2.16	0.46
1:A:287:PRO:HA	1:A:340:LEU:HD21	1.98	0.46
1:B:86:THR:HG22	1:B:115:LEU:HG	1.97	0.46
1:A:14:GLY:O	1:A:18:LYS:N	2.42	0.46
1:B:2:SER:O	1:B:5:MET:N	2.48	0.46
1:B:202:HIS:O	1:B:206:SER:HB2	2.15	0.46
1:C:90:VAL:HG23	1:C:91:LEU:N	2.31	0.46
1:C:98:HIS:HB2	1:D:199:ARG:HE	1.80	0.46
1:D:24:ILE:HG12	1:D:159:THR:HB	1.98	0.46
1:B:77:LYS:CB	1:B:201:VAL:HG12	2.44	0.46
1:B:373:THR:N	1:B:374:MET:CE	2.78	0.46
1:B:421:PHE:O	1:B:424:MET:HB3	2.15	0.46
1:C:318:LEU:HD21	1:C:409:GLY:HA2	1.98	0.46
1:D:236:LEU:HD11	1:D:345:GLN:HA	1.98	0.46
1:A:214:GLY:C	1:A:216:PRO:HD2	2.40	0.46
1:B:167:VAL:HB	1:B:182:PHE:CE2	2.51	0.46
1:C:18:LYS:O	1:C:22:ILE:HG22	2.16	0.46
1:C:80:ILE:CD1	1:C:126:PRO:CB	2.94	0.46
1:C:302:ALA:O	1:C:303:SER:C	2.58	0.46
1:A:75:LYS:CG	1:A:76:PHE:N	2.80	0.45
1:B:124:ASP:CB	1:B:373:THR:HG23	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:HH21	1:B:340:LEU:HD11	1.80	0.45
1:C:340:LEU:O	1:C:340:LEU:CG	2.61	0.45
1:C:393:LEU:HA	1:C:396:TYR:HB3	1.98	0.45
1:D:135:THR:CB	1:D:141:ARG:HG3	2.46	0.45
1:A:216:PRO:HA	1:A:219:THR:OG1	2.16	0.45
1:D:233:LEU:CB	1:D:349:VAL:HG13	2.46	0.45
1:D:239:MET:SD	1:D:299:TRP:CH2	3.09	0.45
1:D:351:ASP:HA	1:D:354:ASP:CB	2.45	0.45
1:B:28:TYR:CE1	1:B:31:TYR:HB2	2.52	0.45
1:B:83:GLY:HA3	1:B:122:ILE:HG21	1.97	0.45
1:B:370:SER:O	1:B:374:MET:CE	2.64	0.45
1:C:7:THR:HG23	1:C:201:VAL:HB	1.98	0.45
1:C:11:TYR:CZ	1:C:130:LEU:HD23	2.52	0.45
1:C:16:PHE:O	1:C:20:PHE:CB	2.65	0.45
1:C:77:LYS:HB2	1:C:201:VAL:CG2	2.43	0.45
1:D:75:LYS:HE3	1:D:76:PHE:CA	2.43	0.45
1:D:387:ILE:HB	1:D:414:MET:SD	2.57	0.45
1:A:28:TYR:O	1:A:29:LEU:C	2.58	0.45
1:A:261:VAL:CG2	1:A:328:VAL:HG23	2.39	0.45
1:B:316:MET:HE3	1:B:316:MET:HB3	1.80	0.45
1:C:241:LEU:HD22	1:C:379:GLY:HA3	1.97	0.45
1:C:279:ASN:HD21	1:C:338:THR:HG23	1.81	0.45
1:D:110:CYS:O	1:D:114:ILE:HB	2.17	0.45
1:A:172:GLY:O	1:A:173:ALA:HB3	2.17	0.45
1:A:240:ALA:O	1:A:243:TYR:N	2.50	0.45
1:A:372:GLN:O	1:A:376:VAL:HG13	2.15	0.45
1:D:286:PHE:O	1:D:290:VAL:HG22	2.16	0.45
1:D:386:PHE:HA	1:D:389:LEU:HB2	1.98	0.45
1:A:287:PRO:CA	1:A:340:LEU:HD21	2.46	0.45
1:B:99:LEU:CD2	1:B:180:GLN:CD	2.90	0.45
1:D:125:ILE:O	1:D:369:TYR:OH	2.32	0.45
1:B:120:TYR:HA	1:B:123:MET:HB2	1.98	0.45
1:B:403:SER:OG	1:B:404:ALA:N	2.50	0.45
1:C:49:LEU:O	1:C:52:ARG:HG2	2.17	0.45
1:C:279:ASN:HA	1:C:336:ILE:HA	1.98	0.45
1:D:375:VAL:HG23	1:D:376:VAL:N	2.32	0.45
1:A:41:VAL:HG11	1:A:105:GLN:HG2	1.98	0.45
1:A:190:PHE:O	1:A:193:SER:N	2.47	0.45
1:B:351:ASP:O	1:B:433:TYR:CE2	2.69	0.45
1:B:428:LEU:HD12	1:B:428:LEU:HA	1.84	0.45
1:D:114:ILE:O	1:D:118:MET:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:MET:HE1	1:B:429:TYR:CG	2.52	0.45
1:B:261:VAL:HG22	1:B:262:ILE:H	1.82	0.45
1:C:148:PRO:C	1:C:150:PHE:N	2.75	0.45
1:D:257:TYR:HE1	1:D:316:MET:HE3	1.82	0.45
1:D:416:VAL:HG13	1:D:417:LEU:N	2.31	0.45
1:A:35:ASP:OD2	1:A:175:ARG:NE	2.50	0.45
1:A:202:HIS:C	1:A:203:GLU:OE1	2.59	0.45
1:A:375:VAL:O	1:A:376:VAL:C	2.58	0.45
1:B:13:PHE:O	1:B:193:SER:OG	2.32	0.45
1:B:16:PHE:HB2	1:B:151:PHE:CE2	2.52	0.45
1:B:86:THR:O	1:B:90:VAL:HG23	2.17	0.45
1:C:24:ILE:O	1:C:28:TYR:N	2.37	0.45
1:C:125:ILE:N	1:C:126:PRO:CD	2.80	0.45
1:C:329:ALA:O	1:C:332:ILE:HG12	2.17	0.45
1:D:131:VAL:N	1:D:132:PRO:CD	2.80	0.45
1:D:420:LEU:HD23	1:D:420:LEU:C	2.42	0.45
1:A:147:PHE:N	1:A:148:PRO:CD	2.80	0.44
1:A:253:PHE:CE2	1:A:414:MET:SD	3.10	0.44
1:B:299:TRP:HD1	1:B:344:LEU:HD13	1.81	0.44
1:A:128:TRP:NE1	1:A:346:VAL:HG11	2.31	0.44
1:B:163:THR:CG2	1:B:182:PHE:HZ	2.27	0.44
1:C:28:TYR:O	1:C:29:LEU:C	2.60	0.44
1:C:131:VAL:HG12	1:C:145:VAL:HG22	1.99	0.44
1:D:75:LYS:C	1:D:77:LYS:N	2.72	0.44
1:D:258:PHE:HA	1:D:261:VAL:HG22	1.99	0.44
1:A:286:PHE:O	1:A:298:LEU:HD21	2.17	0.44
1:A:351:ASP:HA	1:A:354:ASP:HB2	1.98	0.44
1:A:383:ALA:HA	1:A:386:PHE:HB3	2.00	0.44
1:B:76:PHE:O	1:B:80:ILE:HG23	2.18	0.44
1:B:353:VAL:O	1:B:357:GLU:N	2.42	0.44
1:C:175:ARG:HD2	1:C:175:ARG:C	2.39	0.44
1:C:235:CYS:SG	1:C:428:LEU:HD11	2.58	0.44
1:C:299:TRP:HA	1:C:302:ALA:HB3	1.99	0.44
1:D:233:LEU:HA	1:D:349:VAL:HG22	1.98	0.44
1:D:333:PHE:O	1:D:336:ILE:HG13	2.18	0.44
1:A:148:PRO:C	1:A:150:PHE:N	2.75	0.44
1:B:270:TYR:HD2	1:B:271:TYR:CD1	2.36	0.44
1:C:86:THR:HA	1:C:89:LEU:HD12	1.98	0.44
1:A:105:GLN:HE21	1:A:105:GLN:H	1.59	0.44
1:B:59:ASP:HA	1:B:374:MET:SD	2.57	0.44
1:B:77:LYS:HB3	1:B:78:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:N	1:B:146:PRO:HD3	2.32	0.44
1:B:353:VAL:HG11	1:B:365:GLU:O	2.18	0.44
1:B:387:ILE:CG2	1:B:417:LEU:HD22	2.48	0.44
1:C:253:PHE:CZ	1:C:414:MET:HE2	2.52	0.44
1:A:266:ASP:OD1	1:A:266:ASP:N	2.48	0.44
1:B:373:THR:HB	1:B:374:MET:CE	2.48	0.44
1:D:90:VAL:HG11	1:D:116:TRP:HB2	1.99	0.44
1:D:182:PHE:O	1:D:186:LEU:HD13	2.18	0.44
1:D:244:ASN:HB3	1:D:376:VAL:HG21	2.00	0.44
1:A:287:PRO:O	1:A:295:ARG:NH1	2.51	0.44
1:B:35:ASP:HA	1:B:38:GLY:CA	2.42	0.44
1:C:353:VAL:O	1:C:357:GLU:HB2	2.17	0.44
1:D:62:MET:C	1:D:370:SER:HB3	2.42	0.44
1:D:129:SER:HB2	1:D:369:TYR:OH	2.13	0.44
1:B:439:MET:CB	1:B:440:LEU:HD12	2.47	0.44
1:C:95:PHE:CE1	1:C:184:LEU:HD11	2.52	0.44
1:D:83:GLY:O	1:D:119:THR:CB	2.66	0.44
1:A:32:TYR:CD1	1:A:35:ASP:HB3	2.53	0.44
1:A:75:LYS:HD3	1:A:202:HIS:HA	1.99	0.44
1:A:388:ALA:O	1:A:392:GLY:CA	2.66	0.44
1:B:40:SER:O	1:B:40:SER:OG	2.30	0.44
1:C:16:PHE:CE2	1:C:151:PHE:HD2	2.35	0.44
1:C:77:LYS:CE	1:C:201:VAL:HG22	2.47	0.44
1:D:37:VAL:O	1:D:38:GLY:C	2.61	0.44
1:D:71:SER:O	1:D:72:ARG:C	2.60	0.44
1:D:387:ILE:HG13	1:D:388:ALA:N	2.32	0.44
1:A:148:PRO:O	1:A:150:PHE:N	2.50	0.43
1:A:156:GLY:C	1:A:158:VAL:H	2.26	0.43
1:A:157:PHE:HB3	1:A:158:VAL:HG23	2.00	0.43
1:A:282:THR:HG21	1:A:337:GLY:HA2	1.99	0.43
1:B:240:ALA:HA	1:B:345:GLN:NE2	2.32	0.43
1:C:142:GLU:HB3	1:C:344:LEU:CD2	2.48	0.43
1:D:75:LYS:HB3	1:D:77:LYS:H	1.83	0.43
1:D:383:ALA:O	1:D:387:ILE:HG23	2.18	0.43
1:A:243:TYR:CZ	1:A:341:PHE:CD2	3.02	0.43
1:C:127:PHE:CZ	1:C:131:VAL:HG21	2.52	0.43
1:A:157:PHE:CE1	1:A:277:ALA:HB1	2.54	0.43
1:A:204:VAL:HA	1:A:207:SER:OG	2.18	0.43
1:A:392:GLY:O	1:A:393:LEU:HD22	2.18	0.43
1:B:197:THR:O	1:B:201:VAL:HG23	2.19	0.43
1:A:383:ALA:O	1:A:386:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:PRO:O	1:B:307:VAL:C	2.61	0.43
1:C:66:VAL:O	1:C:67:ASN:CG	2.62	0.43
1:C:72:ARG:CG	1:C:73:TRP:N	2.81	0.43
1:D:33:TYR:O	1:D:33:TYR:CD1	2.70	0.43
1:D:145:VAL:N	1:D:146:PRO:CD	2.81	0.43
1:D:147:PHE:HD1	1:D:150:PHE:CD2	2.28	0.43
1:B:20:PHE:CD2	1:B:186:LEU:HA	2.53	0.43
1:B:164:LEU:N	1:B:165:PRO:HD2	2.34	0.43
1:C:79:TRP:HZ2	1:C:125:ILE:HG23	1.83	0.43
1:D:370:SER:C	1:D:372:GLN:H	2.27	0.43
1:A:127:PHE:CD1	1:A:127:PHE:O	2.71	0.43
1:A:195:ILE:HG23	1:A:196:VAL:HG23	2.00	0.43
1:A:429:TYR:CD2	1:A:429:TYR:O	2.71	0.43
1:B:271:TYR:C	1:B:273:SER:N	2.75	0.43
1:B:290:VAL:CG1	1:B:295:ARG:HG2	2.35	0.43
1:C:138:LYS:C	1:C:139:ARG:CG	2.91	0.43
1:D:125:ILE:O	1:D:128:TRP:CD1	2.72	0.43
1:D:245:ILE:CG1	1:D:376:VAL:HG23	2.43	0.43
1:A:87:ASN:O	1:A:90:VAL:HB	2.18	0.43
1:A:390:VAL:CG1	1:A:413:ILE:HG23	2.49	0.43
1:A:397:THR:O	1:A:398:PRO:C	2.62	0.43
1:B:93:LEU:CD1	1:B:112:THR:HG21	2.24	0.43
1:C:139:ARG:HB3	1:C:141:ARG:HH11	1.83	0.43
1:C:255:ILE:O	1:C:258:PHE:HB3	2.19	0.43
1:D:332:ILE:C	1:D:334:LEU:N	2.77	0.43
1:A:56:ALA:O	1:A:60:PRO:HD2	2.19	0.43
1:B:61:ILE:HD12	1:B:61:ILE:HA	1.87	0.43
1:B:352:THR:N	1:B:433:TYR:HE2	2.16	0.43
1:A:105:GLN:CA	1:A:105:GLN:NE2	2.80	0.43
1:A:302:ALA:O	1:A:306:PRO:HD3	2.19	0.43
1:B:62:MET:SD	1:B:122:ILE:HD11	2.58	0.43
1:B:256:TYR:O	1:B:260:TYR:N	2.52	0.43
1:B:290:VAL:O	1:B:290:VAL:HG12	2.19	0.43
1:C:62:MET:HE2	1:C:122:ILE:HD12	2.00	0.43
1:C:66:VAL:C	1:C:67:ASN:CG	2.87	0.43
1:D:117:GLY:O	1:D:120:TYR:N	2.52	0.43
1:A:5:MET:SD	1:A:135:THR:HG23	2.59	0.43
1:A:77:LYS:N	1:A:78:PRO:HD2	2.34	0.43
1:A:145:VAL:HG13	1:A:146:PRO:HD3	2.01	0.43
1:B:59:ASP:OD1	1:B:374:MET:HG3	2.19	0.43
1:B:80:ILE:CG1	1:B:81:LEU:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PHE:CZ	1:B:425:THR:HG21	2.53	0.43
1:C:58:ASN:CB	1:C:121:THR:HG21	2.48	0.43
1:C:216:PRO:C	1:C:219:THR:HG1	2.26	0.43
1:C:332:ILE:O	1:C:335:ASN:HB2	2.18	0.43
1:D:237:LEU:HD22	1:D:371:VAL:HB	2.01	0.43
1:A:128:TRP:HD1	1:A:369:TYR:HE1	1.62	0.42
1:A:245:ILE:HG21	1:A:417:LEU:HD21	1.99	0.42
1:C:241:LEU:CA	1:C:376:VAL:HG13	2.48	0.42
1:C:313:LEU:HD13	1:C:330:ALA:O	2.18	0.42
1:D:76:PHE:HB3	1:D:80:ILE:CG2	2.49	0.42
1:D:368:ALA:O	1:D:369:TYR:C	2.61	0.42
1:D:420:LEU:HD22	1:D:421:PHE:CD1	2.54	0.42
1:A:150:PHE:CD1	1:A:150:PHE:C	2.95	0.42
1:A:164:LEU:HA	1:A:167:VAL:HG12	2.01	0.42
1:B:417:LEU:O	1:B:421:PHE:CG	2.72	0.42
1:C:278:ALA:O	1:C:336:ILE:HG22	2.19	0.42
1:A:81:LEU:HD12	1:A:85:LEU:HD12	2.01	0.42
1:A:351:ASP:HA	1:A:354:ASP:HB3	2.02	0.42
1:B:239:MET:HE1	1:B:429:TYR:HB2	2.00	0.42
1:C:148:PRO:C	1:C:150:PHE:H	2.26	0.42
1:C:249:ILE:O	1:C:253:PHE:HB2	2.18	0.42
1:C:349:VAL:HB	1:C:372:GLN:CB	2.49	0.42
1:D:137:ASP:O	1:D:138:LYS:CG	2.50	0.42
1:D:386:PHE:CD1	1:D:389:LEU:HD12	2.54	0.42
1:A:27:MET:HE2	1:A:159:THR:O	2.19	0.42
1:A:91:LEU:HD12	1:A:94:LEU:HD13	2.01	0.42
1:A:123:MET:HE1	1:A:190:PHE:CZ	2.54	0.42
1:A:278:ALA:HB1	1:A:336:ILE:CG2	2.45	0.42
1:B:268:PHE:O	1:B:269:PRO:C	2.62	0.42
1:C:88:SER:O	1:C:92:PHE:N	2.51	0.42
1:C:279:ASN:OD1	1:C:338:THR:O	2.36	0.42
1:D:55:ASP:OD1	1:D:375:VAL:HB	2.20	0.42
1:D:73:TRP:CB	1:D:209:ASN:HB2	2.50	0.42
1:A:98:HIS:HB2	1:B:199:ARG:HD2	2.02	0.42
1:B:12:GLY:O	1:B:15:ALA:HB3	2.19	0.42
1:B:248:ASN:OD1	1:B:377:LYS:HG2	2.19	0.42
1:C:116:TRP:O	1:C:119:THR:HB	2.20	0.42
1:D:320:ASP:HB2	1:D:323:ASN:HB3	2.01	0.42
1:A:334:LEU:O	1:A:336:ILE:N	2.52	0.42
1:B:236:LEU:HD21	1:B:345:GLN:O	2.19	0.42
1:B:415:ILE:N	1:B:415:ILE:CD1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ASP:O	1:C:36:VAL:C	2.62	0.42
1:C:92:PHE:HD1	1:C:187:ILE:HD13	1.85	0.42
1:D:413:ILE:O	1:D:414:MET:C	2.61	0.42
1:A:1:MET:SD	1:A:4:SER:N	2.90	0.42
1:A:31:TYR:O	1:A:34:THR:HB	2.19	0.42
1:A:241:LEU:HD11	1:A:375:VAL:HG12	2.01	0.42
1:A:254:ALA:HB1	1:A:272:LEU:HD21	2.01	0.42
1:A:417:LEU:HD23	1:A:418:PRO:N	2.34	0.42
1:B:125:ILE:HD11	1:B:369:TYR:CD1	2.54	0.42
1:B:167:VAL:HB	1:B:182:PHE:HE2	1.85	0.42
1:B:235:CYS:SG	1:B:236:LEU:N	2.92	0.42
1:B:281:LEU:HD23	1:B:284:ILE:HD11	2.00	0.42
1:D:391:LEU:HD12	1:D:395:GLY:HA3	2.02	0.42
1:A:100:PHE:CE1	1:A:108:PHE:HB2	2.55	0.42
1:A:143:GLN:HA	1:A:295:ARG:HH21	1.84	0.42
1:B:237:LEU:HD13	1:B:371:VAL:HG21	2.01	0.42
1:D:413:ILE:HD13	1:D:413:ILE:H	1.85	0.42
1:A:45:GLY:O	1:A:48:PHE:HB2	2.20	0.42
1:B:81:LEU:CD1	1:B:198:LEU:HD23	2.50	0.42
1:B:91:LEU:HD13	1:B:186:LEU:HD22	2.02	0.42
1:B:237:LEU:O	1:B:241:LEU:HG	2.19	0.42
1:C:33:TYR:HA	1:C:36:VAL:HG13	2.02	0.42
1:C:202:HIS:ND1	1:C:202:HIS:C	2.78	0.42
1:C:413:ILE:HA	1:C:416:VAL:HG12	2.02	0.42
1:A:81:LEU:HD11	1:A:85:LEU:CD1	2.49	0.42
1:A:107:VAL:HB	1:A:108:PHE:H	1.67	0.42
1:A:299:TRP:CZ2	1:A:341:PHE:CZ	3.08	0.42
1:A:342:TRP:CD1	1:A:346:VAL:HG22	2.55	0.42
1:B:250:ILE:O	1:B:251:ASN:C	2.62	0.42
1:C:118:MET:O	1:C:122:ILE:HG22	2.20	0.42
1:C:233:LEU:HD12	1:C:233:LEU:HA	1.87	0.42
1:D:118:MET:HE2	1:D:118:MET:HA	2.02	0.42
1:D:380:SER:O	1:D:384:ALA:HB2	2.19	0.42
1:A:62:MET:HE3	1:A:122:ILE:HD12	2.01	0.41
1:A:76:PHE:HE2	1:A:126:PRO:HA	1.84	0.41
1:A:279:ASN:HA	1:A:335:ASN:O	2.19	0.41
1:A:287:PRO:CB	1:A:340:LEU:HD21	2.50	0.41
1:B:32:TYR:CD1	1:B:176:GLY:CA	2.95	0.41
1:B:310:CYS:SG	1:B:311:ALA:N	2.89	0.41
1:A:282:THR:HG23	1:A:286:PHE:HD1	1.79	0.41
1:B:333:PHE:CZ	1:B:336:ILE:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLY:CA	1:D:190:PHE:HD1	2.33	0.41
1:D:21:ALA:O	1:D:25:VAL:CG2	2.68	0.41
1:D:320:ASP:CB	1:D:323:ASN:HB2	2.50	0.41
1:A:8:LYS:HG3	1:A:131:VAL:HG22	2.01	0.41
1:A:98:HIS:HD2	1:A:99:LEU:HB2	1.80	0.41
1:B:95:PHE:O	1:B:180:GLN:NE2	2.46	0.41
1:C:128:TRP:O	1:C:132:PRO:HD3	2.21	0.41
1:C:417:LEU:HD23	1:C:418:PRO:HD3	2.02	0.41
1:D:77:LYS:HE3	1:D:81:LEU:HD22	2.03	0.41
1:B:162:ILE:O	1:B:162:ILE:CG2	2.68	0.41
1:B:305:MET:HB2	1:B:306:PRO:HD3	2.02	0.41
1:B:396:TYR:O	1:B:396:TYR:HD1	2.03	0.41
1:C:32:TYR:O	1:C:36:VAL:HG12	2.20	0.41
1:C:76:PHE:CE1	1:C:79:TRP:CE3	3.09	0.41
1:A:41:VAL:HB	1:A:105:GLN:CD	2.45	0.41
1:A:81:LEU:CD1	1:A:85:LEU:CD1	2.98	0.41
1:A:194:THR:O	1:A:198:LEU:HG	2.21	0.41
1:B:34:THR:HG23	1:B:43:LEU:CD2	2.50	0.41
1:C:372:GLN:O	1:C:376:VAL:HG23	2.19	0.41
1:C:399:ASN:C	1:C:401:ALA:H	2.29	0.41
1:D:344:LEU:HD22	1:D:348:MET:HE1	2.03	0.41
1:A:209:ASN:O	1:A:210:GLY:C	2.64	0.41
1:A:346:VAL:HG12	1:A:369:TYR:CD1	2.56	0.41
1:C:16:PHE:CE2	1:C:151:PHE:CD2	3.09	0.41
1:C:83:GLY:CA	1:C:122:ILE:HG23	2.51	0.41
1:C:299:TRP:CZ2	1:C:341:PHE:CZ	3.08	0.41
1:C:333:PHE:C	1:C:335:ASN:H	2.28	0.41
1:D:147:PHE:N	1:D:148:PRO:HD2	2.36	0.41
1:A:174:ASP:O	1:A:178:GLY:N	2.53	0.41
1:A:256:TYR:HA	1:A:259:THR:HB	2.02	0.41
1:A:307:VAL:CG2	1:A:422:PHE:CD2	3.04	0.41
1:B:77:LYS:O	1:B:81:LEU:CB	2.65	0.41
1:C:77:LYS:HA	1:C:80:ILE:CG1	2.42	0.41
1:C:242:ALA:HA	1:C:245:ILE:CG1	2.49	0.41
1:C:417:LEU:HA	1:C:420:LEU:HB2	2.02	0.41
1:D:342:TRP:O	1:D:345:GLN:HB2	2.21	0.41
1:D:418:PRO:O	1:D:422:PHE:HD1	2.03	0.41
1:A:240:ALA:O	1:A:243:TYR:HB3	2.21	0.41
1:A:271:TYR:OH	1:A:329:ALA:CB	2.69	0.41
1:B:99:LEU:CD1	1:B:177:PHE:HB2	2.47	0.41
1:C:2:SER:O	1:C:6:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASN:C	1:C:230:ASN:ND2	2.79	0.41
1:C:240:ALA:HA	1:C:345:GLN:HE22	1.86	0.41
1:D:91:LEU:HD12	1:D:94:LEU:HB3	2.01	0.41
1:D:426:LEU:O	1:D:426:LEU:HD23	2.20	0.41
1:A:56:ALA:O	1:A:374:MET:HE3	2.21	0.41
1:A:75:LYS:HG2	1:A:77:LYS:H	1.86	0.41
1:B:76:PHE:HA	1:B:79:TRP:HB3	2.02	0.41
1:B:81:LEU:HD11	1:B:198:LEU:HD23	2.03	0.41
1:B:415:ILE:O	1:B:416:VAL:C	2.64	0.41
1:C:27:MET:O	1:C:27:MET:HG2	2.21	0.41
1:C:58:ASN:ND2	1:C:121:THR:HG21	2.36	0.41
1:C:127:PHE:CE1	1:C:131:VAL:HG21	2.56	0.41
1:C:141:ARG:NH2	1:C:351:ASP:OD1	2.53	0.41
1:C:241:LEU:N	1:C:376:VAL:HG13	2.36	0.41
1:D:19:ASP:HB3	1:D:155:ALA:HB3	2.03	0.41
1:D:192:ALA:O	1:D:195:ILE:HG22	2.21	0.41
1:D:269:PRO:O	1:D:272:LEU:HB3	2.20	0.41
1:A:90:VAL:HG21	1:A:116:TRP:CA	2.51	0.41
1:B:10:SER:O	1:B:13:PHE:N	2.54	0.41
1:B:21:ALA:CB	1:B:87:ASN:ND2	2.83	0.41
1:B:28:TYR:O	1:B:29:LEU:C	2.63	0.41
1:C:175:ARG:O	1:C:175:ARG:CD	2.62	0.41
1:C:215:ARG:H	1:C:216:PRO:HD2	1.80	0.41
1:B:76:PHE:O	1:B:79:TRP:N	2.54	0.40
1:D:145:VAL:N	1:D:146:PRO:HD3	2.36	0.40
1:D:316:MET:O	1:D:317:ALA:HB2	2.19	0.40
1:A:32:TYR:HA	1:A:35:ASP:HB3	2.02	0.40
1:A:77:LYS:O	1:A:80:ILE:HG13	2.22	0.40
1:A:78:PRO:O	1:A:82:ILE:N	2.55	0.40
1:A:82:ILE:O	1:A:86:THR:CB	2.70	0.40
1:A:116:TRP:C	1:A:116:TRP:CD1	2.99	0.40
1:C:136:LEU:O	1:C:138:LYS:N	2.53	0.40
1:C:402:GLN:HG3	1:C:403:SER:N	2.35	0.40
1:D:257:TYR:O	1:D:260:TYR:HB3	2.21	0.40
1:A:33:TYR:CD1	1:A:33:TYR:C	2.99	0.40
1:A:305:MET:HE2	1:A:305:MET:HB3	1.84	0.40
1:B:239:MET:CE	1:B:429:TYR:HB2	2.52	0.40
1:B:260:TYR:OH	1:B:317:ALA:CB	2.69	0.40
1:B:410:MET:HB3	1:B:413:ILE:HD11	2.04	0.40
1:C:56:ALA:O	1:C:60:PRO:CD	2.68	0.40
1:C:72:ARG:HE	1:C:72:ARG:HB3	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:PHE:HD1	1:D:283:LEU:HD21	1.78	0.40
1:D:236:LEU:HA	1:D:236:LEU:HD12	1.90	0.40
1:B:241:LEU:O	1:B:245:ILE:CG1	2.69	0.40
1:C:238:GLY:HA2	1:C:241:LEU:HD12	2.03	0.40
1:D:322:HIS:O	1:D:326:LEU:HD13	2.22	0.40
1:A:14:GLY:O	1:A:18:LYS:HB2	2.21	0.40
1:B:35:ASP:CG	1:B:175:ARG:NH1	2.80	0.40
1:C:75:LYS:CD	1:C:202:HIS:O	2.66	0.40
1:C:376:VAL:O	1:C:377:LYS:C	2.61	0.40
1:D:63:GLY:N	1:D:370:SER:HB3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/486 (92%)	365 (82%)	65 (15%)	16 (4%)	2	15
1	B	422/486 (87%)	360 (85%)	54 (13%)	8 (2%)	6	25
1	C	429/486 (88%)	358 (83%)	63 (15%)	8 (2%)	6	25
1	D	374/486 (77%)	314 (84%)	52 (14%)	8 (2%)	5	23
All	All	1671/1944 (86%)	1397 (84%)	234 (14%)	40 (2%)	4	21

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ILE
1	A	269	PRO
1	A	271	TYR
1	B	430	PHE
1	C	134	ILE

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Mol	Chain	Res	Type
1	C	269	PRO
1	C	271	TYR
1	D	369	TYR
1	A	96	SER
1	A	107	VAL
1	A	214	GLY
1	A	369	TYR
1	A	392	GLY
1	A	398	PRO
1	B	384	ALA
1	C	137	ASP
1	C	339	ALA
1	C	401	ALA
1	C	422	PHE
1	D	38	GLY
1	D	78	PRO
1	D	371	VAL
1	A	433	TYR
1	D	125	ILE
1	D	317	ALA
1	A	111	VAL
1	A	373	THR
1	A	379	GLY
1	A	432	TYR
1	B	35	ASP
1	A	335	ASN
1	D	268	PHE
1	A	42	GLY
1	B	245	ILE
1	B	337	GLY
1	C	397	THR
1	D	146	PRO
1	B	45	GLY
1	B	249	ILE
1	B	409	GLY

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	354/406 (87%)	300 (85%)	54 (15%)	3	10
1	B	331/406 (82%)	274 (83%)	57 (17%)	2	8
1	C	353/406 (87%)	271 (77%)	82 (23%)	1	2
1	D	302/406 (74%)	255 (84%)	47 (16%)	2	10
All	All	1340/1624 (82%)	1100 (82%)	240 (18%)	2	7

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	LEU
1	A	11	TYR
1	A	22	ILE
1	A	29	LEU
1	A	46	THR
1	A	52	ARG
1	A	55	ASP
1	A	59	ASP
1	A	62	MET
1	A	69	THR
1	A	77	LYS
1	A	80	ILE
1	A	86	THR
1	A	92	PHE
1	A	96	SER
1	A	103	THR
1	A	105	GLN
1	A	107	VAL
1	A	111	VAL
1	A	114	ILE
1	A	121	THR
1	A	128	TRP
1	A	134	ILE
1	A	141	ARG
1	A	149	ARG
1	A	151	PHE
1	A	187	ILE
1	A	191	ILE
1	A	203	GLU
1	A	204	VAL

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Mol	Chain	Res	Type
1	A	207	SER
1	A	227	ILE
1	A	229	LYS
1	A	230	ASN
1	A	248	ASN
1	A	259	THR
1	A	261	VAL
1	A	262	ILE
1	A	264	ASP
1	A	266	ASP
1	A	280	LEU
1	A	281	LEU
1	A	282	THR
1	A	285	VAL
1	A	291	LYS
1	A	303	SER
1	A	358	PHE
1	A	359	LYS
1	A	361	ASN
1	A	417	LEU
1	A	421	PHE
1	A	422	PHE
1	A	428	LEU
1	B	5	MET
1	B	35	ASP
1	B	48	PHE
1	B	49	LEU
1	B	54	TRP
1	B	59	ASP
1	B	61	ILE
1	B	66	VAL
1	B	70	ARG
1	B	75	LYS
1	B	80	ILE
1	B	86	THR
1	B	92	PHE
1	B	95	PHE
1	B	111	VAL
1	B	114	ILE
1	B	125	ILE
1	B	130	LEU
1	B	145	VAL

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Mol	Chain	Res	Type
1	B	154	LEU
1	B	175	ARG
1	B	191	ILE
1	B	194	THR
1	B	195	ILE
1	B	197	THR
1	B	200	ASN
1	B	205	TYR
1	B	208	ASP
1	B	253	PHE
1	B	259	THR
1	B	269	PRO
1	B	283	LEU
1	B	289	LEU
1	B	295	ARG
1	B	297	ILE
1	B	299	TRP
1	B	305	MET
1	B	314	PHE
1	B	316	MET
1	B	321	ILE
1	B	326	LEU
1	B	336	ILE
1	B	345	GLN
1	B	366	SER
1	B	369	TYR
1	B	374	MET
1	B	380	SER
1	B	389	LEU
1	B	390	VAL
1	B	410	MET
1	B	413	ILE
1	B	415	ILE
1	B	419	VAL
1	B	420	LEU
1	B	423	MET
1	B	425	THR
1	B	428	LEU
1	C	1	MET
1	C	5	MET
1	C	6	THR
1	C	11	TYR

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Mol	Chain	Res	Type
1	C	28	TYR
1	C	29	LEU
1	C	30	MET
1	C	33	TYR
1	C	35	ASP
1	C	36	VAL
1	C	37	VAL
1	C	61	ILE
1	C	62	MET
1	C	65	ILE
1	C	67	ASN
1	C	70	ARG
1	C	72	ARG
1	C	77	LYS
1	C	85	LEU
1	C	110	CYS
1	C	114	ILE
1	C	118	MET
1	C	121	THR
1	C	128	TRP
1	C	130	LEU
1	C	135	THR
1	C	136	LEU
1	C	137	ASP
1	C	139	ARG
1	C	141	ARG
1	C	142	GLU
1	C	143	GLN
1	C	148	PRO
1	C	154	LEU
1	C	158	VAL
1	C	175	ARG
1	C	181	MET
1	C	187	ILE
1	C	198	LEU
1	C	203	GLU
1	C	212	THR
1	C	227	ILE
1	C	229	LYS
1	C	230	ASN
1	C	236	LEU
1	C	248	ASN

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Mol	Chain	Res	Type
1	C	255	ILE
1	C	259	THR
1	C	271	TYR
1	C	272	LEU
1	C	281	LEU
1	C	282	THR
1	C	288	ARG
1	C	293	LEU
1	C	313	LEU
1	C	314	PHE
1	C	323	ASN
1	C	326	LEU
1	C	327	ILE
1	C	328	VAL
1	C	345	GLN
1	C	351	ASP
1	C	360	LEU
1	C	363	ARG
1	C	367	ILE
1	C	372	GLN
1	C	374	MET
1	C	375	VAL
1	C	385	PHE
1	C	386	PHE
1	C	391	LEU
1	C	393	LEU
1	C	398	PRO
1	C	400	VAL
1	C	403	SER
1	C	406	THR
1	C	407	LEU
1	C	408	GLN
1	C	411	GLN
1	C	412	PHE
1	C	422	PHE
1	C	426	LEU
1	D	13	PHE
1	D	27	MET
1	D	33	TYR
1	D	37	VAL
1	D	49	LEU
1	D	53	ILE

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Mol	Chain	Res	Type
1	D	59	ASP
1	D	61	ILE
1	D	66	VAL
1	D	75	LYS
1	D	80	ILE
1	D	86	THR
1	D	89	LEU
1	D	93	LEU
1	D	110	CYS
1	D	123	MET
1	D	124	ASP
1	D	134	ILE
1	D	141	ARG
1	D	143	GLN
1	D	144	LEU
1	D	175	ARG
1	D	191	ILE
1	D	194	THR
1	D	195	ILE
1	D	199	ARG
1	D	204	VAL
1	D	208	ASP
1	D	235	CYS
1	D	257	TYR
1	D	270	TYR
1	D	273	SER
1	D	282	THR
1	D	284	ILE
1	D	292	MET
1	D	299	TRP
1	D	304	VAL
1	D	318	LEU
1	D	326	LEU
1	D	344	LEU
1	D	387	ILE
1	D	393	LEU
1	D	394	ILE
1	D	413	ILE
1	D	414	MET
1	D	415	ILE
1	D	419	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	98	HIS
1	A	105	GLN
1	A	217	HIS
1	A	244	ASN
1	A	322	HIS
1	A	323	ASN
1	A	335	ASN
1	A	345	GLN
1	A	361	ASN
1	A	411	GLN
1	B	67	ASN
1	B	143	GLN
1	B	244	ASN
1	B	279	ASN
1	B	323	ASN
1	B	335	ASN
1	C	67	ASN
1	C	105	GLN
1	C	230	ASN
1	C	402	GLN
1	C	411	GLN
1	D	180	GLN
1	D	244	ASN
1	D	248	ASN
1	D	251	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	448/486 (92%)	1.72	143 (31%)	11	4, 75, 180, 265	25 (5%)
1	B	426/486 (87%)	2.45	193 (45%)	00	28, 89, 247, 360	9 (2%)
1	C	431/486 (88%)	1.61	124 (28%)	12	24, 76, 168, 340	0
1	D	382/486 (78%)	2.22	154 (40%)	00	31, 85, 220, 331	1 (0%)
All	All	1687/1944 (86%)	1.99	614 (36%)	11	4, 81, 212, 360	35 (2%)

All (614) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	ASP	22.9
1	A	432	TYR	22.7
1	B	411	GLN	19.8
1	D	364	CYS	17.9
1	D	366	SER	17.6
1	A	446	HIS	16.3
1	C	321	ILE	15.9
1	D	362	ILE	15.4
1	D	351	ASP	14.3
1	B	364	CYS	14.1
1	D	411	GLN	14.1
1	D	412	PHE	13.6
1	D	350	ALA	13.3
1	C	320	ASP	12.9
1	B	350	ALA	12.7
1	A	434	ARG	12.2
1	B	363	ARG	11.4
1	B	432	TYR	11.2
1	A	433	TYR	11.1
1	B	374	MET	11.1
1	B	365	GLU	11.1

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Mol	Chain	Res	Type	RSRZ
1	C	5	MET	11.0
1	D	157	PHE	10.8
1	A	366	SER	10.6
1	C	319	ALA	10.6
1	B	352	THR	10.4
1	C	358	PHE	10.3
1	A	445	ILE	10.3
1	B	101	GLU	10.0
1	D	361	ASN	9.9
1	A	443	ILE	9.8
1	B	349	VAL	9.8
1	B	354	ASP	9.5
1	C	323	ASN	9.2
1	B	100	PHE	9.1
1	B	108	PHE	9.0
1	D	363	ARG	9.0
1	D	349	VAL	8.9
1	A	408	GLN	8.8
1	A	323	ASN	8.7
1	A	324	ALA	8.7
1	D	66	VAL	8.5
1	B	96	SER	8.4
1	B	33	TYR	8.3
1	B	70	ARG	8.2
1	A	73	TRP	8.1
1	A	181	MET	8.1
1	C	178	GLY	8.0
1	C	322	HIS	8.0
1	D	352	THR	8.0
1	A	447	LEU	8.0
1	D	169	TYR	7.9
1	B	141	ARG	7.9
1	A	442	LYS	7.8
1	A	365	GLU	7.8
1	D	201	VAL	7.7
1	A	363	ARG	7.7
1	B	139	ARG	7.7
1	D	374	MET	7.5
1	C	363	ARG	7.3
1	A	367	ILE	7.2
1	C	200	ASN	7.1
1	B	366	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	150	PHE	7.1
1	A	320	ASP	7.1
1	D	163	THR	7.0
1	B	143	GLN	7.0
1	B	369	TYR	7.0
1	C	338	THR	7.0
1	B	343	VAL	7.0
1	D	367	ILE	6.8
1	D	67	ASN	6.8
1	D	357	GLU	6.7
1	B	412	PHE	6.6
1	C	99	LEU	6.6
1	C	318	LEU	6.6
1	B	106	VAL	6.6
1	B	122	ILE	6.6
1	B	133	THR	6.6
1	B	95	PHE	6.5
1	D	16	PHE	6.5
1	B	373	THR	6.5
1	D	13	PHE	6.5
1	B	129	SER	6.5
1	D	130	LEU	6.5
1	B	367	ILE	6.5
1	A	105	GLN	6.5
1	B	257	TYR	6.4
1	D	369	TYR	6.3
1	B	132	PRO	6.3
1	D	343	VAL	6.3
1	A	440	LEU	6.3
1	A	8	LYS	6.2
1	D	202	HIS	6.2
1	D	141	ARG	6.2
1	D	353	VAL	6.2
1	B	109	VAL	6.1
1	C	421	PHE	6.1
1	B	439	MET	6.1
1	B	63	GLY	6.1
1	B	65	ILE	6.1
1	A	439	MET	6.0
1	B	399	ASN	6.0
1	A	325	ALA	6.0
1	D	368	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	131	VAL	5.8
1	A	361	ASN	5.8
1	C	163	THR	5.8
1	B	436	ASN	5.8
1	B	144	LEU	5.8
1	B	16	PHE	5.8
1	B	146	PRO	5.8
1	C	367	ILE	5.8
1	C	355	TYR	5.7
1	B	265	ALA	5.7
1	B	107	VAL	5.7
1	B	175	ARG	5.7
1	D	166	PHE	5.6
1	B	258	PHE	5.6
1	D	154	LEU	5.6
1	A	100	PHE	5.5
1	A	421	PHE	5.5
1	D	341	PHE	5.5
1	A	204	VAL	5.5
1	D	365	GLU	5.5
1	D	354	ASP	5.5
1	D	70	ARG	5.5
1	B	358	PHE	5.5
1	C	412	PHE	5.5
1	B	444	GLN	5.5
1	C	289	LEU	5.4
1	D	375	VAL	5.4
1	B	272	LEU	5.4
1	A	438	ASP	5.4
1	C	362	ILE	5.4
1	C	198	LEU	5.3
1	D	299	TRP	5.3
1	A	441	ARG	5.3
1	B	362	ILE	5.3
1	D	267	LEU	5.3
1	B	361	ASN	5.3
1	D	131	VAL	5.3
1	D	122	ILE	5.3
1	B	375	VAL	5.3
1	A	444	GLN	5.2
1	B	410	MET	5.1
1	A	436	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	165	PRO	5.1
1	D	373	THR	5.1
1	B	98	HIS	5.1
1	D	175	ARG	5.1
1	A	362	ILE	5.0
1	D	255	ILE	5.0
1	C	422	PHE	5.0
1	C	37	VAL	5.0
1	C	314	PHE	5.0
1	B	438	ASP	5.0
1	B	166	PHE	5.0
1	A	234	SER	5.0
1	A	171	GLY	5.0
1	D	142	GLU	4.9
1	C	258	PHE	4.9
1	C	9	LEU	4.9
1	D	158	VAL	4.9
1	C	59	ASP	4.9
1	D	124	ASP	4.8
1	D	372	GLN	4.8
1	B	164	LEU	4.8
1	C	72	ARG	4.8
1	A	139	ARG	4.8
1	D	132	PRO	4.7
1	C	324	ALA	4.7
1	B	55	ASP	4.7
1	D	125	ILE	4.7
1	A	296	ARG	4.7
1	D	75	LYS	4.6
1	A	437	GLY	4.6
1	D	144	LEU	4.6
1	D	58	ASN	4.6
1	B	29	LEU	4.6
1	D	69	THR	4.6
1	D	257	TYR	4.6
1	D	266	ASP	4.6
1	C	164	LEU	4.6
1	A	99	LEU	4.5
1	A	435	LEU	4.5
1	D	200	ASN	4.5
1	C	128	TRP	4.5
1	B	337	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	417	LEU	4.5
1	D	370	SER	4.5
1	C	139	ARG	4.5
1	B	69	THR	4.5
1	C	125	ILE	4.4
1	A	355	TYR	4.4
1	D	340	LEU	4.4
1	C	71	SER	4.4
1	B	372	GLN	4.4
1	D	8	LYS	4.4
1	B	445	ILE	4.3
1	D	254	ALA	4.3
1	A	319	ALA	4.3
1	A	143	GLN	4.3
1	B	126	PRO	4.3
1	B	405	GLN	4.3
1	D	160	ALA	4.3
1	D	17	GLY	4.3
1	B	25	VAL	4.3
1	B	359	LYS	4.2
1	D	331	GLY	4.2
1	B	66	VAL	4.2
1	B	75	LYS	4.2
1	C	316	MET	4.2
1	C	317	ALA	4.2
1	A	369	TYR	4.2
1	A	286	PHE	4.1
1	B	134	ILE	4.1
1	C	172	GLY	4.1
1	A	222	THR	4.1
1	D	65	ILE	4.1
1	C	124	ASP	4.1
1	D	413	ILE	4.1
1	B	62	MET	4.1
1	D	127	PHE	4.1
1	A	96	SER	4.1
1	C	387	ILE	4.1
1	D	21	ALA	4.1
1	B	147	PHE	4.0
1	D	258	PHE	4.0
1	D	126	PRO	4.0
1	B	376	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	258	PHE	4.0
1	B	356	GLY	4.0
1	D	358	PHE	4.0
1	C	201	VAL	4.0
1	C	352	THR	4.0
1	D	360	LEU	3.9
1	A	210	GLY	3.9
1	C	405	GLN	3.9
1	D	129	SER	3.9
1	B	353	VAL	3.9
1	B	271	TYR	3.9
1	B	355	TYR	3.9
1	A	30	MET	3.9
1	D	71	SER	3.9
1	A	272	LEU	3.9
1	C	121	THR	3.8
1	B	336	ILE	3.8
1	B	440	LEU	3.8
1	B	201	VAL	3.8
1	B	130	LEU	3.8
1	A	322	HIS	3.8
1	D	140	GLU	3.8
1	A	164	LEU	3.8
1	A	229	LYS	3.7
1	B	67	ASN	3.7
1	C	4	SER	3.7
1	B	437	GLY	3.7
1	C	255	ILE	3.7
1	B	256	TYR	3.7
1	B	177	PHE	3.7
1	C	100	PHE	3.7
1	A	203	GLU	3.6
1	D	134	ILE	3.6
1	D	162	ILE	3.6
1	B	104	ALA	3.6
1	B	275	ALA	3.6
1	B	397	THR	3.6
1	A	422	PHE	3.6
1	A	175	ARG	3.6
1	D	109	VAL	3.6
1	D	29	LEU	3.6
1	A	103	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	103	THR	3.6
1	D	133	THR	3.6
1	C	175	ARG	3.5
1	B	401	ALA	3.5
1	B	448	LEU	3.5
1	D	123	MET	3.5
1	D	348	MET	3.5
1	B	13	PHE	3.5
1	A	167	VAL	3.5
1	A	317	ALA	3.5
1	A	339	ALA	3.5
1	B	73	TRP	3.5
1	C	344	LEU	3.5
1	C	62	MET	3.5
1	C	389	LEU	3.5
1	A	124	ASP	3.5
1	A	144	LEU	3.4
1	D	355	TYR	3.4
1	D	83	GLY	3.4
1	A	306	PRO	3.4
1	D	164	LEU	3.4
1	A	178	GLY	3.4
1	A	388	ALA	3.4
1	B	435	LEU	3.4
1	C	32	TYR	3.4
1	D	80	ILE	3.4
1	B	433	TYR	3.4
1	A	126	PRO	3.4
1	B	79	TRP	3.3
1	B	200	ASN	3.3
1	B	145	VAL	3.3
1	D	68	ALA	3.3
1	B	105	GLN	3.3
1	A	431	ARG	3.3
1	D	15	ALA	3.3
1	A	59	ASP	3.3
1	D	9	LEU	3.3
1	A	345	GLN	3.3
1	B	368	ALA	3.3
1	C	315	ALA	3.3
1	C	171	GLY	3.3
1	B	403	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	345	GLN	3.2
1	C	7	THR	3.2
1	C	357	GLU	3.2
1	A	141	ARG	3.2
1	B	35	ASP	3.2
1	D	135	THR	3.2
1	B	58	ASN	3.2
1	D	396	TYR	3.2
1	A	353	VAL	3.2
1	A	163	THR	3.2
1	C	374	MET	3.2
1	D	428	LEU	3.2
1	A	36	VAL	3.2
1	B	48	PHE	3.2
1	A	401	ALA	3.2
1	D	59	ASP	3.1
1	A	448	LEU	3.1
1	B	136	LEU	3.1
1	C	179	PHE	3.1
1	A	350	ALA	3.1
1	D	418	PRO	3.1
1	B	135	THR	3.1
1	C	207	SER	3.1
1	D	165	PRO	3.1
1	A	411	GLN	3.1
1	D	233	LEU	3.1
1	A	166	PHE	3.1
1	D	18	LYS	3.1
1	B	32	TYR	3.1
1	A	179	PHE	3.1
1	B	92	PHE	3.0
1	B	140	GLU	3.0
1	B	266	ASP	3.0
1	B	49	LEU	3.0
1	C	65	ILE	3.0
1	C	144	LEU	3.0
1	B	97	ALA	3.0
1	B	238	GLY	3.0
1	D	161	GLY	3.0
1	A	170	VAL	3.0
1	C	66	VAL	3.0
1	B	121	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	128	TRP	3.0
1	A	330	ALA	3.0
1	D	156	GLY	3.0
1	B	37	VAL	3.0
1	D	204	VAL	3.0
1	A	121	THR	3.0
1	D	22	ILE	3.0
1	D	359	LYS	2.9
1	C	369	TYR	2.9
1	D	238	GLY	2.9
1	A	21	ALA	2.9
1	B	260	TYR	2.9
1	A	106	VAL	2.9
1	C	372	GLN	2.9
1	A	101	GLU	2.9
1	A	218	LEU	2.9
1	B	27	MET	2.9
1	D	332	ILE	2.9
1	B	447	LEU	2.9
1	B	449	ASP	2.9
1	C	365	GLU	2.9
1	D	342	TRP	2.9
1	C	204	VAL	2.9
1	B	17	GLY	2.9
1	D	74	GLY	2.9
1	C	143	GLN	2.9
1	B	188	ALA	2.9
1	D	32	TYR	2.9
1	B	24	ILE	2.9
1	C	411	GLN	2.8
1	B	338	THR	2.8
1	A	430	PHE	2.8
1	B	169	TYR	2.8
1	B	280	LEU	2.8
1	C	166	PHE	2.8
1	D	63	GLY	2.8
1	B	400	VAL	2.8
1	A	314	PHE	2.8
1	B	441	ARG	2.8
1	B	128	TRP	2.8
1	A	256	TYR	2.8
1	D	265	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	328	VAL	2.8
1	B	357	GLU	2.8
1	C	313	LEU	2.8
1	D	159	THR	2.8
1	B	421	PHE	2.8
1	A	373	THR	2.8
1	D	116	TRP	2.7
1	A	5	MET	2.7
1	A	127	PHE	2.7
1	B	161	GLY	2.7
1	C	409	GLY	2.7
1	B	264	ASP	2.7
1	A	257	TYR	2.7
1	A	368	ALA	2.7
1	A	151	PHE	2.7
1	A	327	ILE	2.7
1	A	107	VAL	2.7
1	A	328	VAL	2.7
1	C	167	VAL	2.7
1	D	190	PHE	2.7
1	C	8	LYS	2.7
1	D	7	THR	2.7
1	C	97	ALA	2.7
1	A	41	VAL	2.7
1	A	318	LEU	2.7
1	C	187	ILE	2.7
1	D	191	ILE	2.7
1	A	168	SER	2.7
1	B	99	LEU	2.7
1	C	142	GLU	2.6
1	A	338	THR	2.6
1	A	407	LEU	2.6
1	B	204	VAL	2.6
1	A	191	ILE	2.6
1	C	327	ILE	2.6
1	B	50	VAL	2.6
1	B	344	LEU	2.6
1	C	98	HIS	2.6
1	C	165	PRO	2.6
1	B	320	ASP	2.6
1	D	19	ASP	2.6
1	D	337	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	272	LEU	2.6
1	D	397	THR	2.6
1	B	59	ASP	2.6
1	C	373	THR	2.6
1	B	18	LYS	2.6
1	B	179	PHE	2.6
1	B	102	GLY	2.6
1	B	142	GLU	2.6
1	C	36	VAL	2.6
1	C	126	PRO	2.5
1	B	71	SER	2.5
1	D	344	LEU	2.5
1	A	346	VAL	2.5
1	D	11	TYR	2.5
1	B	262	ILE	2.5
1	C	79	TRP	2.5
1	D	30	MET	2.5
1	A	102	GLY	2.5
1	C	141	ARG	2.5
1	C	161	GLY	2.5
1	C	221	LYS	2.5
1	C	96	SER	2.5
1	B	187	ILE	2.5
1	C	253	PHE	2.5
1	B	360	LEU	2.5
1	C	241	LEU	2.5
1	D	271	TYR	2.5
1	D	272	LEU	2.5
1	A	111	VAL	2.5
1	B	290	VAL	2.5
1	B	413	ILE	2.5
1	D	336	ILE	2.5
1	B	34	THR	2.5
1	C	73	TRP	2.5
1	D	85	LEU	2.5
1	B	176	GLY	2.5
1	C	416	VAL	2.5
1	A	329	ALA	2.4
1	D	128	TRP	2.4
1	B	241	LEU	2.4
1	A	202	HIS	2.4
1	C	339	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	80	ILE	2.4
1	C	122	ILE	2.4
1	A	233	LEU	2.4
1	B	125	ILE	2.4
1	C	275	ALA	2.4
1	A	47	LEU	2.4
1	B	85	LEU	2.4
1	C	391	LEU	2.4
1	C	6	THR	2.4
1	A	349	VAL	2.4
1	C	131	VAL	2.4
1	B	14	GLY	2.4
1	B	429	TYR	2.4
1	A	97	ALA	2.4
1	D	339	ALA	2.4
1	B	8	LYS	2.4
1	A	37	VAL	2.4
1	B	158	VAL	2.4
1	C	55	ASP	2.4
1	B	295	ARG	2.4
1	C	286	PHE	2.4
1	A	313	LEU	2.4
1	A	142	GLU	2.4
1	C	194	THR	2.3
1	C	58	ASN	2.3
1	B	120	TYR	2.3
1	C	169	TYR	2.3
1	C	228	TYR	2.3
1	B	313	LEU	2.3
1	A	201	VAL	2.3
1	D	371	VAL	2.3
1	D	168	SER	2.3
1	D	34	THR	2.3
1	C	254	ALA	2.3
1	D	62	MET	2.3
1	A	4	SER	2.3
1	B	267	LEU	2.3
1	D	268	PHE	2.3
1	D	145	VAL	2.3
1	B	148	PRO	2.3
1	A	206	SER	2.3
1	D	10	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	226	LEU	2.3
1	D	430	PHE	2.3
1	A	232	GLN	2.3
1	B	442	LYS	2.3
1	A	343	VAL	2.3
1	B	196	VAL	2.3
1	D	90	VAL	2.3
1	B	269	PRO	2.3
1	D	246	ALA	2.3
1	A	93	LEU	2.3
1	B	103	THR	2.3
1	B	163	THR	2.3
1	D	121	THR	2.3
1	A	177	PHE	2.3
1	D	189	PHE	2.3
1	C	138	LYS	2.3
1	C	335	ASN	2.3
1	A	405	GLN	2.3
1	A	321	ILE	2.2
1	D	187	ILE	2.2
1	A	104	ALA	2.2
1	B	339	ALA	2.2
1	A	147	PHE	2.2
1	B	159	THR	2.2
1	B	197	THR	2.2
1	C	120	TYR	2.2
1	D	167	VAL	2.2
1	A	165	PRO	2.2
1	B	398	PRO	2.2
1	A	389	LEU	2.2
1	A	54	TRP	2.2
1	B	54	TRP	2.2
1	B	64	TRP	2.2
1	B	342	TRP	2.2
1	B	190	PHE	2.2
1	A	228	TYR	2.2
1	C	19	ASP	2.2
1	D	176	GLY	2.2
1	D	199	ARG	2.2
1	C	311	ALA	2.2
1	B	6	THR	2.2
1	C	406	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	6	THR	2.2
1	D	86	THR	2.2
1	B	443	ILE	2.2
1	C	366	SER	2.2
1	D	57	ILE	2.2
1	D	303	SER	2.2
1	B	414	MET	2.2
1	A	18	LYS	2.2
1	A	255	ILE	2.1
1	B	239	MET	2.1
1	B	427	VAL	2.1
1	B	167	VAL	2.1
1	B	236	LEU	2.1
1	C	176	GLY	2.1
1	C	400	VAL	2.1
1	C	342	TRP	2.1
1	A	125	ILE	2.1
1	A	420	LEU	2.1
1	C	105	GLN	2.1
1	C	408	GLN	2.1
1	D	43	LEU	2.1
1	D	250	ILE	2.1
1	C	243	TYR	2.1
1	A	92	PHE	2.1
1	A	386	PHE	2.1
1	C	146	PRO	2.1
1	B	335	ASN	2.0
1	D	239	MET	2.0
1	B	155	ALA	2.0
1	D	84	THR	2.0
1	D	188	ALA	2.0
1	A	180	GLN	2.0
1	C	225	GLY	2.0
1	D	269	PRO	2.0
1	D	286	PHE	2.0
1	B	138	LYS	2.0
1	A	61	ILE	2.0
1	B	191	ILE	2.0
1	C	53	ILE	2.0
1	B	5	MET	2.0
1	A	197	THR	2.0
1	B	7	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	155	ALA	2.0
1	B	23	GLY	2.0
1	B	377	LYS	2.0
1	A	285	VAL	2.0
1	B	9	LEU	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.