



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:59 PM UTC

PDB ID : 1MDA / pdb_00001mda
Title : CRYSTAL STRUCTURE OF AN ELECTRON-TRANSFER COMPLEX BETWEEN METHYLAMINE DEHYDROGENASE AND AMICYANIN
Authors : Chen, L.; Durley, R.; Mathews, F.S.
Deposited on : 1992-03-02
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

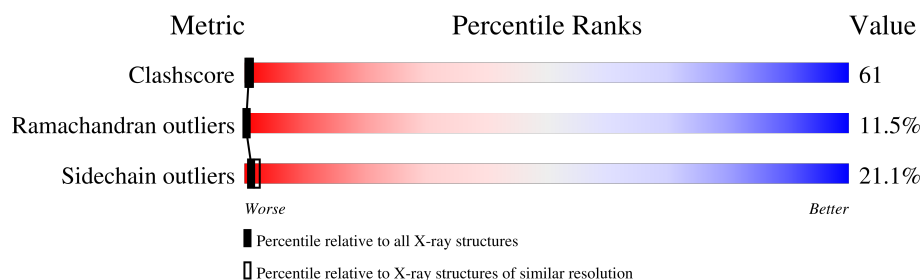
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	368	36% 41% 18% 5%
1	J	368	39% 39% 17% 6%
2	L	121	40% 40% 15% 5%
2	M	121	28% 52% 14% 6%
3	A	103	8% 35% 38% 19%
3	B	103	15% 32% 32% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRQ	M	57	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8567 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 METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	368	Total	C	N	O	S	0	0	0
			2582	1585	451	532	14			
1	J	368	Total	C	N	O	S	0	0	0
			2583	1585	451	533	14			

- Molecule 2 is a protein called METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	121	Total	C	N	O	S	0	0	0
			910	558	155	184	13			
2	M	121	Total	C	N	O	S	0	0	0
			910	558	155	184	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	TRQ	TRP	conflict	UNP A44544
M	57	TRQ	TRP	conflict	UNP A44544

- Molecule 3 is a protein called AMICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	103	Total	C	N	O	S	0	0	0
			790	506	130	148	6			
3	B	103	Total	C	N	O	S	0	0	0
			790	506	130	148	6			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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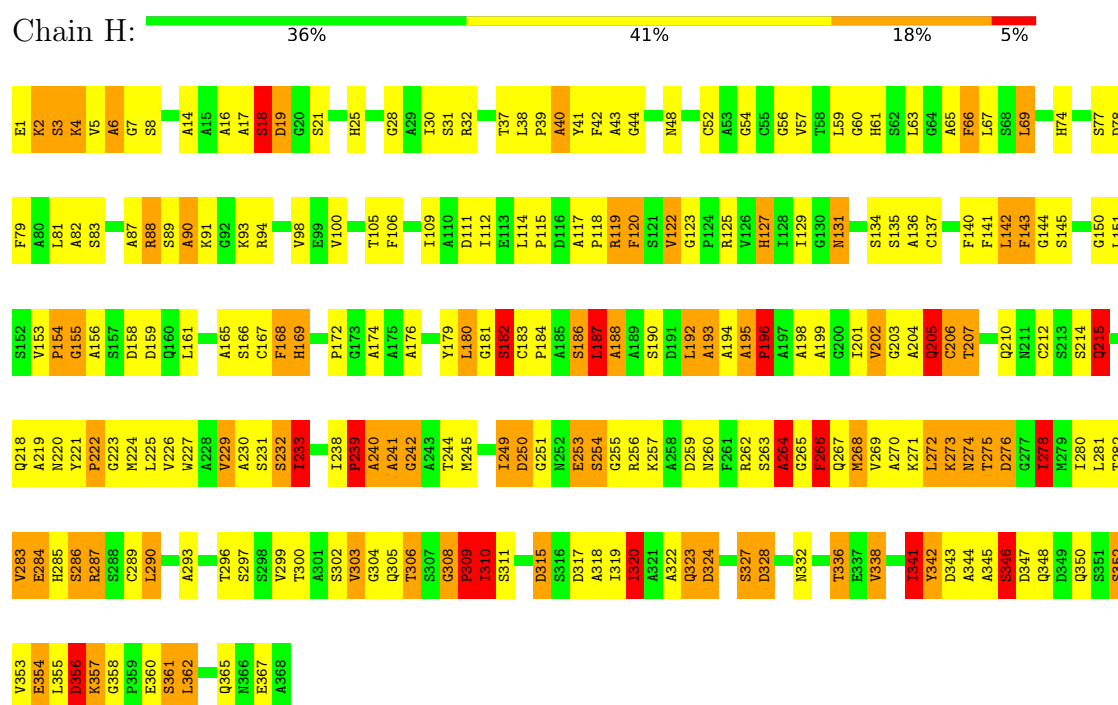
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cu	0	0
			1	1		

3 Residue-property plots

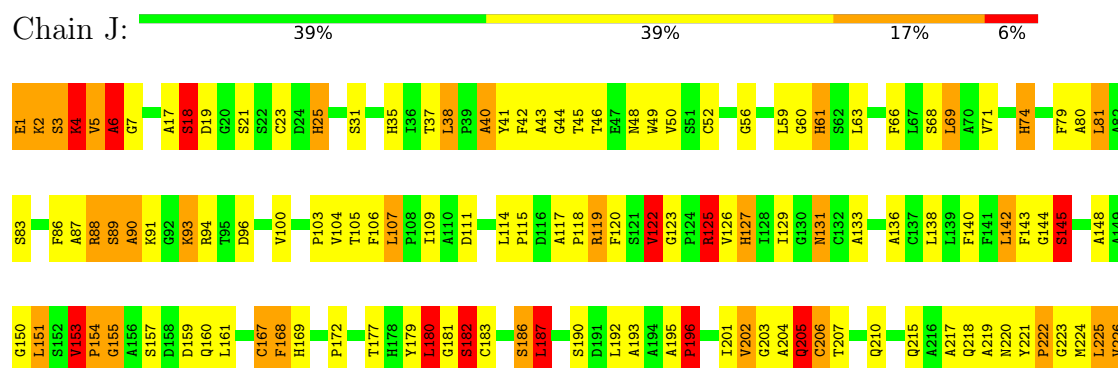
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

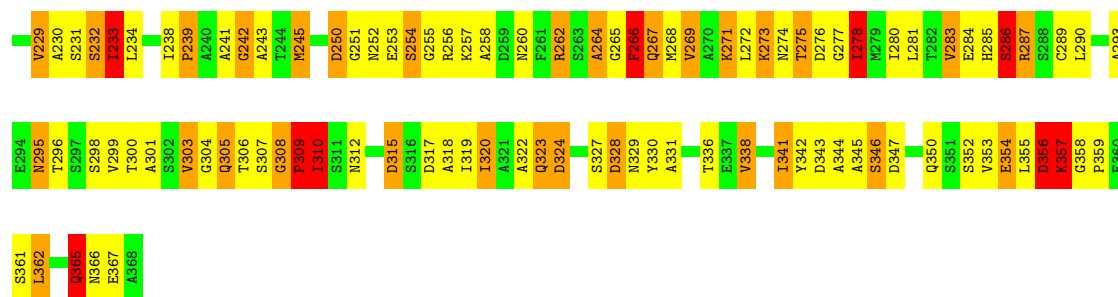
Note EDS was not executed.

• Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)



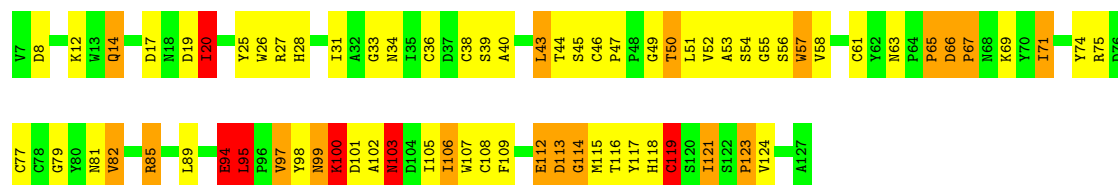
• Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)





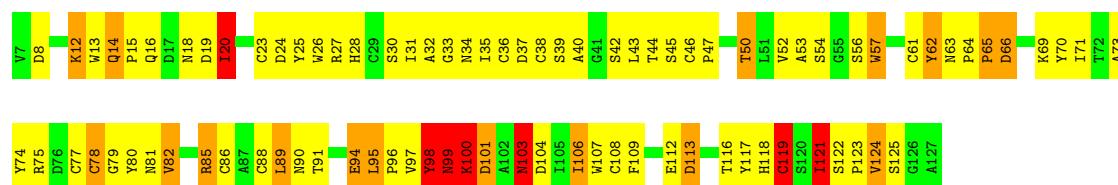
• Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain L: 40% 40% 15% 5%



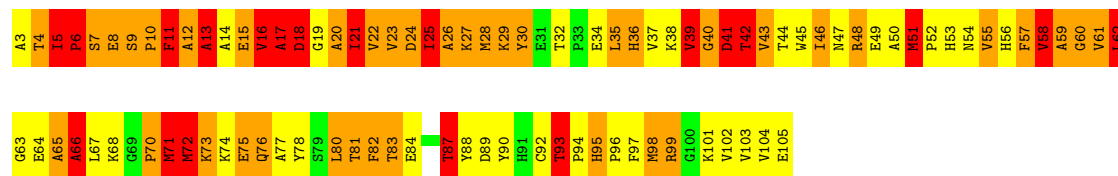
• Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain M: 28% 52% 14% 6%



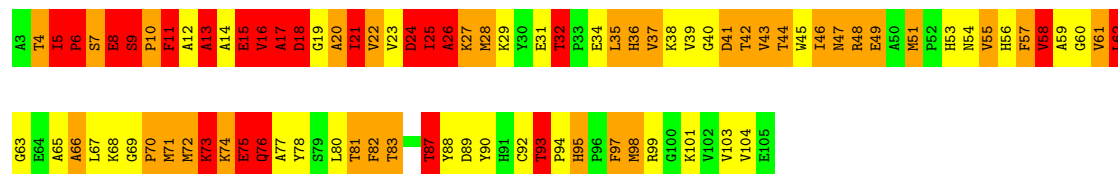
• Molecule 3: AMICYANIN

Chain A: 8% 35% 38% 19%



• Molecule 3: AMICYANIN

Chain B: 15% 32% 32% 21%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.70Å 124.70Å 247.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, TNT	Depositor
R, R_{free}	0.285 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8567	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRQ, CU

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	H	1.09	3/2629 (0.1%)	2.15	128/3577 (3.6%)
1	J	1.05	0/2630	2.02	101/3577 (2.8%)
2	L	1.03	0/917	1.92	29/1250 (2.3%)
2	M	0.98	0/917	1.91	33/1250 (2.6%)
3	A	1.33	3/811 (0.4%)	2.39	47/1102 (4.3%)
3	B	1.38	4/811 (0.5%)	2.47	56/1102 (5.1%)
All	All	1.12	10/8715 (0.1%)	2.12	394/11858 (3.3%)

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	H	3	0
1	J	1	1
2	M	1	1
3	B	0	1
All	All	5	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	21	ILE	C-N	-8.52	1.28	1.33
3	A	41	ASP	C-O	-7.98	1.16	1.24
1	H	240	ALA	CA-C	-7.47	1.43	1.52
1	H	241	ALA	N-CA	-6.98	1.37	1.46
1	H	239	PRO	C-N	-5.95	1.26	1.33
3	B	26	ALA	CA-C	-5.58	1.45	1.52
3	B	8	GLU	CA-C	-5.53	1.48	1.53
3	A	18	ASP	N-CA	-5.30	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	41	ASP	CA-C	-5.26	1.46	1.53
3	B	17	ALA	N-CA	-5.11	1.39	1.46

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5	ILE	C-N-CD	-19.12	78.54	120.60
3	B	5	ILE	C-N-CD	-18.21	80.53	120.60
1	H	61	HIS	CA-CB-CG	14.03	127.83	113.80
1	J	61	HIS	CA-CB-CG	13.21	127.01	113.80
1	H	240	ALA	N-CA-CB	-13.08	90.45	109.94
3	B	10	PRO	N-CA-C	12.51	130.53	110.40
1	J	232	SER	N-CA-C	12.16	127.26	109.14
2	L	94	GLU	N-CA-C	11.98	124.34	111.28
3	A	11	PHE	CB-CA-C	-11.75	94.91	111.95
1	H	347	ASP	CA-CB-CG	11.23	123.83	112.60
1	H	320	ILE	N-CA-CB	10.95	129.29	111.23
1	H	232	SER	N-CA-C	10.75	126.18	109.52
3	B	10	PRO	N-CA-CB	10.73	116.06	102.86
1	H	6	ALA	N-CA-C	-10.73	94.72	110.06
1	H	308	GLY	CA-C-N	10.70	133.22	119.84
1	H	308	GLY	C-N-CA	10.70	133.22	119.84
3	B	21	ILE	CA-C-N	-10.59	111.38	121.97
3	B	21	ILE	C-N-CA	-10.59	111.38	121.97
2	M	94	GLU	N-CA-C	10.30	123.80	111.33
3	B	10	PRO	CA-N-CD	-10.18	97.75	112.00
3	B	11	PHE	CB-CA-C	-10.17	96.25	111.70
3	A	49	GLU	N-CA-C	9.86	123.86	110.55
1	J	183	CYS	CB-CA-C	-9.86	96.86	110.37
1	H	65	ALA	N-CA-C	9.62	117.99	108.75
1	J	182	SER	N-CA-CB	9.54	126.61	110.49
1	H	4	LYS	N-CA-CB	-9.44	96.52	110.49
1	H	182	SER	N-CA-CB	9.31	126.22	110.49
1	H	74	HIS	CA-CB-CG	-9.29	104.50	113.80
1	H	238	ILE	N-CA-C	9.24	118.12	107.77
1	J	3	SER	CA-C-N	9.22	136.38	121.99
1	J	3	SER	C-N-CA	9.22	136.38	121.99
1	H	303	VAL	N-CA-CB	-9.17	100.55	111.83
1	J	287	ARG	N-CA-C	-9.12	99.43	113.02
2	M	119	CYS	N-CA-CB	-9.12	97.70	111.56
1	H	4	LYS	N-CA-C	-9.10	101.70	113.17
1	H	18	SER	N-CA-C	8.94	129.84	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	220	ASN	CA-CB-CG	8.89	121.49	112.60
1	J	4	LYS	N-CA-C	-8.87	99.87	113.89
1	J	310	ILE	N-CA-C	8.85	127.75	109.34
1	J	233	ILE	N-CA-C	8.85	127.74	109.34
1	H	155	GLY	N-CA-C	-8.84	92.23	113.18
3	A	80	LEU	N-CA-CB	8.78	125.57	110.81
1	H	3	SER	CA-C-N	8.78	137.02	122.54
1	H	3	SER	C-N-CA	8.78	137.02	122.54
1	H	119	ARG	N-CA-C	8.72	125.76	111.37
1	J	167	CYS	N-CA-CB	-8.72	96.13	111.39
1	H	233	ILE	N-CA-C	8.67	127.37	109.34
1	J	168	PHE	N-CA-C	8.61	124.16	111.34
1	J	119	ARG	N-CA-C	8.58	125.52	111.37
1	J	155	GLY	N-CA-C	-8.57	92.86	113.18
1	J	320	ILE	N-CA-CB	8.57	125.37	111.23
3	B	11	PHE	N-CA-C	8.57	123.28	107.60
2	L	103	ASN	N-CA-C	8.55	123.44	112.92
1	J	180	LEU	N-CA-C	-8.52	96.84	109.62
3	A	41	ASP	CA-C-O	-8.50	111.88	120.80
3	A	24	ASP	N-CA-CB	-8.49	96.14	110.49
1	J	18	SER	N-CA-C	8.45	128.80	110.80
1	H	78	ASP	CA-CB-CG	8.30	120.90	112.60
1	J	354	GLU	N-CA-C	8.29	122.58	111.30
1	H	156	ALA	N-CA-C	8.29	123.41	111.56
1	H	310	ILE	N-CA-C	8.29	126.58	109.34
1	J	6	ALA	CA-C-N	8.22	137.53	121.41
1	J	6	ALA	C-N-CA	8.22	137.53	121.41
1	J	127	HIS	CA-CB-CG	-8.22	105.58	113.80
1	H	220	ASN	CA-CB-CG	8.17	120.77	112.60
2	M	99	ASN	N-CA-C	8.16	128.18	110.80
2	L	99	ASN	N-CA-C	8.11	128.07	110.80
2	L	98	TYR	CA-C-N	8.10	137.01	121.54
2	L	98	TYR	C-N-CA	8.10	137.01	121.54
1	J	153	VAL	N-CA-C	8.08	116.25	107.60
1	H	239	PRO	CA-C-N	8.06	131.42	120.54
1	H	239	PRO	C-N-CA	8.06	131.42	120.54
1	J	61	HIS	N-CA-CB	-8.05	99.08	111.56
1	J	25	HIS	CA-CB-CG	8.05	121.85	113.80
1	J	74	HIS	CA-CB-CG	-7.99	105.81	113.80
3	A	13	ALA	N-CA-C	-7.98	93.81	110.80
3	B	13	ALA	N-CA-C	-7.95	93.87	110.80
1	H	168	PHE	CA-CB-CG	-7.93	105.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	8	GLU	CA-C-O	-7.91	112.00	120.71
1	H	240	ALA	O-C-N	7.89	130.30	122.09
3	A	6	PRO	N-CA-CB	7.84	111.23	102.60
3	B	58	VAL	N-CA-CB	7.82	124.13	111.23
3	A	21	ILE	CA-C-N	-7.80	107.94	121.97
3	A	21	ILE	C-N-CA	-7.80	107.94	121.97
3	B	13	ALA	CA-C-N	-7.73	107.32	120.23
3	B	13	ALA	C-N-CA	-7.73	107.32	120.23
1	H	287	ARG	N-CA-CB	7.72	125.94	111.43
1	J	193	ALA	N-CA-C	7.70	120.52	110.43
3	A	11	PHE	CA-CB-CG	7.70	121.50	113.80
1	H	25	HIS	CA-CB-CG	7.69	121.49	113.80
2	L	99	ASN	CA-C-N	7.67	136.19	121.54
2	L	99	ASN	C-N-CA	7.67	136.19	121.54
1	J	308	GLY	CA-C-N	7.67	129.42	119.84
1	J	308	GLY	C-N-CA	7.67	129.42	119.84
2	L	119	CYS	N-CA-CB	-7.66	98.88	111.66
3	B	49	GLU	N-CA-C	7.65	121.84	110.52
3	A	13	ALA	CA-C-N	-7.62	106.98	121.54
3	A	13	ALA	C-N-CA	-7.62	106.98	121.54
3	B	55	VAL	CB-CA-C	7.61	119.09	110.41
1	H	239	PRO	N-CA-CB	7.58	111.21	103.25
3	A	23	VAL	N-CA-C	-7.53	97.88	109.78
3	A	71	MET	N-CA-CB	-7.53	98.25	111.49
2	L	101	ASP	N-CA-C	-7.52	103.22	113.30
1	J	347	ASP	CA-CB-CG	7.48	120.08	112.60
3	B	87	THR	CB-CA-C	7.48	122.46	110.19
3	B	16	VAL	CA-CB-CG1	7.48	123.11	110.40
1	H	332	ASN	CA-CB-CG	7.45	120.05	112.60
1	J	309	PRO	CA-C-N	7.45	135.37	121.97
1	J	309	PRO	C-N-CA	7.45	135.37	121.97
3	B	32	THR	CA-C-N	7.43	129.13	119.84
3	B	32	THR	C-N-CA	7.43	129.13	119.84
1	J	154	PRO	CA-C-N	7.42	135.96	121.41
1	J	154	PRO	C-N-CA	7.42	135.96	121.41
2	M	99	ASN	CA-C-N	7.42	135.71	121.54
2	M	99	ASN	C-N-CA	7.42	135.71	121.54
3	A	16	VAL	CA-CB-CG1	7.39	122.96	110.40
3	B	6	PRO	N-CA-CB	7.36	110.70	102.60
1	J	17	ALA	N-CA-C	7.36	120.92	109.07
2	L	100	LYS	N-CA-C	7.36	126.47	110.80
2	L	101	ASP	CA-C-N	7.31	132.89	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	101	ASP	C-N-CA	7.31	132.89	121.99
1	H	193	ALA	N-CA-C	7.29	119.74	110.33
3	B	58	VAL	CB-CA-C	7.29	123.24	111.29
1	H	131	ASN	CA-CB-CG	7.28	119.88	112.60
1	H	232	SER	CA-C-N	7.26	135.03	121.97
1	H	232	SER	C-N-CA	7.26	135.03	121.97
1	J	346	SER	N-CA-C	7.24	126.23	110.80
3	B	9	SER	C-N-CD	-7.22	95.41	125.00
2	M	20	ILE	N-CA-CB	7.21	123.13	111.23
3	B	8	GLU	N-CA-C	7.19	124.52	110.56
1	J	3	SER	N-CA-C	-7.18	95.50	110.80
3	A	10	PRO	N-CA-CB	7.16	110.77	103.25
1	H	168	PHE	N-CA-C	7.15	126.03	110.80
1	H	240	ALA	CA-C-O	7.13	128.53	120.90
1	H	215	GLN	CB-CA-C	-7.12	100.95	111.77
1	H	273	LYS	N-CA-C	7.08	119.08	111.36
3	A	82	PHE	N-CA-C	7.05	120.16	109.23
2	M	98	TYR	CA-C-N	7.05	135.00	121.54
2	M	98	TYR	C-N-CA	7.05	135.00	121.54
1	J	356	ASP	N-CA-C	7.04	125.79	110.80
2	M	103	ASN	N-CA-C	7.02	121.93	112.88
2	M	101	ASP	N-CA-C	-6.99	103.93	113.30
3	A	28	MET	CA-C-O	-6.99	114.17	122.27
1	H	48	ASN	CA-CB-CG	6.98	119.58	112.60
3	B	11	PHE	CA-CB-CG	6.96	120.76	113.80
1	J	25	HIS	N-CA-CB	6.95	123.58	111.00
1	H	287	ARG	N-CA-C	-6.93	102.25	113.19
1	H	354	GLU	N-CA-C	6.90	120.93	111.54
1	H	127	HIS	CA-CB-CG	-6.88	106.92	113.80
1	H	81	LEU	N-CA-CB	-6.87	98.69	111.13
2	M	99	ASN	CA-CB-CG	-6.87	105.73	112.60
1	H	25	HIS	N-CA-CB	6.84	123.83	111.37
3	A	65	ALA	CB-CA-C	-6.83	108.68	116.54
1	H	266	PHE	N-CA-CB	6.83	122.03	110.49
1	J	275	THR	N-CA-CB	6.83	121.88	110.14
1	H	77	SER	N-CA-C	6.82	120.82	112.23
3	A	11	PHE	N-CA-C	6.79	122.00	107.67
2	M	112	GLU	N-CA-C	-6.76	105.56	113.88
1	J	6	ALA	N-CA-C	-6.76	96.40	110.80
1	H	309	PRO	CA-C-N	6.75	134.12	121.97
1	H	309	PRO	C-N-CA	6.75	134.12	121.97
3	A	11	PHE	N-CA-CB	-6.75	100.65	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	19	ASP	N-CA-CB	6.73	121.87	110.49
3	B	25	ILE	N-CA-CB	-6.72	100.14	111.23
3	A	14	ALA	CA-C-N	-6.70	113.48	122.72
3	A	14	ALA	C-N-CA	-6.70	113.48	122.72
1	H	196	PRO	N-CA-C	6.69	126.26	112.47
2	L	94	GLU	N-CA-CB	6.69	119.95	110.12
3	B	11	PHE	N-CA-CB	-6.65	100.50	112.27
2	M	100	LYS	N-CA-C	6.65	124.97	110.80
1	H	240	ALA	CB-CA-C	-6.64	100.18	110.81
1	H	154	PRO	N-CA-CB	6.63	110.21	103.25
3	B	82	PHE	N-CA-C	6.62	120.31	109.06
3	A	10	PRO	N-CA-C	6.57	126.01	112.47
3	B	93	THR	N-CA-C	6.57	121.79	113.25
2	M	66	ASP	CA-CB-CG	6.57	119.17	112.60
1	H	180	LEU	CA-C-N	6.57	130.33	121.01
1	H	180	LEU	C-N-CA	6.57	130.33	121.01
1	H	40	ALA	N-CA-C	6.54	120.61	112.24
1	H	187	LEU	N-CA-C	6.53	124.72	110.80
3	A	71	MET	CA-C-O	-6.52	114.15	121.25
1	H	201	ILE	N-CA-C	6.51	117.95	108.58
2	L	123	PRO	CB-CA-C	-6.50	102.56	111.21
1	H	347	ASP	N-CA-C	6.50	119.66	110.23
1	J	315	ASP	CA-CB-CG	6.50	119.09	112.60
2	L	119	CYS	CA-CB-SG	-6.49	99.48	114.40
1	J	329	ASN	CA-CB-CG	6.48	119.08	112.60
1	H	336	THR	CB-CA-C	6.45	120.86	110.09
1	J	125	ARG	CD-NE-CZ	-6.43	115.40	124.40
2	M	94	GLU	N-CA-CB	6.43	119.70	110.06
3	B	48	ARG	CB-CA-C	6.42	120.34	109.55
1	J	183	CYS	N-CA-C	-6.41	100.76	108.14
1	H	346	SER	N-CA-C	6.40	124.44	110.80
3	B	42	THR	CA-C-O	-6.38	114.28	121.81
2	L	102	ALA	N-CA-C	6.38	118.55	108.67
1	J	48	ASN	CA-CB-CG	6.35	118.95	112.60
3	A	17	ALA	N-CA-C	-6.35	97.28	110.80
3	B	68	LYS	N-CA-CB	6.34	120.50	110.23
1	J	365	GLN	N-CA-CB	6.34	120.50	110.23
1	H	174	ALA	N-CA-CB	-6.27	101.33	111.24
2	M	99	ASN	O-C-N	6.27	130.93	122.59
3	A	48	ARG	N-CA-C	-6.27	105.67	113.38
1	J	88	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	J	250	ASP	CA-CB-CG	6.25	118.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	101	ASP	O-C-N	6.24	129.79	122.24
3	B	8	GLU	O-C-N	6.22	129.09	122.38
1	H	180	LEU	N-CA-C	-6.21	101.07	110.70
1	H	324	ASP	N-CA-C	6.21	118.90	109.95
1	H	238	ILE	CB-CA-C	6.21	117.92	110.78
1	J	18	SER	N-CA-CB	-6.18	100.04	110.49
3	B	98	MET	N-CA-C	-6.16	100.53	109.59
1	H	183	CYS	CB-CA-C	-6.16	98.04	110.17
1	J	168	PHE	CA-CB-CG	-6.16	107.64	113.80
1	J	157	SER	N-CA-C	6.15	118.51	108.55
1	H	268	MET	N-CA-C	6.15	118.06	111.36
2	M	66	ASP	N-CA-C	-6.14	101.91	109.65
3	A	58	VAL	N-CA-CB	6.13	121.35	111.23
1	J	25	HIS	N-CA-C	6.12	119.47	109.24
1	H	341	ILE	CB-CA-C	6.10	119.13	110.84
1	J	327	SER	N-CA-C	6.09	119.83	110.20
1	H	194	ALA	CB-CA-C	-6.09	109.54	116.54
1	J	123	GLY	N-CA-C	-6.08	99.94	112.34
1	H	355	LEU	N-CA-C	-6.08	104.46	112.72
3	A	8	GLU	N-CA-C	6.06	123.72	110.80
2	M	119	CYS	N-CA-C	6.06	117.75	108.42
1	J	133	ALA	N-CA-C	6.05	119.50	111.75
3	B	26	ALA	O-C-N	6.04	130.63	122.59
3	B	8	GLU	N-CA-CB	6.04	119.69	110.39
2	L	98	TYR	CB-CA-C	6.04	122.43	110.42
3	A	23	VAL	CA-CB-CG2	-6.03	100.14	110.40
1	H	154	PRO	CA-C-N	6.03	133.23	121.41
1	H	154	PRO	C-N-CA	6.03	133.23	121.41
3	B	76	GLN	O-C-N	-6.03	114.57	122.59
1	H	17	ALA	N-CA-C	6.02	118.54	108.73
3	B	75	GLU	CA-C-O	-5.99	111.94	120.51
1	H	315	ASP	CA-CB-CG	5.97	118.57	112.60
1	J	286	SER	N-CA-CB	-5.97	100.40	110.49
1	J	278	ILE	N-CA-CB	5.94	118.94	111.46
1	H	5	VAL	CA-C-N	5.94	132.29	122.62
1	H	5	VAL	C-N-CA	5.94	132.29	122.62
2	L	66	ASP	N-CA-C	-5.93	100.99	109.24
1	J	6	ALA	O-C-N	5.93	130.48	122.59
1	H	17	ALA	CA-C-N	5.93	132.87	121.54
1	H	17	ALA	C-N-CA	5.93	132.87	121.54
1	J	31	SER	N-CA-C	5.92	117.73	111.28
1	J	232	SER	CA-C-N	5.90	132.60	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	232	SER	C-N-CA	5.90	132.60	121.97
1	J	66	PHE	N-CA-C	5.87	117.61	109.15
1	J	2	LYS	CA-C-N	5.87	132.75	121.54
1	J	2	LYS	C-N-CA	5.87	132.75	121.54
1	J	347	ASP	N-CA-C	5.86	118.31	110.35
1	H	4	LYS	CA-CB-CG	5.84	125.77	114.10
1	J	68	SER	N-CA-C	5.82	118.70	110.50
2	L	112	GLU	N-CA-C	-5.82	106.32	113.41
1	J	114	LEU	CA-C-N	5.81	127.11	119.84
1	J	114	LEU	C-N-CA	5.81	127.11	119.84
1	J	17	ALA	CA-C-N	5.81	132.64	121.54
1	J	17	ALA	C-N-CA	5.81	132.64	121.54
1	H	4	LYS	CB-CA-C	5.81	119.78	110.09
1	H	327	SER	N-CA-C	5.80	119.07	110.48
1	H	328	ASP	CA-CB-CG	5.79	118.39	112.60
1	J	7	GLY	N-CA-C	-5.78	99.49	113.18
3	B	9	SER	N-CA-CB	-5.78	100.09	110.37
1	J	5	VAL	CA-C-O	5.76	127.98	120.78
1	H	272	LEU	N-CA-CB	5.76	119.66	110.16
1	H	367	GLU	N-CA-C	5.75	119.20	109.76
2	L	82	VAL	N-CA-CB	5.74	117.63	110.05
1	J	40	ALA	N-CA-C	5.73	119.33	111.54
3	B	97	PHE	N-CA-C	5.73	118.63	111.24
1	J	81	LEU	CB-CA-C	5.71	119.53	109.89
3	A	72	MET	N-CA-CB	5.71	120.13	110.49
1	H	123	GLY	N-CA-C	-5.70	100.71	112.34
3	B	17	ALA	N-CA-C	-5.70	98.67	110.80
1	J	122	VAL	CB-CA-C	-5.66	103.42	111.40
1	H	182	SER	CB-CA-C	5.65	121.66	110.42
1	J	355	LEU	CA-C-N	5.65	132.33	121.54
1	J	355	LEU	C-N-CA	5.65	132.33	121.54
1	J	182	SER	CB-CA-C	5.65	121.66	110.42
2	M	32	ALA	N-CA-CB	5.63	120.69	110.95
3	A	87	THR	CB-CA-C	5.62	119.48	110.16
3	B	14	ALA	N-CA-C	5.58	121.98	112.99
1	H	346	SER	CA-C-N	5.58	128.63	120.71
1	H	346	SER	C-N-CA	5.58	128.63	120.71
1	J	43	ALA	CA-C-N	5.57	126.27	120.03
1	J	43	ALA	C-N-CA	5.57	126.27	120.03
1	H	61	HIS	CB-CA-C	-5.57	100.25	111.17
2	M	124	VAL	CB-CA-C	5.57	117.24	111.23
3	B	14	ALA	CA-C-N	-5.56	115.32	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	14	ALA	C-N-CA	-5.56	115.32	123.00
1	H	169	HIS	CA-CB-CG	-5.55	108.25	113.80
3	A	16	VAL	CB-CA-C	5.54	120.38	111.29
1	H	195	ALA	CA-C-N	5.53	126.76	119.84
1	H	195	ALA	C-N-CA	5.53	126.76	119.84
1	H	158	ASP	N-CA-CB	5.53	118.10	109.97
2	M	54	SER	N-CA-C	-5.51	105.68	112.90
1	H	8	SER	N-CA-C	-5.49	105.31	112.23
1	H	205	GLN	CB-CG-CD	5.49	121.94	112.60
1	H	355	LEU	CA-C-N	5.49	132.03	121.54
1	H	355	LEU	C-N-CA	5.49	132.03	121.54
2	M	98	TYR	CB-CA-C	5.49	121.34	110.42
1	J	266	PHE	N-CA-CB	5.49	119.76	110.49
2	M	121	ILE	N-CA-CB	-5.48	101.39	111.91
1	H	141	PHE	N-CA-C	5.47	118.55	109.46
1	H	284	GLU	CA-C-N	5.46	131.97	121.54
1	H	284	GLU	C-N-CA	5.46	131.97	121.54
1	H	54	GLY	N-CA-C	-5.46	100.24	113.18
1	H	238	ILE	CA-C-O	5.46	123.18	119.20
3	A	66	ALA	CA-C-O	-5.45	112.72	120.51
3	B	10	PRO	O-C-N	5.43	129.68	122.89
3	B	24	ASP	CA-C-N	5.43	131.74	121.97
3	B	24	ASP	C-N-CA	5.43	131.74	121.97
3	B	71	MET	CB-CA-C	-5.43	101.25	109.99
2	M	36	CYS	CA-CB-SG	-5.42	101.92	114.40
1	J	88	ARG	NE-CZ-NH2	5.42	124.08	119.20
2	L	66	ASP	CA-CB-CG	5.41	118.01	112.60
3	B	41	ASP	CA-CB-CG	5.41	118.01	112.60
1	H	276	ASP	N-CA-C	-5.40	103.96	110.44
1	H	356	ASP	N-CA-C	5.38	122.27	110.80
3	A	32	THR	CA-C-N	5.38	126.56	119.84
3	A	32	THR	C-N-CA	5.38	126.56	119.84
1	H	342	TYR	CB-CA-C	-5.38	98.77	109.79
1	J	274	ASN	CA-CB-CG	5.38	117.97	112.60
2	M	37	ASP	CA-CB-CG	-5.37	107.23	112.60
1	J	74	HIS	N-CA-C	5.36	117.88	111.71
2	M	30	SER	N-CA-C	5.34	116.71	110.41
3	A	64	GLU	N-CA-CB	5.33	119.72	110.07
1	H	350	GLN	CB-CG-CD	5.31	121.63	112.60
3	B	15	GLU	O-C-N	5.31	129.55	123.29
2	L	36	CYS	N-CA-CB	5.30	118.50	110.28
3	B	73	LYS	O-C-N	5.30	128.73	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	79	PHE	N-CA-CB	5.30	120.91	111.69
2	L	119	CYS	N-CA-C	5.30	117.12	109.07
3	B	47	ASN	N-CA-CB	5.30	117.87	109.71
1	H	308	GLY	O-C-N	5.29	127.06	121.77
1	H	172	PRO	N-CA-CB	5.28	107.74	103.36
1	H	6	ALA	CA-C-N	5.27	131.74	121.41
1	H	6	ALA	C-N-CA	5.27	131.74	121.41
3	A	71	MET	O-C-N	5.27	128.52	123.04
3	B	60	GLY	N-CA-C	-5.27	100.69	113.18
3	B	9	SER	CA-C-N	5.26	126.61	120.98
3	B	9	SER	C-N-CA	5.26	126.61	120.98
2	M	98	TYR	N-CA-CB	5.26	119.38	110.49
1	J	155	GLY	CA-C-N	5.25	130.19	122.63
1	J	155	GLY	C-N-CA	5.25	130.19	122.63
3	B	7	SER	N-CA-C	5.25	121.99	110.80
2	M	101	ASP	CA-C-N	5.25	129.00	121.50
2	M	101	ASP	C-N-CA	5.25	129.00	121.50
1	H	83	SER	N-CA-C	5.23	116.93	109.14
2	L	98	TYR	N-CA-CB	5.23	119.33	110.49
1	J	187	LEU	N-CA-C	5.22	121.92	110.80
2	M	62	TYR	N-CA-C	5.21	116.80	108.41
1	H	7	GLY	N-CA-C	-5.20	100.85	113.18
1	J	262	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	A	23	VAL	O-C-N	-5.20	117.27	122.62
1	H	188	ALA	N-CA-C	5.20	117.44	109.07
3	A	66	ALA	N-CA-CB	-5.18	101.73	110.49
1	H	143	PHE	CA-C-N	5.17	125.58	120.31
1	H	143	PHE	C-N-CA	5.17	125.58	120.31
2	L	20	ILE	N-CA-CB	5.17	119.76	111.23
2	M	78	CYS	N-CA-C	5.16	117.39	109.95
1	J	160	GLN	N-CA-CB	-5.16	102.36	111.39
3	B	21	ILE	CA-CB-CG2	-5.16	101.73	110.50
1	H	264	ALA	N-CA-C	5.15	121.77	110.80
1	J	196	PRO	N-CA-C	5.15	123.08	112.47
3	A	93	THR	N-CA-C	5.14	121.17	109.81
3	A	5	ILE	CA-CB-CG2	5.14	119.24	110.50
2	L	67	PRO	N-CA-CB	5.13	105.84	102.25
3	A	49	GLU	N-CA-CB	5.13	118.25	110.45
1	J	366	ASN	CA-CB-CG	5.13	117.73	112.60
1	H	18	SER	N-CA-CB	-5.13	101.82	110.49
1	H	3	SER	CA-C-O	5.12	127.83	120.51
1	J	305	GLN	N-CA-C	5.12	118.28	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	89	SER	N-CA-C	5.11	121.68	110.80
1	H	131	ASN	CB-CA-C	-5.10	101.11	109.53
1	J	328	ASP	CA-CB-CG	5.10	117.70	112.60
2	L	112	GLU	CA-C-O	5.09	125.17	119.41
2	M	27	ARG	N-CA-C	5.09	117.57	111.71
1	H	278	ILE	N-CA-CB	5.09	117.10	110.99
1	J	312	ASN	N-CA-C	5.08	118.74	112.54
1	H	66	PHE	CA-CB-CG	5.08	118.88	113.80
3	A	12	ALA	CB-CA-C	5.07	120.51	110.42
1	J	286	SER	CA-C-N	5.06	130.13	122.08
1	J	286	SER	C-N-CA	5.06	130.13	122.08
1	J	83	SER	N-CA-C	5.05	116.49	108.96
1	H	57	VAL	N-CA-C	5.05	116.23	108.71
2	L	99	ASN	O-C-N	5.04	129.30	122.59
1	J	205	GLN	CB-CG-CD	5.04	121.17	112.60
1	J	324	ASP	N-CA-C	5.04	117.55	110.14
3	A	49	GLU	O-C-N	5.04	128.59	122.85
1	H	361	SER	N-CA-C	5.03	117.68	109.59
3	A	60	GLY	N-CA-C	-5.03	101.27	113.18
1	H	5	VAL	N-CA-CB	5.02	119.52	111.23
2	M	113	ASP	N-CA-CB	5.01	118.95	110.49
1	H	306	THR	N-CA-CB	5.00	118.03	109.87

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	232	SER	CA
1	H	310	ILE	CA
1	H	320	ILE	CA
1	J	232	SER	CA
2	M	94	GLU	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	11	PHE	Mainchain
1	J	180	LEU	Mainchain
2	M	98	TYR	Mainchain

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	H	2582	0	2472	219	0
1	J	2583	0	2472	239	0
2	L	910	0	808	87	0
2	M	910	0	809	110	0
3	A	790	0	774	231	0
3	B	790	0	774	212	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8567	0	8109	1025	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 61.

All (1025) 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)
3:B:6:PRO:HB3	3:B:83:THR:HG23	1.22	1.19
3:A:54:ASN:HB3	3:A:71:MET:HE3	1.25	1.18
1:H:222:PRO:HG3	1:H:273:LYS:HD2	1.21	1.15
2:M:121:ILE:HG23	2:M:123:PRO:HD3	1.22	1.15
2:L:121:ILE:HG23	2:L:123:PRO:HD3	1.27	1.12
1:J:205:GLN:HG2	1:J:245:MET:HE2	1.22	1.10
2:L:81:ASN:H	1:J:63:LEU:HD11	1.16	1.10
3:A:52:PRO:HD3	3:A:73:LYS:HE3	1.29	1.10
1:J:272:LEU:HD23	1:J:275:THR:HG22	1.25	1.08
2:L:43:LEU:HD13	2:L:44:THR:HG23	1.33	1.06
1:J:222:PRO:HG3	1:J:273:LYS:HD2	1.29	1.05
3:B:54:ASN:HB3	3:B:71:MET:HE2	1.36	1.04
2:M:57:TRQ:HZ3	2:M:107:TRP:H	1.20	1.04
1:J:69:LEU:HG	1:J:129:ILE:HB	1.33	1.04
3:B:21:ILE:HG21	3:B:42:THR:O	1.59	1.02
1:J:303:VAL:HG12	1:J:305:GLN:HG2	1.39	1.01
1:J:353:VAL:HG13	1:J:354:GLU:HG2	1.42	1.01
3:B:25:ILE:HG22	3:B:48:ARG:HB3	1.41	1.01
3:A:6:PRO:HB3	3:A:83:THR:HG23	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:303:VAL:HG12	1:H:305:GLN:HG2	1.40	1.00
1:J:186:SER:HB3	1:J:205:GLN:HE21	1.20	1.00
1:H:270:ALA:HB2	1:H:320:ILE:HG22	1.43	0.99
3:B:25:ILE:HG23	3:B:26:ALA:N	1.75	0.99
3:B:25:ILE:CG2	3:B:48:ARG:HB3	1.91	0.99
3:B:25:ILE:HG21	3:B:48:ARG:C	1.90	0.96
1:J:44:GLY:H	2:M:81:ASN:ND2	1.65	0.95
1:H:205:GLN:HG2	1:H:245:MET:HE2	1.50	0.94
1:J:205:GLN:HG2	1:J:245:MET:CE	1.98	0.94
3:B:46:ILE:HD11	3:B:48:ARG:HH12	1.33	0.94
3:A:12:ALA:HB1	3:A:76:GLN:CD	1.94	0.92
2:M:99:ASN:HB3	2:M:100:LYS:HD3	1.51	0.92
3:A:10:PRO:HA	3:A:11:PHE:HD1	1.34	0.92
3:B:46:ILE:HD11	3:B:48:ARG:NH1	1.85	0.92
1:J:254:SER:HA	1:J:257:LYS:HE3	1.52	0.91
1:H:205:GLN:CG	1:H:245:MET:HE2	2.00	0.91
1:H:195:ALA:HB3	1:H:196:PRO:HD3	1.51	0.91
3:A:12:ALA:HA	3:A:77:ALA:H	1.34	0.90
1:H:273:LYS:H	1:H:323:GLN:NE2	1.70	0.90
1:H:296:THR:HG23	1:H:310:ILE:HB	1.53	0.90
3:B:8:GLU:O	3:B:9:SER:HB2	1.70	0.90
3:A:47:ASN:ND2	3:A:52:PRO:HA	1.88	0.89
3:B:39:VAL:HG12	3:B:104:VAL:HG12	1.53	0.89
1:H:222:PRO:CG	1:H:273:LYS:HD2	2.03	0.89
2:L:20:ILE:HG21	1:J:6:ALA:HB1	1.53	0.88
3:A:5:ILE:HG13	3:A:6:PRO:HD3	1.54	0.88
3:A:54:ASN:CB	3:A:71:MET:HE3	2.02	0.88
3:A:58:VAL:O	3:A:66:ALA:HB1	1.72	0.88
3:A:6:PRO:HG2	3:A:82:PHE:HA	1.56	0.88
3:A:39:VAL:HG12	3:A:104:VAL:HG12	1.56	0.87
3:A:25:ILE:HD11	3:A:98:MET:HE3	1.57	0.87
1:H:353:VAL:HG13	1:H:354:GLU:HG2	1.55	0.87
3:A:21:ILE:HG22	3:A:43:VAL:HA	1.56	0.86
1:H:38:LEU:HD11	1:H:358:GLY:H	1.41	0.86
2:L:57:TRQ:HB2	2:L:107:TRP:NE1	1.90	0.86
3:B:16:VAL:CG1	3:B:17:ALA:H	1.88	0.86
1:H:38:LEU:CD1	1:H:358:GLY:H	1.89	0.86
1:H:63:LEU:HD11	2:M:81:ASN:H	1.41	0.86
3:A:23:VAL:HG21	3:A:45:TRP:CD2	2.10	0.86
3:B:24:ASP:HB3	3:B:46:ILE:HG23	1.57	0.86
1:J:341:ILE:HD12	1:J:342:TYR:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:22:VAL:CG1	3:A:44:THR:HB	2.05	0.85
3:B:6:PRO:HB2	3:B:82:PHE:HA	1.56	0.85
1:J:272:LEU:HD23	1:J:275:THR:CG2	2.05	0.85
1:J:278:ILE:HG23	1:J:299:VAL:HG23	1.58	0.85
3:B:16:VAL:HG12	3:B:17:ALA:H	1.41	0.85
3:B:31:GLU:HG2	3:B:32:THR:N	1.90	0.85
2:M:77:CYS:HB2	2:M:119:CYS:HB3	1.59	0.85
3:A:67:LEU:HD21	3:A:78:TYR:CE2	2.11	0.85
1:J:205:GLN:CG	1:J:245:MET:HE2	2.07	0.85
1:J:300:THR:HB	1:J:303:VAL:O	1.77	0.84
3:B:37:VAL:HG12	3:B:41:ASP:OD2	1.77	0.84
3:B:25:ILE:HG23	3:B:26:ALA:H	1.40	0.84
1:J:186:SER:HB3	1:J:205:GLN:NE2	1.92	0.84
1:H:215:GLN:HG3	1:H:266:PHE:O	1.77	0.84
3:A:47:ASN:HD21	3:A:52:PRO:HA	1.42	0.83
1:H:207:THR:HG23	1:H:210:GLN:HE21	1.42	0.83
1:H:229:VAL:HG22	1:H:232:SER:H	1.44	0.83
3:B:21:ILE:O	3:B:44:THR:HG23	1.78	0.83
1:H:229:VAL:HG22	1:H:232:SER:N	1.93	0.83
2:M:31:ILE:HD12	2:M:88:CYS:HB2	1.58	0.83
3:A:16:VAL:CG1	3:A:17:ALA:H	1.90	0.83
1:J:331:ALA:HB3	1:J:342:TYR:HE1	1.42	0.83
3:B:59:ALA:CB	3:B:66:ALA:HB2	2.08	0.83
3:B:59:ALA:HB2	3:B:66:ALA:HB2	1.59	0.83
3:B:6:PRO:CG	3:B:83:THR:H	1.92	0.83
1:J:267:GLN:HE22	1:J:362:LEU:H	1.25	0.83
3:A:52:PRO:CD	3:A:73:LYS:HE3	2.06	0.83
1:H:270:ALA:CB	1:H:320:ILE:HG22	2.09	0.83
3:A:67:LEU:HD21	3:A:78:TYR:HE2	1.42	0.82
2:M:20:ILE:HG22	2:M:25:TYR:CE2	2.12	0.82
1:J:239:PRO:HD2	1:J:242:GLY:O	1.79	0.82
3:B:25:ILE:HD12	3:B:49:GLU:HG3	1.61	0.82
3:A:22:VAL:HG12	3:A:44:THR:HB	1.60	0.81
1:J:38:LEU:CD1	1:J:358:GLY:H	1.94	0.81
1:J:195:ALA:HB3	1:J:196:PRO:HD3	1.60	0.81
3:B:58:VAL:HG12	3:B:59:ALA:H	1.46	0.81
2:L:97:VAL:C	2:L:99:ASN:H	1.89	0.81
1:H:229:VAL:HG23	1:H:231:SER:H	1.46	0.80
3:A:67:LEU:HD22	3:A:80:LEU:HD13	1.62	0.80
1:H:273:LYS:H	1:H:323:GLN:HE22	1.30	0.80
1:H:278:ILE:HG12	1:H:299:VAL:CG2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:25:ILE:HG13	3:B:49:GLU:HB2	1.64	0.79
1:H:38:LEU:HD21	1:H:357:LYS:HB2	1.65	0.79
3:A:12:ALA:N	3:A:77:ALA:O	2.15	0.79
1:H:69:LEU:HG	1:H:129:ILE:HB	1.63	0.79
1:J:1:GLU:O	1:J:4:LYS:HB2	1.83	0.79
3:A:23:VAL:HB	3:A:45:TRP:NE1	1.98	0.79
3:A:10:PRO:HA	3:A:11:PHE:CD1	2.17	0.79
3:B:12:ALA:HA	3:B:77:ALA:H	1.45	0.79
1:H:222:PRO:HG3	1:H:273:LYS:CD	2.08	0.78
2:L:81:ASN:N	1:J:63:LEU:HD11	1.97	0.78
1:H:207:THR:HG23	1:H:210:GLN:NE2	1.99	0.78
3:B:10:PRO:HA	3:B:11:PHE:HD1	1.48	0.78
1:H:296:THR:CG2	1:H:310:ILE:HB	2.14	0.78
3:A:42:THR:HA	3:A:81:THR:HA	1.65	0.78
2:L:51:LEU:CD1	2:L:112:GLU:HB2	2.13	0.78
3:B:6:PRO:CB	3:B:83:THR:HG23	2.10	0.78
3:B:25:ILE:CG2	3:B:26:ALA:N	2.40	0.78
2:M:57:TRQ:HZ3	2:M:107:TRP:N	1.99	0.77
1:H:6:ALA:HB2	2:M:20:ILE:HG12	1.67	0.77
1:J:296:THR:CG2	1:J:310:ILE:HB	2.15	0.77
1:J:229:VAL:HG22	1:J:232:SER:N	1.98	0.77
3:B:47:ASN:HB3	3:B:73:LYS:O	1.84	0.77
3:B:6:PRO:HG2	3:B:82:PHE:HA	1.67	0.77
3:A:44:THR:HG22	3:A:46:ILE:HG22	1.65	0.77
3:B:57:PHE:CE2	3:B:88:TYR:HB3	2.19	0.77
1:J:169:HIS:O	1:J:180:LEU:HD12	1.85	0.77
1:H:239:PRO:HD2	1:H:242:GLY:O	1.85	0.76
1:J:229:VAL:HG23	1:J:231:SER:H	1.50	0.76
1:J:238:ILE:HG22	1:J:243:ALA:HA	1.66	0.76
3:B:87:THR:HB	3:B:103:VAL:HG22	1.67	0.76
2:L:63:ASN:OD1	2:L:65:PRO:HD2	1.85	0.76
3:A:57:PHE:CE2	3:A:88:TYR:HB3	2.19	0.76
3:B:4:THR:H	3:B:63:GLY:HA3	1.51	0.76
1:H:186:SER:HB3	1:H:205:GLN:HE21	1.50	0.75
3:A:16:VAL:HG12	3:A:17:ALA:H	1.48	0.75
3:A:20:ALA:O	3:A:21:ILE:HB	1.84	0.75
3:B:21:ILE:CG2	3:B:43:VAL:HA	2.16	0.75
3:B:6:PRO:CB	3:B:82:PHE:HA	2.15	0.75
1:H:38:LEU:HD22	1:H:356:ASP:O	1.86	0.75
2:M:79:GLY:H	2:M:116:THR:HG23	1.51	0.75
2:L:124:VAL:HG12	1:J:19:ASP:OD2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:97:PHE:O	3:B:99:ARG:HG2	1.86	0.75
1:J:283:VAL:HG11	1:J:293:ALA:HA	1.67	0.74
2:M:121:ILE:HG23	2:M:123:PRO:CD	2.10	0.74
3:B:57:PHE:HE2	3:B:88:TYR:HB3	1.51	0.74
1:J:44:GLY:H	2:M:81:ASN:HD21	1.34	0.74
1:J:238:ILE:HG22	1:J:243:ALA:CB	2.17	0.74
3:B:47:ASN:HD21	3:B:53:HIS:HD2	1.34	0.74
1:H:111:ASP:OD2	1:J:88:ARG:NH1	2.21	0.74
1:H:362:LEU:HD12	1:H:362:LEU:N	2.02	0.74
2:L:121:ILE:CG2	2:L:123:PRO:HD3	2.11	0.74
3:A:58:VAL:HG12	3:A:59:ALA:N	2.03	0.74
1:H:253:GLU:H	1:H:256:ARG:HD2	1.53	0.74
1:J:254:SER:CA	1:J:257:LYS:HE3	2.18	0.74
3:A:6:PRO:HG2	3:A:82:PHE:CA	2.17	0.74
1:J:221:TYR:CB	1:J:222:PRO:HD3	2.18	0.73
1:H:229:VAL:HG13	1:H:232:SER:O	1.89	0.73
3:A:27:LYS:O	3:A:29:LYS:HD2	1.88	0.73
1:J:222:PRO:CG	1:J:273:LYS:HD2	2.12	0.73
1:H:44:GLY:H	2:L:81:ASN:ND2	1.86	0.73
3:A:25:ILE:HD11	3:A:98:MET:CE	2.18	0.73
1:H:114:LEU:HD13	1:H:140:PHE:CZ	2.24	0.72
1:J:283:VAL:HG12	1:J:293:ALA:CB	2.19	0.72
3:B:61:VAL:O	3:B:62:LEU:HB2	1.88	0.72
1:H:44:GLY:H	2:L:81:ASN:HD21	1.37	0.72
2:M:15:PRO:HB2	2:M:64:PRO:HG3	1.70	0.72
3:A:61:VAL:O	3:A:62:LEU:HB2	1.89	0.72
3:B:75:GLU:O	3:B:76:GLN:O	2.06	0.72
3:A:22:VAL:HG12	3:A:44:THR:CB	2.19	0.72
1:J:362:LEU:HD12	1:J:362:LEU:N	2.04	0.72
3:A:5:ILE:CG1	3:A:6:PRO:HD3	2.19	0.72
1:J:222:PRO:HG3	1:J:273:LYS:CD	2.15	0.72
3:A:87:THR:HB	3:A:103:VAL:HG22	1.70	0.72
1:H:167:CYS:HB3	1:H:180:LEU:HG	1.72	0.72
3:A:21:ILE:CG2	3:A:43:VAL:HA	2.19	0.71
2:L:46:CYS:HB3	2:L:50:THR:CG2	2.19	0.71
2:L:81:ASN:H	1:J:63:LEU:CD1	2.00	0.71
2:L:17:ASP:OD2	2:L:65:PRO:HG2	1.90	0.71
3:A:9:SER:HB3	3:A:10:PRO:HD2	1.71	0.71
1:J:233:ILE:N	1:J:233:ILE:HD13	2.06	0.71
1:J:253:GLU:H	1:J:256:ARG:HD2	1.56	0.71
3:B:20:ALA:O	3:B:21:ILE:HB	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:25:ILE:HG13	3:B:49:GLU:N	2.06	0.71
3:B:39:VAL:HG12	3:B:104:VAL:CG1	2.21	0.71
3:A:51:MET:N	3:A:73:LYS:HE2	2.05	0.70
3:B:10:PRO:CA	3:B:11:PHE:HD1	2.04	0.70
3:B:10:PRO:C	3:B:11:PHE:HD1	1.98	0.70
1:H:319:ILE:O	1:H:320:ILE:HG23	1.91	0.70
1:H:6:ALA:HB1	2:M:20:ILE:HG21	1.74	0.70
3:A:6:PRO:CG	3:A:82:PHE:HA	2.22	0.70
3:A:41:ASP:O	3:A:42:THR:HG22	1.91	0.70
3:B:6:PRO:CG	3:B:82:PHE:HA	2.21	0.70
3:A:72:MET:HB3	3:A:76:GLN:OE1	1.91	0.70
3:A:70:PRO:C	3:A:71:MET:HG2	2.13	0.70
3:B:54:ASN:HB2	3:B:69:GLY:O	1.90	0.70
3:B:25:ILE:HD12	3:B:26:ALA:H	1.56	0.70
3:B:89:ASP:OD1	3:B:101:LYS:HD3	1.92	0.70
2:M:125:SER:O	3:B:73:LYS:HE3	1.91	0.70
3:B:27:LYS:O	3:B:29:LYS:N	2.24	0.70
1:H:38:LEU:CD2	1:H:357:LYS:HB2	2.22	0.69
1:J:264:ALA:HB2	1:J:293:ALA:CB	2.22	0.69
1:J:219:ALA:HB1	1:J:222:PRO:HD2	1.72	0.69
1:J:238:ILE:HG22	1:J:243:ALA:CA	2.22	0.69
1:J:229:VAL:HG22	1:J:232:SER:H	1.57	0.69
3:B:25:ILE:HG21	3:B:49:GLU:N	2.07	0.69
1:J:272:LEU:CD2	1:J:275:THR:HG22	2.13	0.69
1:J:303:VAL:CG1	1:J:305:GLN:HG2	2.21	0.69
3:B:25:ILE:CG2	3:B:48:ARG:CB	2.68	0.69
1:J:278:ILE:HG23	1:J:299:VAL:CG2	2.23	0.69
1:H:205:GLN:HG3	1:H:245:MET:HE2	1.74	0.68
3:A:6:PRO:CG	3:A:83:THR:H	2.06	0.68
2:M:28:HIS:HB3	2:M:31:ILE:CD1	2.23	0.68
2:M:57:TRQ:NE1	2:M:74:TYR:HB2	2.08	0.68
1:J:298:SER:OG	1:J:310:ILE:HD11	1.93	0.68
3:B:21:ILE:O	3:B:21:ILE:HG22	1.92	0.68
2:M:63:ASN:OD1	2:M:65:PRO:HD2	1.93	0.68
1:H:278:ILE:HG23	1:H:299:VAL:HG23	1.74	0.68
1:H:90:ALA:O	2:L:116:THR:HG21	1.93	0.68
1:J:320:ILE:HG12	1:J:362:LEU:HB2	1.75	0.68
3:A:25:ILE:HG22	3:A:48:ARG:H	1.58	0.68
3:A:39:VAL:HG12	3:A:104:VAL:CG1	2.23	0.68
3:A:59:ALA:CB	3:A:66:ALA:HB2	2.24	0.68
1:J:217:ALA:HB3	1:J:226:VAL:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:28:HIS:HB3	2:M:31:ILE:HD13	1.74	0.68
1:H:6:ALA:CB	2:M:20:ILE:HG12	2.24	0.68
3:B:6:PRO:HG2	3:B:82:PHE:CA	2.24	0.68
1:H:143:PHE:HE2	2:L:99:ASN:HD21	1.40	0.67
1:H:272:LEU:HD22	1:H:275:THR:CG2	2.25	0.67
1:H:341:ILE:HD12	1:H:342:TYR:N	2.09	0.67
3:B:25:ILE:HG13	3:B:49:GLU:H	1.59	0.67
3:B:25:ILE:HB	3:B:48:ARG:H	1.58	0.67
3:B:21:ILE:HG21	3:B:42:THR:C	2.19	0.67
3:B:58:VAL:O	3:B:66:ALA:HB1	1.93	0.67
3:B:72:MET:CB	3:B:76:GLN:HB2	2.24	0.67
3:B:10:PRO:HA	3:B:11:PHE:CD1	2.29	0.67
1:J:262:ARG:HG3	1:J:285:HIS:HB2	1.77	0.67
3:B:12:ALA:N	3:B:77:ALA:O	2.27	0.67
1:H:136:ALA:O	1:H:154:PRO:HD2	1.94	0.67
2:L:108:CYS:HB3	2:L:114:GLY:O	1.94	0.67
3:B:23:VAL:HG21	3:B:45:TRP:NE1	2.10	0.67
3:B:25:ILE:CG1	3:B:49:GLU:HB2	2.24	0.67
1:H:222:PRO:O	1:H:224:MET:N	2.28	0.67
3:A:12:ALA:HB1	3:A:76:GLN:NE2	2.09	0.67
1:J:142:LEU:HD23	1:J:143:PHE:N	2.10	0.66
1:J:283:VAL:HG22	1:J:284:GLU:H	1.59	0.66
3:B:67:LEU:HD21	3:B:78:TYR:CE2	2.31	0.66
1:H:303:VAL:O	1:H:305:GLN:N	2.26	0.66
1:J:254:SER:N	1:J:257:LYS:HE3	2.11	0.66
1:H:6:ALA:HB1	2:M:20:ILE:CG2	2.25	0.66
1:H:357:LYS:CE	1:J:357:LYS:HE2	2.26	0.66
1:J:267:GLN:HB3	1:J:318:ALA:HB1	1.77	0.66
1:J:37:THR:CG2	1:J:361:SER:HB2	2.25	0.66
3:A:6:PRO:HB2	3:A:82:PHE:HA	1.78	0.66
1:H:274:ASN:OD1	1:H:274:ASN:N	2.29	0.66
1:H:357:LYS:HE2	1:J:357:LYS:HE2	1.77	0.66
1:H:272:LEU:HD23	1:H:275:THR:H	1.61	0.66
1:J:222:PRO:O	1:J:224:MET:N	2.28	0.66
2:M:46:CYS:HB3	2:M:50:THR:CG2	2.26	0.66
3:A:23:VAL:HG11	3:A:45:TRP:CZ2	2.31	0.65
3:B:25:ILE:CD1	3:B:49:GLU:HB2	2.25	0.65
1:H:151:LEU:HD22	1:H:159:ASP:HB3	1.77	0.65
3:A:10:PRO:C	3:A:11:PHE:HD1	2.03	0.65
3:A:58:VAL:HG12	3:A:59:ALA:H	1.59	0.65
1:H:303:VAL:CG1	1:H:305:GLN:HG2	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:89:ASP:OD1	3:A:101:LYS:HD3	1.97	0.65
3:B:59:ALA:HB2	3:B:66:ALA:CB	2.25	0.65
1:H:272:LEU:HD22	1:H:275:THR:HG22	1.78	0.65
2:L:51:LEU:HD13	2:L:112:GLU:HB2	1.78	0.65
1:J:286:SER:OG	2:M:12:LYS:HD2	1.97	0.65
1:J:296:THR:HG23	1:J:310:ILE:HD12	1.78	0.65
1:H:343:ASP:C	1:H:345:ALA:H	2.03	0.64
3:A:23:VAL:HG21	3:A:45:TRP:CE2	2.32	0.64
3:A:41:ASP:O	3:A:81:THR:CB	2.46	0.64
1:J:303:VAL:O	1:J:305:GLN:N	2.28	0.64
2:M:97:VAL:C	2:M:99:ASN:H	2.02	0.64
3:A:28:MET:O	3:A:29:LYS:HB3	1.97	0.64
3:B:28:MET:HE1	3:B:51:MET:HG2	1.79	0.64
1:H:229:VAL:CG2	1:H:231:SER:H	2.09	0.64
2:L:20:ILE:HG21	1:J:6:ALA:CB	2.27	0.64
1:J:264:ALA:HB2	1:J:293:ALA:HB3	1.80	0.64
3:A:42:THR:HB	3:A:81:THR:HB	1.77	0.64
3:B:23:VAL:HG23	3:B:45:TRP:CD1	2.31	0.64
3:B:25:ILE:HG22	3:B:48:ARG:CB	2.23	0.64
1:J:253:GLU:O	1:J:255:GLY:N	2.31	0.64
2:M:44:THR:O	2:M:121:ILE:HD11	1.98	0.64
1:H:281:LEU:HD22	1:H:293:ALA:HB3	1.79	0.64
3:A:7:SER:CB	3:A:81:THR:HG23	2.26	0.64
2:L:43:LEU:HD13	2:L:44:THR:CG2	2.20	0.64
3:A:48:ARG:NH1	3:A:75:GLU:OE1	2.29	0.64
3:A:45:TRP:C	3:A:46:ILE:HG22	2.22	0.64
3:B:17:ALA:HB1	3:B:18:ASP:OD1	1.97	0.64
3:B:21:ILE:HG22	3:B:43:VAL:HA	1.79	0.64
3:B:38:LYS:N	3:B:41:ASP:OD2	2.31	0.64
1:J:169:HIS:O	1:J:180:LEU:HA	1.97	0.63
3:B:5:ILE:HG13	3:B:6:PRO:HD3	1.79	0.63
2:L:20:ILE:HG22	2:L:25:TYR:CZ	2.33	0.63
3:A:53:HIS:O	3:A:71:MET:HB3	1.99	0.63
1:J:221:TYR:HB2	1:J:222:PRO:HD3	1.79	0.63
1:J:296:THR:O	1:J:310:ILE:HG13	1.97	0.63
2:L:99:ASN:HB3	2:L:100:LYS:HD3	1.79	0.63
2:M:99:ASN:C	2:M:100:LYS:HD3	2.23	0.63
3:A:95:HIS:HB3	3:A:97:PHE:CE2	2.33	0.63
1:J:229:VAL:C	1:J:231:SER:H	2.04	0.63
1:H:42:PHE:HD1	1:H:67:LEU:HD21	1.63	0.63
1:J:37:THR:HG22	1:J:361:SER:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:ALA:O	1:J:154:PRO:HD2	1.99	0.63
3:B:58:VAL:CG1	3:B:59:ALA:H	2.11	0.63
1:H:254:SER:HA	1:H:257:LYS:HE3	1.81	0.62
1:H:117:ALA:N	1:H:118:PRO:HD3	2.14	0.62
1:J:283:VAL:HG12	1:J:293:ALA:HB1	1.80	0.62
2:L:100:LYS:HD2	3:A:28:MET:HE1	1.80	0.62
1:J:219:ALA:CB	1:J:222:PRO:HD2	2.29	0.62
1:H:275:THR:OG1	1:H:276:ASP:N	2.28	0.62
2:M:20:ILE:HG22	2:M:25:TYR:CZ	2.34	0.62
3:B:5:ILE:O	3:B:62:LEU:HD23	1.99	0.62
1:J:362:LEU:H	1:J:362:LEU:HD12	1.64	0.62
3:A:7:SER:HB2	3:A:81:THR:HG23	1.82	0.62
3:A:21:ILE:HG23	3:A:43:VAL:HG13	1.81	0.62
1:J:60:GLY:HA3	1:J:106:PHE:CE2	2.34	0.62
2:M:33:GLY:HA3	2:M:117:TYR:OH	1.98	0.62
1:H:38:LEU:O	1:H:38:LEU:HG	2.00	0.62
3:A:21:ILE:HG22	3:A:21:ILE:O	1.99	0.62
2:M:28:HIS:O	2:M:31:ILE:HG12	2.01	0.61
3:A:67:LEU:CD2	3:A:80:LEU:HD13	2.29	0.61
1:J:319:ILE:O	1:J:320:ILE:HG23	2.00	0.61
3:B:16:VAL:CG1	3:B:17:ALA:N	2.63	0.61
3:B:25:ILE:HD12	3:B:49:GLU:CG	2.29	0.61
1:J:117:ALA:N	1:J:118:PRO:HD3	2.15	0.61
3:A:57:PHE:HE2	3:A:88:TYR:HB3	1.61	0.61
3:B:95:HIS:C	3:B:97:PHE:H	2.06	0.61
1:J:195:ALA:CB	1:J:196:PRO:HD3	2.28	0.61
3:A:35:LEU:HD13	3:A:35:LEU:O	2.01	0.61
1:J:90:ALA:O	2:M:116:THR:HG21	2.00	0.61
3:A:88:TYR:O	3:A:101:LYS:HG3	2.01	0.61
3:B:4:THR:O	3:B:5:ILE:HG23	2.00	0.61
3:B:15:GLU:O	3:B:16:VAL:O	2.18	0.61
1:H:39:PRO:HG2	1:H:360:GLU:OE1	2.01	0.61
1:J:296:THR:HG23	1:J:310:ILE:HB	1.82	0.61
2:M:38:CYS:O	2:M:85:ARG:HD3	1.99	0.61
3:A:21:ILE:HG23	3:A:43:VAL:CG1	2.30	0.61
3:A:39:VAL:HB	3:A:83:THR:O	2.01	0.61
3:A:71:MET:O	3:A:72:MET:HB2	1.99	0.61
3:A:53:HIS:ND1	3:A:95:HIS:HE1	1.98	0.61
3:B:57:PHE:HA	3:B:90:TYR:HA	1.81	0.61
3:A:50:ALA:C	3:A:73:LYS:HZ3	2.08	0.61
1:H:328:ASP:HB3	1:H:341:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:51:MET:H	3:A:73:LYS:HE2	1.65	0.60
1:H:69:LEU:CG	1:H:129:ILE:HB	2.31	0.60
1:H:186:SER:HB3	1:H:205:GLN:NE2	2.16	0.60
3:A:10:PRO:CA	3:A:11:PHE:HD1	2.10	0.60
3:A:6:PRO:CB	3:A:83:THR:HG23	2.27	0.60
1:J:328:ASP:HB3	1:J:341:ILE:HD13	1.82	0.60
3:A:4:THR:O	3:A:5:ILE:HG23	2.01	0.60
3:A:72:MET:HB3	3:A:76:GLN:CD	2.26	0.60
1:J:38:LEU:HG	1:J:38:LEU:O	2.00	0.60
3:A:44:THR:HG22	3:A:46:ILE:CG2	2.31	0.60
3:A:57:PHE:HA	3:A:90:TYR:HA	1.83	0.60
3:B:72:MET:HB3	3:B:76:GLN:HB2	1.82	0.60
1:H:233:ILE:HB	1:H:249:ILE:HG12	1.82	0.60
3:B:10:PRO:C	3:B:11:PHE:CD1	2.79	0.60
1:J:229:VAL:CG2	1:J:231:SER:H	2.15	0.60
3:A:29:LYS:O	3:A:29:LYS:HD3	2.02	0.60
1:H:264:ALA:HB2	1:H:293:ALA:HB2	1.84	0.60
2:M:12:LYS:HZ3	2:M:12:LYS:HA	1.67	0.60
3:A:6:PRO:CB	3:A:82:PHE:HA	2.31	0.60
3:A:29:LYS:O	3:A:30:TYR:C	2.43	0.60
1:H:283:VAL:HG22	1:H:284:GLU:H	1.66	0.60
2:L:27:ARG:NH1	2:L:43:LEU:HD11	2.17	0.60
1:J:138:LEU:C	1:J:138:LEU:HD23	2.27	0.60
1:H:18:SER:OG	1:H:19:ASP:N	2.32	0.59
1:J:254:SER:H	1:J:257:LYS:HE3	1.67	0.59
3:A:22:VAL:HG12	3:A:44:THR:O	2.02	0.59
3:A:92:CYS:SG	3:A:94:PRO:HD2	2.42	0.59
3:B:34:GLU:OE1	3:B:101:LYS:NZ	2.30	0.59
1:J:38:LEU:O	1:J:46:THR:HB	2.03	0.59
1:H:87:ALA:O	1:H:91:LYS:O	2.20	0.59
1:J:74:HIS:O	1:J:367:GLU:HG2	2.03	0.59
3:A:9:SER:HB3	3:A:10:PRO:CD	2.31	0.59
2:L:57:TRQ:HB2	2:L:107:TRP:HE1	1.66	0.59
3:A:25:ILE:HG23	3:A:26:ALA:N	2.17	0.59
1:J:38:LEU:HD11	1:J:358:GLY:H	1.66	0.59
3:B:6:PRO:HG2	3:B:83:THR:H	1.66	0.59
2:M:16:GLN:HG3	2:M:24:ASP:O	2.01	0.59
1:H:267:GLN:HB3	1:H:318:ALA:HB1	1.84	0.59
3:A:95:HIS:HB3	3:A:97:PHE:CZ	2.37	0.59
2:L:20:ILE:HD13	1:J:6:ALA:HB2	1.85	0.59
1:J:87:ALA:O	1:J:91:LYS:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:GLU:O	3:A:16:VAL:O	2.21	0.59
3:B:43:VAL:CG2	3:B:82:PHE:HE1	2.15	0.59
1:H:361:SER:C	1:H:362:LEU:HD12	2.27	0.58
3:B:87:THR:CB	3:B:103:VAL:HG22	2.32	0.58
1:H:272:LEU:HA	1:H:323:GLN:HE22	1.68	0.58
1:H:59:LEU:C	2:M:40:ALA:HB2	2.28	0.58
1:H:300:THR:HB	1:H:303:VAL:O	2.02	0.58
1:J:283:VAL:HG22	1:J:284:GLU:N	2.17	0.58
3:A:98:MET:O	3:A:98:MET:HG2	2.03	0.58
3:B:5:ILE:HB	3:B:6:PRO:HG3	1.84	0.58
1:H:169:HIS:O	1:H:180:LEU:HD12	2.04	0.58
1:J:303:VAL:HG11	1:J:305:GLN:NE2	2.18	0.58
3:A:23:VAL:HB	3:A:45:TRP:CD1	2.39	0.58
3:B:23:VAL:CG2	3:B:45:TRP:CD1	2.87	0.58
1:J:143:PHE:HE2	2:M:99:ASN:HD21	1.51	0.58
1:H:229:VAL:C	1:H:231:SER:H	2.10	0.58
1:H:264:ALA:O	1:H:289:CYS:O	2.20	0.58
2:L:49:GLY:HA2	1:J:107:LEU:CD2	2.33	0.58
2:M:42:SER:OG	2:M:45:SER:HB2	2.03	0.58
3:B:28:MET:HE3	3:B:53:HIS:HE1	1.68	0.58
1:H:28:GLY:O	1:H:30:ILE:HG23	2.03	0.58
1:J:107:LEU:N	1:J:107:LEU:HD23	2.18	0.58
1:J:153:VAL:HG12	1:J:159:ASP:HB2	1.86	0.58
3:B:25:ILE:HG13	3:B:49:GLU:CB	2.32	0.58
1:J:252:ASN:O	1:J:257:LYS:HE2	2.04	0.58
3:B:29:LYS:HG2	3:B:29:LYS:O	2.02	0.58
3:B:26:ALA:O	3:B:27:LYS:O	2.21	0.58
3:B:12:ALA:HA	3:B:77:ALA:N	2.17	0.57
3:B:38:LYS:HG3	3:B:41:ASP:OD2	2.03	0.57
3:B:72:MET:HB3	3:B:76:GLN:CB	2.33	0.57
3:B:72:MET:HB2	3:B:76:GLN:HB2	1.85	0.57
1:H:267:GLN:HE22	1:H:362:LEU:H	1.53	0.57
1:J:86:PHE:HA	1:J:93:LYS:O	2.04	0.57
3:B:31:GLU:HG2	3:B:32:THR:H	1.65	0.57
3:A:51:MET:N	3:A:73:LYS:CE	2.67	0.57
3:A:90:TYR:HE1	3:A:102:VAL:HG23	1.68	0.57
1:H:283:VAL:HG22	1:H:284:GLU:N	2.20	0.57
3:A:16:VAL:CG1	3:A:17:ALA:N	2.67	0.57
1:J:331:ALA:HB3	1:J:342:TYR:CE1	2.33	0.57
3:A:17:ALA:HB1	3:A:18:ASP:OD1	2.04	0.57
3:A:46:ILE:HD11	3:A:48:ARG:NH2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:43:LEU:CD1	2:L:44:THR:HG23	2.21	0.57
3:B:25:ILE:HG21	3:B:48:ARG:CA	2.34	0.57
3:A:41:ASP:O	3:A:81:THR:HB	2.05	0.57
2:L:51:LEU:HD11	2:L:112:GLU:HB2	1.84	0.57
1:J:229:VAL:HG23	1:J:231:SER:N	2.19	0.57
1:J:356:ASP:O	1:J:357:LYS:HB2	2.05	0.57
3:B:92:CYS:SG	3:B:94:PRO:HD2	2.45	0.57
2:L:46:CYS:HB3	2:L:50:THR:HG21	1.87	0.56
1:H:143:PHE:HE2	2:L:99:ASN:ND2	2.04	0.56
1:H:179:TYR:C	1:H:181:GLY:H	2.12	0.56
2:L:81:ASN:HB3	1:J:63:LEU:HD21	1.86	0.56
1:J:229:VAL:HG13	1:J:232:SER:O	2.04	0.56
3:B:4:THR:O	3:B:62:LEU:O	2.22	0.56
3:B:47:ASN:O	3:B:75:GLU:HA	2.05	0.56
1:H:38:LEU:HD21	1:H:40:ALA:HB2	1.85	0.56
2:L:44:THR:C	2:L:121:ILE:HD11	2.29	0.56
1:J:343:ASP:C	1:J:345:ALA:H	2.13	0.56
3:B:57:PHE:HE2	3:B:88:TYR:CB	2.18	0.56
3:B:58:VAL:CG1	3:B:59:ALA:N	2.68	0.56
3:B:25:ILE:CD1	3:B:26:ALA:H	2.17	0.56
3:B:95:HIS:HB3	3:B:97:PHE:CE2	2.40	0.56
2:M:100:LYS:HD3	2:M:100:LYS:N	2.21	0.56
3:A:11:PHE:CD1	3:A:11:PHE:N	2.74	0.56
2:L:100:LYS:HD2	3:A:97:PHE:HZ	1.70	0.56
1:J:272:LEU:HA	1:J:323:GLN:HE22	1.71	0.56
3:B:27:LYS:O	3:B:29:LYS:HD2	2.06	0.56
1:H:341:ILE:HD12	1:H:341:ILE:C	2.30	0.56
2:M:14:GLN:H	2:M:14:GLN:CD	2.14	0.56
3:B:88:TYR:CD1	3:B:88:TYR:N	2.73	0.56
1:J:255:GLY:O	1:J:258:ALA:HB3	2.06	0.56
1:H:4:LYS:HA	2:M:18:ASN:O	2.06	0.56
2:L:19:ASP:O	2:L:20:ILE:HG12	2.06	0.56
1:J:262:ARG:CG	1:J:285:HIS:HB2	2.35	0.55
3:B:99:ARG:HG3	3:B:99:ARG:HH11	1.71	0.55
3:A:12:ALA:HB1	3:A:76:GLN:CG	2.36	0.55
3:A:54:ASN:HA	3:A:70:PRO:O	2.05	0.55
3:B:6:PRO:HB2	3:B:81:THR:O	2.06	0.55
1:J:272:LEU:O	1:J:275:THR:O	2.24	0.55
2:M:46:CYS:HB3	2:M:50:THR:HG21	1.88	0.55
3:A:88:TYR:CD1	3:A:88:TYR:N	2.75	0.55
1:J:168:PHE:N	1:J:168:PHE:CD1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:13:TRP:CH2	2:M:24:ASP:HA	2.41	0.55
2:L:55:GLY:O	2:L:75:ARG:HG2	2.06	0.55
3:A:42:THR:CA	3:A:81:THR:HA	2.34	0.55
1:H:336:THR:O	1:H:338:VAL:HG12	2.06	0.55
1:J:241:ALA:O	1:J:242:GLY:O	2.24	0.55
2:M:100:LYS:HD2	3:B:97:PHE:HZ	1.71	0.55
1:H:285:HIS:O	1:H:286:SER:HB2	2.07	0.55
2:M:79:GLY:N	2:M:116:THR:HG23	2.18	0.55
2:L:20:ILE:CG2	1:J:6:ALA:CB	2.85	0.55
1:J:264:ALA:HB2	1:J:293:ALA:HB2	1.89	0.55
3:A:21:ILE:O	3:A:22:VAL:HG13	2.07	0.55
3:B:37:VAL:HG12	3:B:41:ASP:CG	2.31	0.55
1:H:283:VAL:CG2	1:H:284:GLU:H	2.20	0.55
1:H:354:GLU:C	1:H:356:ASP:H	2.15	0.55
3:A:23:VAL:CG2	3:A:45:TRP:CD2	2.88	0.55
3:A:35:LEU:HD13	3:A:35:LEU:C	2.32	0.55
1:J:179:TYR:HD2	1:J:187:LEU:CD2	2.20	0.54
2:M:31:ILE:HD12	2:M:88:CYS:CB	2.35	0.54
2:M:57:TRQ:CZ3	2:M:107:TRP:HB2	2.37	0.54
3:B:29:LYS:HA	3:B:98:MET:HB3	1.89	0.54
3:A:24:ASP:O	3:A:25:ILE:HB	2.06	0.54
3:B:40:GLY:N	3:B:82:PHE:O	2.39	0.54
3:A:26:ALA:O	3:A:28:MET:N	2.40	0.54
1:H:111:ASP:CG	1:J:88:ARG:HH12	2.15	0.54
2:L:77:CYS:HB2	2:L:119:CYS:HB3	1.88	0.54
2:M:12:LYS:HA	2:M:12:LYS:NZ	2.22	0.54
3:A:99:ARG:HH11	3:A:99:ARG:CG	2.20	0.54
1:H:362:LEU:N	1:H:362:LEU:CD1	2.70	0.54
3:A:42:THR:HA	3:A:81:THR:CA	2.37	0.54
3:B:11:PHE:CD1	3:B:11:PHE:N	2.76	0.54
2:L:20:ILE:HD13	1:J:6:ALA:CB	2.38	0.54
2:L:47:PRO:O	2:L:50:THR:HG22	2.07	0.54
3:A:59:ALA:HB2	3:A:66:ALA:CB	2.38	0.54
2:M:77:CYS:HB2	2:M:119:CYS:CB	2.36	0.54
3:B:25:ILE:CB	3:B:48:ARG:HB3	2.37	0.54
1:H:192:LEU:C	1:H:192:LEU:HD22	2.32	0.54
2:L:66:ASP:O	2:L:66:ASP:OD1	2.26	0.54
2:L:97:VAL:C	2:L:99:ASN:N	2.63	0.54
1:J:283:VAL:CG1	1:J:293:ALA:HA	2.37	0.54
2:M:79:GLY:H	2:M:116:THR:CG2	2.19	0.54
3:A:11:PHE:O	3:A:12:ALA:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:51:MET:N	3:A:73:LYS:NZ	2.55	0.54
3:B:22:VAL:CG2	3:B:23:VAL:N	2.70	0.54
1:J:225:LEU:HD23	1:J:226:VAL:N	2.23	0.53
3:A:4:THR:H	3:A:63:GLY:HA3	1.72	0.53
3:A:65:ALA:O	3:A:66:ALA:HB2	2.08	0.53
2:L:40:ALA:HB2	1:J:59:LEU:C	2.33	0.53
3:A:5:ILE:HG12	3:A:5:ILE:O	2.07	0.53
3:A:7:SER:HB2	3:A:81:THR:CG2	2.38	0.53
2:M:12:LYS:HZ2	2:M:13:TRP:H	1.57	0.53
3:A:87:THR:CB	3:A:103:VAL:HG22	2.38	0.53
3:B:21:ILE:C	3:B:22:VAL:HG12	2.33	0.53
3:B:35:LEU:CD2	3:B:37:VAL:HG22	2.38	0.53
1:J:207:THR:H	1:J:210:GLN:HE21	1.57	0.53
1:H:166:SER:O	1:H:184:PRO:HD2	2.08	0.53
2:M:99:ASN:HB3	2:M:100:LYS:CD	2.33	0.53
3:A:6:PRO:HG3	3:A:83:THR:H	1.72	0.53
3:B:16:VAL:O	3:B:17:ALA:HB2	2.09	0.53
3:B:65:ALA:O	3:B:66:ALA:HB2	2.08	0.53
3:A:51:MET:CA	3:A:73:LYS:CE	2.86	0.53
1:J:142:LEU:HD21	1:J:144:GLY:O	2.08	0.53
1:J:283:VAL:CG2	1:J:284:GLU:H	2.21	0.53
3:B:28:MET:CE	3:B:53:HIS:HE1	2.22	0.53
3:B:45:TRP:O	3:B:77:ALA:HB1	2.09	0.53
3:B:47:ASN:ND2	3:B:53:HIS:HD2	2.05	0.53
1:H:60:GLY:N	2:M:40:ALA:HB2	2.24	0.53
1:H:63:LEU:HD11	2:M:81:ASN:N	2.18	0.53
1:J:265:GLY:O	1:J:317:ASP:O	2.27	0.53
1:J:296:THR:HG23	1:J:310:ILE:CG1	2.39	0.53
2:M:44:THR:HA	2:M:121:ILE:HG12	1.91	0.53
2:M:77:CYS:O	2:M:118:HIS:HB3	2.09	0.53
1:J:167:CYS:SG	1:J:180:LEU:O	2.67	0.53
1:J:267:GLN:NE2	1:J:362:LEU:HD12	2.24	0.53
2:M:14:GLN:CD	2:M:14:GLN:N	2.67	0.53
1:H:221:TYR:CB	1:H:222:PRO:HD3	2.38	0.52
2:L:58:VAL:HB	2:L:71:ILE:HD12	1.91	0.52
1:H:219:ALA:HB1	1:H:222:PRO:HD2	1.90	0.52
2:L:52:VAL:HG23	1:J:23:CYS:SG	2.49	0.52
2:M:70:TYR:HB3	2:M:124:VAL:CG2	2.39	0.52
3:A:10:PRO:C	3:A:11:PHE:CD1	2.87	0.52
3:B:27:LYS:O	3:B:28:MET:C	2.51	0.52
3:B:24:ASP:O	3:B:25:ILE:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:264:ALA:O	1:J:289:CYS:O	2.27	0.52
1:J:296:THR:HG23	1:J:296:THR:O	2.10	0.52
1:J:322:ALA:HB3	1:J:328:ASP:H	1.74	0.52
2:M:121:ILE:CG2	2:M:123:PRO:HD3	2.16	0.52
3:A:95:HIS:C	3:A:97:PHE:H	2.17	0.52
1:H:229:VAL:HG23	1:H:231:SER:N	2.20	0.52
1:H:241:ALA:O	1:H:242:GLY:O	2.28	0.52
3:A:94:PRO:HG2	3:A:95:HIS:CE1	2.44	0.52
1:J:229:VAL:O	1:J:231:SER:N	2.43	0.52
1:J:231:SER:O	1:J:232:SER:OG	2.25	0.52
3:A:3:ALA:O	3:A:4:THR:HG23	2.09	0.52
3:B:94:PRO:HB2	3:B:95:HIS:CD2	2.44	0.52
1:H:273:LYS:N	1:H:323:GLN:HE22	2.02	0.52
1:H:343:ASP:O	1:H:345:ALA:N	2.42	0.52
1:J:232:SER:CB	1:J:251:GLY:H	2.22	0.52
3:B:70:PRO:O	3:B:71:MET:HG2	2.10	0.52
1:H:42:PHE:CD1	1:H:67:LEU:HD21	2.43	0.52
1:J:105:THR:O	1:J:106:PHE:HB2	2.08	0.52
2:M:39:SER:O	2:M:40:ALA:HB3	2.09	0.52
3:A:38:LYS:HG3	3:A:39:VAL:O	2.09	0.52
3:B:20:ALA:O	3:B:21:ILE:CB	2.58	0.52
1:H:202:VAL:HG13	1:H:203:GLY:N	2.25	0.52
2:L:40:ALA:CB	1:J:59:LEU:C	2.83	0.52
2:L:47:PRO:HD2	2:L:50:THR:HG21	1.92	0.52
2:L:94:GLU:O	2:L:95:LEU:O	2.28	0.52
1:H:125:ARG:HD2	1:H:125:ARG:N	2.25	0.52
1:H:232:SER:CB	1:H:251:GLY:H	2.23	0.51
1:H:303:VAL:HG11	1:H:305:GLN:NE2	2.24	0.51
3:A:5:ILE:HD11	3:A:88:TYR:CE2	2.45	0.51
3:A:53:HIS:C	3:A:71:MET:HB3	2.36	0.51
1:H:180:LEU:O	1:H:188:ALA:HB3	2.10	0.51
1:H:205:GLN:O	1:H:206:CYS:O	2.27	0.51
2:L:39:SER:O	2:L:40:ALA:HB3	2.10	0.51
1:J:281:LEU:HD23	1:J:295:ASN:O	2.09	0.51
1:J:331:ALA:CB	1:J:342:TYR:HE1	2.19	0.51
2:M:57:TRQ:CD1	2:M:74:TYR:HB2	2.40	0.51
3:B:5:ILE:HA	3:B:6:PRO:CG	2.41	0.51
1:H:179:TYR:C	1:H:181:GLY:N	2.67	0.51
2:M:73:ALA:O	2:M:123:PRO:HD2	2.11	0.51
3:A:45:TRP:C	3:A:46:ILE:CG2	2.82	0.51
3:A:55:VAL:O	3:A:68:LYS:O	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:99:ARG:HH11	3:A:99:ARG:HG3	1.74	0.51
1:J:100:VAL:CG1	1:J:109:ILE:HD11	2.41	0.51
1:H:63:LEU:HD13	1:J:90:ALA:HB3	1.92	0.51
1:J:238:ILE:HG22	1:J:243:ALA:HB2	1.92	0.51
1:J:303:VAL:C	1:J:305:GLN:H	2.16	0.51
3:A:53:HIS:CE1	3:A:95:HIS:CE1	2.99	0.51
2:L:20:ILE:CD1	1:J:6:ALA:HB2	2.40	0.51
1:J:303:VAL:HG12	1:J:305:GLN:CG	2.28	0.51
3:A:59:ALA:HB2	3:A:66:ALA:HB2	1.91	0.51
3:B:21:ILE:CG2	3:B:42:THR:O	2.47	0.51
3:B:95:HIS:C	3:B:97:PHE:N	2.69	0.51
1:H:265:GLY:O	1:H:317:ASP:O	2.28	0.51
1:J:269:VAL:HG13	1:J:280:ILE:HD13	1.93	0.51
1:J:296:THR:CG2	1:J:310:ILE:HD12	2.41	0.51
2:M:97:VAL:C	2:M:99:ASN:N	2.68	0.51
3:B:54:ASN:HB3	3:B:70:PRO:O	2.11	0.51
1:H:342:TYR:CE2	1:H:348:GLN:HB2	2.45	0.51
1:J:181:GLY:O	1:J:182:SER:O	2.29	0.51
1:J:275:THR:OG1	1:J:276:ASP:N	2.42	0.51
3:A:25:ILE:O	3:A:26:ALA:HB2	2.10	0.51
3:A:26:ALA:C	3:A:28:MET:N	2.67	0.51
3:A:36:HIS:HB3	3:A:105:GLU:OE2	2.10	0.51
3:B:25:ILE:HD11	3:B:53:HIS:NE2	2.25	0.51
3:B:59:ALA:HB1	3:B:65:ALA:O	2.11	0.51
1:H:125:ARG:HG2	1:H:214:SER:O	2.10	0.51
2:M:47:PRO:HD2	2:M:50:THR:HG21	1.93	0.51
3:A:47:ASN:HB3	3:A:73:LYS:HA	1.93	0.51
3:B:25:ILE:CB	3:B:48:ARG:H	2.24	0.51
1:J:232:SER:HB2	1:J:250:ASP:HA	1.92	0.50
1:J:276:ASP:CG	1:J:301:ALA:HB3	2.36	0.50
3:A:11:PHE:HD1	3:A:11:PHE:N	2.09	0.50
3:B:58:VAL:HG12	3:B:59:ALA:N	2.21	0.50
3:A:57:PHE:HE2	3:A:88:TYR:CB	2.23	0.50
1:H:168:PHE:N	1:H:168:PHE:CD1	2.79	0.50
2:M:99:ASN:CB	2:M:100:LYS:HD3	2.32	0.50
3:A:22:VAL:HG12	3:A:44:THR:CA	2.41	0.50
3:A:47:ASN:HD21	3:A:52:PRO:CA	2.19	0.50
3:B:4:THR:C	3:B:5:ILE:HG23	2.36	0.50
3:B:5:ILE:O	3:B:5:ILE:CG1	2.60	0.50
1:H:31:SER:OG	1:H:324:ASP:HB3	2.12	0.50
1:H:181:GLY:O	1:H:182:SER:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:341:ILE:HD12	1:J:341:ILE:C	2.37	0.50
3:A:58:VAL:CG1	3:A:59:ALA:N	2.73	0.50
1:H:232:SER:HB3	1:H:250:ASP:HA	1.94	0.50
1:J:74:HIS:HA	1:J:365:GLN:HB2	1.94	0.50
1:J:296:THR:HG23	1:J:310:ILE:CB	2.42	0.50
3:B:56:HIS:O	3:B:57:PHE:O	2.30	0.50
1:H:38:LEU:HD21	1:H:357:LYS:CB	2.38	0.50
1:J:202:VAL:HG13	1:J:203:GLY:N	2.27	0.50
1:H:357:LYS:NZ	1:J:357:LYS:CE	2.75	0.50
3:A:34:GLU:OE1	3:A:101:LYS:NZ	2.41	0.50
3:B:12:ALA:HB1	3:B:76:GLN:HB3	1.94	0.50
2:M:106:ILE:HD12	2:M:106:ILE:O	2.12	0.50
3:A:5:ILE:O	3:A:62:LEU:HG	2.12	0.50
3:A:18:ASP:OD1	3:A:18:ASP:N	2.26	0.50
1:J:229:VAL:C	1:J:231:SER:N	2.67	0.49
1:J:296:THR:HG23	1:J:310:ILE:CD1	2.42	0.49
3:B:36:HIS:ND1	3:B:36:HIS:N	2.60	0.49
3:B:95:HIS:O	3:B:97:PHE:N	2.45	0.49
1:H:229:VAL:C	1:H:231:SER:N	2.69	0.49
1:H:262:ARG:CG	1:H:285:HIS:HB2	2.41	0.49
2:L:20:ILE:HG12	1:J:6:ALA:HB3	1.93	0.49
1:J:267:GLN:HE22	1:J:362:LEU:HD12	1.77	0.49
3:B:18:ASP:OD1	3:B:18:ASP:N	2.28	0.49
1:J:266:PHE:O	1:J:268:MET:N	2.45	0.49
2:M:103:ASN:HD22	2:M:103:ASN:C	2.20	0.49
3:A:42:THR:HA	3:A:80:LEU:O	2.12	0.49
3:A:90:TYR:HE1	3:A:102:VAL:CG2	2.24	0.49
2:L:58:VAL:HG22	3:A:51:MET:HE1	1.95	0.49
2:M:35:ILE:HD12	2:M:86:CYS:HB3	1.94	0.49
3:A:41:ASP:O	3:A:81:THR:OG1	2.28	0.49
1:H:60:GLY:HA3	1:H:106:PHE:CE2	2.47	0.49
1:H:137:CYS:HA	1:H:154:PRO:HD2	1.94	0.49
1:J:131:ASN:O	1:J:172:PRO:HG2	2.12	0.49
1:J:303:VAL:HG12	1:J:303:VAL:O	2.10	0.49
3:A:4:THR:O	3:A:62:LEU:O	2.30	0.49
3:B:53:HIS:O	3:B:71:MET:HA	2.12	0.49
3:B:54:ASN:HB3	3:B:71:MET:CE	2.26	0.49
1:H:232:SER:CB	1:H:250:ASP:HA	2.43	0.49
1:H:280:ILE:HG22	1:H:297:SER:O	2.13	0.49
2:L:40:ALA:HB1	1:J:59:LEU:O	2.12	0.49
2:M:70:TYR:HB3	2:M:124:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:99:ASN:ND2	3:B:97:PHE:HE2	2.11	0.49
3:A:25:ILE:CG2	3:A:48:ARG:H	2.26	0.49
3:A:41:ASP:C	3:A:42:THR:HG22	2.37	0.49
1:J:71:VAL:HG23	1:J:80:ALA:HB3	1.95	0.49
3:A:16:VAL:O	3:A:17:ALA:HB2	2.11	0.49
3:B:93:THR:C	3:B:95:HIS:H	2.21	0.49
1:J:79:PHE:HE1	1:J:103:PRO:HA	1.78	0.49
3:A:67:LEU:CD2	3:A:78:TYR:HE2	2.20	0.49
1:H:357:LYS:NZ	1:J:357:LYS:HE3	2.28	0.49
1:J:44:GLY:H	2:M:81:ASN:HD22	1.56	0.49
1:J:93:LYS:HD2	1:J:94:ARG:O	2.13	0.49
2:M:53:ALA:HB2	2:M:108:CYS:HA	1.95	0.49
2:M:61:CYS:O	2:M:69:LYS:HA	2.12	0.49
3:A:22:VAL:HG12	3:A:44:THR:C	2.38	0.49
3:B:43:VAL:HG21	3:B:82:PHE:HE1	1.78	0.49
2:L:53:ALA:O	2:L:75:ARG:HD2	2.12	0.48
1:J:205:GLN:O	1:J:206:CYS:O	2.31	0.48
3:A:9:SER:O	3:A:11:PHE:HE1	1.95	0.48
2:M:106:ILE:HD12	2:M:108:CYS:HB2	1.94	0.48
3:A:7:SER:CB	3:A:81:THR:CG2	2.91	0.48
3:B:16:VAL:HG12	3:B:17:ALA:O	2.13	0.48
3:B:5:ILE:HD12	3:B:88:TYR:OH	2.14	0.48
3:B:81:THR:HG23	3:B:82:PHE:N	2.29	0.48
2:L:28:HIS:HB3	2:L:31:ILE:CD1	2.43	0.48
1:J:167:CYS:SG	1:J:180:LEU:HG	2.53	0.48
1:J:215:GLN:HG3	1:J:266:PHE:O	2.12	0.48
2:M:20:ILE:HG22	2:M:25:TYR:CD2	2.47	0.48
3:B:5:ILE:HA	3:B:6:PRO:HG3	1.94	0.48
3:A:51:MET:HG2	3:A:53:HIS:NE2	2.28	0.48
3:A:55:VAL:O	3:A:55:VAL:HG22	2.13	0.48
3:B:53:HIS:ND1	3:B:98:MET:HE1	2.27	0.48
1:H:303:VAL:C	1:H:305:GLN:H	2.17	0.48
3:A:6:PRO:HB2	3:A:81:THR:O	2.14	0.48
1:H:30:ILE:HG13	1:H:32:ARG:H	1.79	0.48
1:H:98:VAL:N	1:H:112:ILE:O	2.33	0.48
1:H:151:LEU:HD23	1:H:151:LEU:C	2.38	0.48
3:B:35:LEU:HD22	3:B:37:VAL:HG22	1.94	0.48
1:H:122:VAL:HG13	2:L:105:ILE:HA	1.96	0.48
1:H:253:GLU:O	1:H:255:GLY:N	2.46	0.48
2:L:45:SER:CA	2:L:121:ILE:HD11	2.44	0.48
2:L:56:SER:HB3	2:L:75:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ALA:HB2	2:M:20:ILE:CG1	2.41	0.48
1:H:187:LEU:HB3	1:H:202:VAL:HB	1.96	0.48
1:J:202:VAL:CG1	1:J:203:GLY:N	2.77	0.48
1:H:343:ASP:OD2	1:H:345:ALA:HB3	2.14	0.47
1:H:134:SER:O	1:H:135:SER:HB2	2.14	0.47
1:H:272:LEU:HD12	1:H:322:ALA:O	2.14	0.47
2:L:20:ILE:HG12	1:J:6:ALA:CB	2.44	0.47
2:L:25:TYR:HB3	2:L:28:HIS:CD2	2.49	0.47
3:A:23:VAL:CG2	3:A:45:TRP:CG	2.98	0.47
3:A:23:VAL:CB	3:A:45:TRP:CE2	2.97	0.47
3:A:90:TYR:CE1	3:A:102:VAL:HG23	2.48	0.47
3:B:99:ARG:HG3	3:B:99:ARG:NH1	2.28	0.47
2:M:99:ASN:ND2	3:B:97:PHE:CE2	2.82	0.47
3:A:23:VAL:HG21	3:A:45:TRP:CE3	2.47	0.47
3:A:51:MET:CA	3:A:73:LYS:HE2	2.44	0.47
1:H:167:CYS:CB	1:H:180:LEU:HG	2.43	0.47
1:J:38:LEU:HD13	1:J:358:GLY:H	1.78	0.47
3:A:51:MET:N	3:A:73:LYS:HZ3	2.10	0.47
1:H:308:GLY:HA2	1:H:309:PRO:HD3	1.31	0.47
2:M:90:ASN:C	2:M:91:THR:HG23	2.39	0.47
3:B:47:ASN:HD21	3:B:53:HIS:CD2	2.23	0.47
3:A:4:THR:C	3:A:5:ILE:HG23	2.38	0.47
3:A:51:MET:HA	3:A:73:LYS:CE	2.45	0.47
3:B:5:ILE:HG13	3:B:5:ILE:O	2.13	0.47
1:H:52:CYS:O	1:H:56:GLY:N	2.42	0.47
1:H:114:LEU:HD13	1:H:140:PHE:CE2	2.49	0.47
1:H:262:ARG:HG3	1:H:285:HIS:HB2	1.97	0.47
1:H:338:VAL:HA	1:H:352:SER:O	2.15	0.47
3:A:5:ILE:HG12	3:A:62:LEU:HA	1.96	0.47
3:A:16:VAL:HG12	3:A:17:ALA:O	2.14	0.47
3:B:71:MET:C	3:B:72:MET:CG	2.85	0.47
1:H:6:ALA:CB	2:M:20:ILE:CG2	2.92	0.47
1:H:219:ALA:CB	1:H:222:PRO:HD2	2.45	0.47
1:J:35:HIS:HA	1:J:49:TRP:O	2.15	0.47
1:J:218:GLN:HA	1:J:224:MET:O	2.15	0.47
3:B:67:LEU:HD21	3:B:78:TYR:HE2	1.80	0.47
1:H:38:LEU:CD2	1:H:40:ALA:HB2	2.45	0.47
1:H:150:GLY:CA	1:H:161:LEU:HD13	2.45	0.47
1:J:142:LEU:HD23	1:J:143:PHE:H	1.80	0.47
1:J:239:PRO:HG2	1:J:241:ALA:O	2.14	0.47
3:B:5:ILE:CA	3:B:6:PRO:CG	2.89	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:LEU:HD22	1:H:159:ASP:CB	2.44	0.47
1:H:303:VAL:HG12	1:H:305:GLN:CG	2.28	0.47
1:J:25:HIS:HB2	1:J:104:VAL:O	2.15	0.47
3:B:6:PRO:HG2	3:B:83:THR:N	2.29	0.47
2:L:51:LEU:HD13	2:L:112:GLU:H	1.81	0.46
2:L:58:VAL:HG21	3:A:51:MET:HE3	1.98	0.46
1:J:138:LEU:HD23	1:J:138:LEU:O	2.15	0.46
3:B:12:ALA:CB	3:B:76:GLN:HB3	2.45	0.46
3:B:28:MET:CE	3:B:53:HIS:CE1	2.99	0.46
3:B:28:MET:C	3:B:98:MET:SD	2.97	0.46
1:H:100:VAL:O	1:H:109:ILE:HG12	2.15	0.46
1:H:259:ASP:O	1:H:260:ASN:HB2	2.16	0.46
1:H:229:VAL:O	1:H:231:SER:N	2.48	0.46
3:A:47:ASN:O	3:A:75:GLU:HA	2.15	0.46
1:H:38:LEU:HD12	1:H:358:GLY:C	2.41	0.46
2:L:14:GLN:O	2:L:14:GLN:HG2	2.16	0.46
2:L:31:ILE:HG23	2:L:74:TYR:CE1	2.51	0.46
1:J:303:VAL:HG11	1:J:305:GLN:HE21	1.81	0.46
1:H:283:VAL:CG2	1:H:284:GLU:N	2.78	0.46
2:L:51:LEU:HD13	2:L:112:GLU:N	2.30	0.46
3:B:5:ILE:HG21	3:B:5:ILE:HD13	1.70	0.46
3:B:11:PHE:O	3:B:12:ALA:HB3	2.14	0.46
1:H:198:ALA:O	1:H:199:ALA:HB3	2.15	0.46
1:J:167:CYS:HB3	1:J:180:LEU:HD21	1.97	0.46
2:M:57:TRQ:CZ3	2:M:107:TRP:CB	2.91	0.46
3:A:74:LYS:O	3:A:75:GLU:HB2	2.16	0.46
3:B:11:PHE:HD1	3:B:11:PHE:N	2.13	0.46
1:H:142:LEU:HD21	1:H:144:GLY:O	2.15	0.46
2:L:33:GLY:HA3	2:L:117:TYR:OH	2.15	0.46
1:J:120:PHE:CE2	1:J:122:VAL:HG21	2.51	0.46
3:B:67:LEU:HD21	3:B:78:TYR:CZ	2.50	0.46
1:J:150:GLY:HA2	1:J:161:LEU:HD13	1.98	0.46
3:A:21:ILE:CG2	3:A:43:VAL:CG1	2.93	0.46
3:A:83:THR:OG1	3:A:84:GLU:N	2.49	0.46
1:H:69:LEU:HD12	1:H:69:LEU:C	2.40	0.46
1:H:38:LEU:HD11	1:H:40:ALA:HA	1.98	0.46
1:H:94:ARG:NE	1:H:117:ALA:HB1	2.31	0.46
1:H:345:ALA:O	1:H:346:SER:HB2	2.15	0.46
1:J:267:GLN:CB	1:J:318:ALA:HB1	2.43	0.46
1:H:14:ALA:C	1:H:16:ALA:H	2.24	0.45
1:J:125:ARG:HH11	1:J:125:ARG:HD3	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:320:ILE:HD13	1:J:320:ILE:HG21	1.65	0.45
2:L:38:CYS:O	2:L:85:ARG:HD3	2.16	0.45
1:J:283:VAL:CG2	1:J:284:GLU:N	2.79	0.45
2:M:14:GLN:O	2:M:14:GLN:HG2	2.15	0.45
3:A:74:LYS:O	3:A:74:LYS:CG	2.64	0.45
3:B:28:MET:HE1	3:B:51:MET:CG	2.45	0.45
1:H:69:LEU:CD2	1:H:129:ILE:HB	2.47	0.45
2:M:13:TRP:CZ3	2:M:24:ASP:HA	2.52	0.45
2:M:80:TYR:HB2	2:M:118:HIS:HB2	1.98	0.45
3:B:25:ILE:HD11	3:B:49:GLU:HB2	1.98	0.45
3:B:39:VAL:HB	3:B:83:THR:O	2.16	0.45
1:H:176:ALA:HB1	1:H:193:ALA:HB2	1.98	0.45
2:L:82:VAL:HG12	2:L:117:TYR:HD2	1.81	0.45
1:J:322:ALA:HB1	1:J:324:ASP:OD1	2.16	0.45
3:A:23:VAL:HG23	3:A:44:THR:O	2.16	0.45
1:H:41:TYR:O	2:L:82:VAL:HG11	2.16	0.45
3:A:67:LEU:HD21	3:A:78:TYR:CZ	2.50	0.45
1:J:254:SER:HA	1:J:257:LYS:CE	2.35	0.45
1:J:358:GLY:N	1:J:359:PRO:CD	2.80	0.45
3:A:5:ILE:CG1	3:A:5:ILE:O	2.65	0.45
3:A:5:ILE:HD11	3:A:88:TYR:HE2	1.82	0.45
1:H:179:TYR:HD2	1:H:187:LEU:CD2	2.30	0.45
1:J:1:GLU:N	1:J:4:LYS:HD3	2.32	0.45
3:B:5:ILE:CA	3:B:6:PRO:HG3	2.46	0.45
3:B:67:LEU:HD21	3:B:78:TYR:OH	2.17	0.45
1:H:167:CYS:C	1:H:168:PHE:CD1	2.94	0.45
1:H:207:THR:H	1:H:210:GLN:HE21	1.65	0.45
1:H:303:VAL:HG11	1:H:305:GLN:HE21	1.82	0.45
1:J:117:ALA:N	1:J:118:PRO:CD	2.80	0.45
2:M:106:ILE:CD1	2:M:108:CYS:HB2	2.47	0.45
3:A:73:LYS:C	3:A:75:GLU:N	2.75	0.45
3:A:95:HIS:C	3:A:97:PHE:N	2.74	0.45
1:H:63:LEU:HD21	2:M:81:ASN:HB3	1.98	0.45
1:H:253:GLU:N	1:H:256:ARG:HD2	2.27	0.45
2:L:106:ILE:HD11	2:L:115:MET:O	2.17	0.45
1:J:38:LEU:HD22	1:J:356:ASP:O	2.17	0.45
3:A:51:MET:HA	3:A:73:LYS:HZ1	1.82	0.45
1:H:240:ALA:HB3	1:H:241:ALA:H	0.98	0.45
3:B:25:ILE:HG23	3:B:26:ALA:CA	2.44	0.45
3:B:25:ILE:HB	3:B:48:ARG:HB3	1.98	0.45
2:L:94:GLU:O	2:L:95:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:122:SER:N	2:M:123:PRO:HD3	2.32	0.44
3:A:21:ILE:HG21	3:A:42:THR:O	2.17	0.44
3:B:46:ILE:HD11	3:B:48:ARG:CZ	2.45	0.44
1:J:142:LEU:CD2	1:J:143:PHE:N	2.80	0.44
2:M:20:ILE:CG2	2:M:25:TYR:CZ	3.00	0.44
3:A:72:MET:O	3:A:73:LYS:O	2.35	0.44
1:H:63:LEU:HD13	1:J:90:ALA:CB	2.46	0.44
1:J:100:VAL:HG12	1:J:109:ILE:HG12	2.00	0.44
3:A:5:ILE:HA	3:A:6:PRO:CG	2.48	0.44
3:A:39:VAL:O	3:A:40:GLY:O	2.35	0.44
3:B:23:VAL:CG2	3:B:45:TRP:NE1	2.81	0.44
1:H:66:PHE:CZ	1:H:67:LEU:HD12	2.52	0.44
3:A:74:LYS:O	3:A:75:GLU:CB	2.65	0.44
3:A:93:THR:C	3:A:95:HIS:H	2.26	0.44
1:J:100:VAL:HG12	1:J:109:ILE:HD11	1.98	0.44
3:A:12:ALA:HA	3:A:77:ALA:N	2.15	0.44
3:A:66:ALA:O	3:A:67:LEU:C	2.60	0.44
1:H:151:LEU:O	1:H:159:ASP:N	2.48	0.44
2:L:26:TRP:CD1	2:L:26:TRP:C	2.94	0.44
1:J:229:VAL:HG23	1:J:230:ALA:N	2.33	0.44
3:A:24:ASP:O	3:A:25:ILE:CB	2.66	0.44
3:A:53:HIS:C	3:A:71:MET:HE2	2.43	0.44
3:B:6:PRO:CG	3:B:83:THR:N	2.72	0.44
3:B:94:PRO:C	3:B:95:HIS:CD2	2.96	0.44
2:M:26:TRP:HB2	2:M:64:PRO:HD3	2.00	0.44
3:A:46:ILE:CD1	3:A:48:ARG:NH2	2.81	0.44
1:H:151:LEU:O	1:H:159:ASP:HB3	2.18	0.44
1:J:125:ARG:NH2	2:M:104:ASP:HB2	2.32	0.44
3:A:42:THR:CB	3:A:81:THR:HB	2.46	0.44
3:B:22:VAL:HG23	3:B:23:VAL:N	2.33	0.44
1:H:59:LEU:C	2:M:40:ALA:CB	2.90	0.44
1:H:212:CYS:HB3	1:H:227:TRP:NE1	2.33	0.44
1:H:272:LEU:HD22	1:H:275:THR:HG23	1.99	0.44
3:A:12:ALA:O	3:A:13:ALA:HB2	2.17	0.44
3:A:75:GLU:O	3:A:76:GLN:O	2.35	0.44
3:B:12:ALA:O	3:B:13:ALA:HB2	2.17	0.44
1:H:82:ALA:HB1	1:H:119:ARG:HD3	2.00	0.43
1:H:187:LEU:O	1:H:202:VAL:HB	2.18	0.43
1:H:221:TYR:HB2	1:H:222:PRO:HD3	1.99	0.43
2:L:20:ILE:HG22	2:L:25:TYR:CE1	2.52	0.43
1:J:41:TYR:O	2:M:82:VAL:HG11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319:ILE:HA	1:J:330:TYR:O	2.17	0.43
3:B:27:LYS:CB	3:B:29:LYS:HD2	2.48	0.43
1:H:60:GLY:HA2	2:M:40:ALA:CB	2.48	0.43
1:J:71:VAL:CG2	1:J:80:ALA:HB3	2.47	0.43
2:M:57:TRQ:NE1	2:M:74:TYR:CB	2.79	0.43
3:B:43:VAL:HG23	3:B:80:LEU:O	2.19	0.43
3:B:51:MET:O	3:B:53:HIS:CD2	2.71	0.43
1:H:202:VAL:CG1	1:H:203:GLY:N	2.81	0.43
1:H:207:THR:HG23	1:H:207:THR:H	1.46	0.43
1:H:267:GLN:HE22	1:H:361:SER:HA	1.83	0.43
2:L:54:SER:HB2	2:L:109:PHE:O	2.18	0.43
1:J:232:SER:HB3	1:J:233:ILE:H	1.71	0.43
1:J:306:THR:HG23	1:J:306:THR:O	2.18	0.43
3:B:9:SER:O	3:B:11:PHE:HE1	2.01	0.43
1:H:2:LYS:O	1:H:2:LYS:HG3	2.18	0.43
1:H:283:VAL:HG13	1:H:285:HIS:CD2	2.53	0.43
1:H:342:TYR:N	1:H:342:TYR:CD1	2.86	0.43
1:J:341:ILE:HG23	1:J:350:GLN:HB2	2.01	0.43
3:A:29:LYS:O	3:A:29:LYS:CG	2.66	0.43
1:H:3:SER:O	2:M:19:ASP:O	2.36	0.43
1:J:205:GLN:H	1:J:205:GLN:HG3	1.48	0.43
3:A:23:VAL:CB	3:A:45:TRP:NE1	2.76	0.43
3:A:27:LYS:HB3	3:A:29:LYS:HE2	2.00	0.43
3:B:72:MET:SD	3:B:76:GLN:O	2.77	0.43
1:J:106:PHE:N	1:J:106:PHE:CD1	2.87	0.43
3:A:26:ALA:O	3:A:27:LYS:C	2.61	0.43
1:H:63:LEU:CD1	2:M:80:TYR:HA	2.49	0.43
2:L:45:SER:N	2:L:121:ILE:HD11	2.32	0.43
2:L:79:GLY:H	2:L:116:THR:HG23	1.83	0.43
3:A:51:MET:HA	3:A:73:LYS:NZ	2.33	0.43
3:A:56:HIS:HB2	3:A:68:LYS:O	2.19	0.43
1:H:195:ALA:HB3	1:H:196:PRO:CD	2.36	0.43
2:L:71:ILE:HG21	3:A:73:LYS:HZ2	1.84	0.43
1:J:336:THR:O	1:J:338:VAL:HG12	2.19	0.43
1:J:343:ASP:C	1:J:345:ALA:N	2.77	0.43
3:B:18:ASP:CG	3:B:19:GLY:H	2.26	0.43
3:B:51:MET:HE3	3:B:51:MET:HB2	1.65	0.43
1:H:290:LEU:HD12	1:H:290:LEU:HA	1.84	0.42
1:J:52:CYS:O	1:J:56:GLY:N	2.39	0.42
1:J:354:GLU:C	1:J:356:ASP:H	2.27	0.42
2:M:25:TYR:HB3	2:M:28:HIS:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:66:ASP:OD1	2:M:66:ASP:O	2.37	0.42
3:A:23:VAL:CG2	3:A:45:TRP:CE2	2.99	0.42
3:B:81:THR:HG23	3:B:82:PHE:H	1.84	0.42
1:H:264:ALA:O	1:H:268:MET:SD	2.77	0.42
2:M:13:TRP:CZ3	2:M:23:CYS:O	2.73	0.42
1:J:260:ASN:O	1:J:284:GLU:HA	2.19	0.42
2:M:56:SER:HB3	2:M:75:ARG:HG2	1.99	0.42
3:A:71:MET:HB3	3:A:71:MET:HE2	1.97	0.42
3:A:73:LYS:O	3:A:75:GLU:N	2.52	0.42
1:H:282:THR:O	1:H:283:VAL:HB	2.20	0.42
1:J:267:GLN:NE2	1:J:362:LEU:CD1	2.82	0.42
1:J:308:GLY:HA2	1:J:309:PRO:HD3	1.36	0.42
2:M:63:ASN:O	2:M:66:ASP:O	2.37	0.42
2:M:95:LEU:HA	2:M:96:PRO:HD3	1.77	0.42
3:A:51:MET:HE3	3:A:51:MET:HB2	1.92	0.42
3:B:54:ASN:OD1	3:B:93:THR:HG23	2.20	0.42
1:H:88:ARG:HD2	1:J:111:ASP:OD2	2.20	0.42
1:H:229:VAL:HG23	1:H:230:ALA:N	2.33	0.42
3:A:19:GLY:O	3:A:20:ALA:O	2.37	0.42
3:A:51:MET:HG2	3:A:53:HIS:CE1	2.54	0.42
3:B:35:LEU:HD22	3:B:35:LEU:C	2.44	0.42
1:J:119:ARG:O	1:J:120:PHE:HB3	2.19	0.42
2:M:26:TRP:CD1	2:M:62:TYR:C	2.97	0.42
3:A:23:VAL:HG23	3:A:45:TRP:HA	2.00	0.42
1:H:59:LEU:O	2:M:40:ALA:HB1	2.19	0.42
2:L:20:ILE:CG1	1:J:6:ALA:CB	2.98	0.42
1:J:144:GLY:O	1:J:145:SER:HB2	2.19	0.42
1:H:150:GLY:HA2	1:H:161:LEU:HD13	2.01	0.42
2:L:103:ASN:C	2:L:103:ASN:HD22	2.28	0.42
1:J:18:SER:OG	1:J:19:ASP:N	2.52	0.42
1:J:238:ILE:CG2	1:J:243:ALA:CB	2.95	0.42
3:A:21:ILE:O	3:A:22:VAL:CG1	2.67	0.42
3:A:94:PRO:HB2	3:A:95:HIS:NE2	2.35	0.42
3:B:36:HIS:C	3:B:37:VAL:CG2	2.92	0.42
2:M:79:GLY:CA	2:M:116:THR:CG2	2.98	0.42
3:A:99:ARG:CG	3:A:99:ARG:NH1	2.79	0.42
3:B:93:THR:C	3:B:95:HIS:N	2.77	0.42
1:H:165:ALA:O	1:H:167:CYS:N	2.53	0.41
1:J:41:TYR:O	1:J:42:PHE:HB2	2.20	0.41
1:J:129:ILE:HG12	1:J:140:PHE:HA	2.02	0.41
3:A:54:ASN:HD21	3:A:93:THR:HG22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:LEU:CD1	1:H:358:GLY:C	2.93	0.41
1:H:119:ARG:O	1:H:120:PHE:HB3	2.20	0.41
1:J:96:ASP:OD2	1:J:117:ALA:HA	2.20	0.41
2:M:50:THR:HG21	2:M:77:CYS:HB3	2.01	0.41
3:A:29:LYS:O	3:A:29:LYS:CD	2.69	0.41
3:A:40:GLY:N	3:A:82:PHE:O	2.53	0.41
3:A:42:THR:HA	3:A:80:LEU:C	2.46	0.41
3:B:25:ILE:HG21	3:B:48:ARG:CB	2.49	0.41
2:L:63:ASN:O	2:L:67:PRO:HA	2.19	0.41
3:A:72:MET:O	3:A:73:LYS:C	2.63	0.41
1:J:281:LEU:HD23	1:J:281:LEU:HA	1.96	0.41
1:H:143:PHE:CZ	3:A:96:PRO:HD3	2.54	0.41
2:L:50:THR:CG2	2:L:77:CYS:HB3	2.51	0.41
2:L:118:HIS:CD2	2:L:119:CYS:HB2	2.55	0.41
1:J:271:LYS:HA	1:J:277:GLY:O	2.20	0.41
3:A:23:VAL:O	3:A:44:THR:O	2.38	0.41
3:A:94:PRO:HB2	3:A:95:HIS:CD2	2.56	0.41
1:H:222:PRO:CD	1:H:273:LYS:HD2	2.50	0.41
1:J:106:PHE:N	1:J:106:PHE:HD1	2.18	0.41
1:J:120:PHE:CD1	1:J:143:PHE:HB3	2.56	0.41
1:J:177:THR:HA	1:J:190:SER:O	2.20	0.41
1:H:43:ALA:HA	2:L:81:ASN:HD21	1.86	0.41
2:L:58:VAL:CG2	3:A:51:MET:HE1	2.51	0.41
2:M:89:LEU:HA	2:M:89:LEU:HD23	1.73	0.41
2:M:95:LEU:HB2	2:M:101:ASP:HB2	2.02	0.41
3:B:61:VAL:O	3:B:61:VAL:CG2	2.68	0.41
1:H:356:ASP:O	1:H:357:LYS:HB2	2.20	0.41
1:H:357:LYS:CE	1:J:357:LYS:CE	2.96	0.41
1:J:151:LEU:C	1:J:151:LEU:CD2	2.94	0.41
1:J:331:ALA:CB	1:J:342:TYR:CE1	3.00	0.41
2:M:19:ASP:O	2:M:20:ILE:HG12	2.21	0.41
3:A:5:ILE:O	3:A:62:LEU:CG	2.68	0.41
3:A:54:ASN:HD21	3:A:56:HIS:HB3	1.86	0.41
3:B:6:PRO:HB3	3:B:83:THR:CG2	2.16	0.41
3:B:22:VAL:HA	3:B:44:THR:O	2.21	0.41
3:B:39:VAL:CG1	3:B:104:VAL:HG12	2.39	0.41
3:B:59:ALA:HB1	3:B:66:ALA:HB2	1.98	0.41
3:B:81:THR:CG2	3:B:82:PHE:N	2.83	0.41
1:J:38:LEU:CG	1:J:40:ALA:HB2	2.51	0.41
3:A:29:LYS:CD	3:A:29:LYS:N	2.84	0.41
3:B:6:PRO:HG3	3:B:83:THR:H	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:25:ILE:CG2	3:B:48:ARG:CA	2.98	0.41
1:H:275:THR:HG1	1:H:276:ASP:H	1.69	0.40
1:J:38:LEU:HG	1:J:40:ALA:HB2	2.01	0.40
1:J:142:LEU:HB3	1:J:148:ALA:HB3	2.03	0.40
3:B:8:GLU:O	3:B:9:SER:CB	2.55	0.40
1:H:219:ALA:O	1:H:222:PRO:HD2	2.21	0.40
1:J:283:VAL:CG1	1:J:293:ALA:CB	2.94	0.40
2:M:46:CYS:HB3	2:M:50:THR:HG22	2.01	0.40
1:H:283:VAL:HG11	1:H:293:ALA:HA	2.04	0.40
2:L:61:CYS:O	2:L:69:LYS:HA	2.22	0.40
1:H:88:ARG:HD2	1:H:88:ARG:HH11	1.70	0.40
1:J:266:PHE:HB3	1:J:267:GLN:H	1.77	0.40
2:M:31:ILE:CD1	2:M:88:CYS:HB2	2.40	0.40
2:M:121:ILE:HD13	2:M:121:ILE:HG21	1.64	0.40
3:B:5:ILE:O	3:B:62:LEU:CD2	2.67	0.40
3:B:6:PRO:CB	3:B:83:THR:H	2.32	0.40
3:B:25:ILE:CD1	3:B:49:GLU:CG	2.98	0.40
3:B:72:MET:CE	3:B:77:ALA:HA	2.51	0.40
1:H:153:VAL:HG13	1:H:153:VAL:O	2.21	0.40
1:H:278:ILE:HG12	1:H:299:VAL:HG21	1.96	0.40
3:A:4:THR:C	3:A:5:ILE:CG2	2.94	0.40
3:B:46:ILE:HD13	3:B:48:ARG:NH2	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	H	366/368 (100%)	290 (79%)	45 (12%)	31 (8%)	0	0
1	J	366/368 (100%)	291 (80%)	42 (12%)	33 (9%)	0	0
2	L	118/121 (98%)	98 (83%)	12 (10%)	8 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	118/121 (98%)	94 (80%)	14 (12%)	10 (8%)	0	0
3	A	101/103 (98%)	49 (48%)	23 (23%)	29 (29%)	0	0
3	B	101/103 (98%)	60 (59%)	18 (18%)	23 (23%)	0	0
All	All	1170/1184 (99%)	882 (75%)	154 (13%)	134 (12%)	0	0

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	182	SER
1	H	186	SER
1	H	206	CYS
1	H	222	PRO
1	H	223	GLY
1	H	239	PRO
1	H	254	SER
1	H	286	SER
1	H	309	PRO
1	H	346	SER
1	H	356	ASP
1	H	357	LYS
2	L	20	ILE
2	L	100	LYS
2	L	113	ASP
1	J	3	SER
1	J	145	SER
1	J	182	SER
1	J	186	SER
1	J	206	CYS
1	J	222	PRO
1	J	223	GLY
1	J	239	PRO
1	J	242	GLY
1	J	254	SER
1	J	309	PRO
1	J	346	SER
1	J	356	ASP
2	M	20	ILE
2	M	100	LYS
2	M	113	ASP
3	A	6	PRO
3	A	7	SER

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Mol	Chain	Res	Type
3	A	9	SER
3	A	16	VAL
3	A	17	ALA
3	A	20	ALA
3	A	21	ILE
3	A	25	ILE
3	A	57	PHE
3	A	62	LEU
3	A	66	ALA
3	A	72	MET
3	A	73	LYS
3	A	76	GLN
3	B	6	PRO
3	B	7	SER
3	B	9	SER
3	B	16	VAL
3	B	17	ALA
3	B	20	ALA
3	B	25	ILE
3	B	27	LYS
3	B	28	MET
3	B	57	PHE
3	B	62	LEU
3	B	66	ALA
3	B	76	GLN
1	H	90	ALA
1	H	127	HIS
1	H	242	GLY
1	H	266	PHE
1	H	304	GLY
1	H	344	ALA
2	L	65	PRO
1	J	18	SER
1	J	90	ALA
1	J	266	PHE
1	J	286	SER
1	J	304	GLY
1	J	357	LYS
2	M	65	PRO
2	M	85	ARG
3	A	13	ALA
3	A	18	ASP

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Mol	Chain	Res	Type
3	A	26	ALA
3	A	27	LYS
3	A	40	GLY
3	A	58	VAL
3	A	59	ALA
3	A	70	PRO
3	A	75	GLU
3	B	13	ALA
3	B	21	ILE
3	B	70	PRO
3	B	74	LYS
1	H	18	SER
1	H	89	SER
1	H	145	SER
1	H	155	GLY
1	H	283	VAL
2	L	85	ARG
1	J	2	LYS
1	J	89	SER
1	J	204	ALA
1	J	264	ALA
1	J	283	VAL
3	A	30	TYR
3	A	42	THR
3	A	51	MET
1	H	2	LYS
1	H	120	PHE
1	H	320	ILE
2	L	8	ASP
1	J	6	ALA
1	J	196	PRO
1	J	344	ALA
2	M	8	ASP
2	M	99	ASN
3	B	18	ASP
3	B	26	ALA
3	B	58	VAL
3	B	75	GLU
1	H	204	ALA
1	H	264	ALA
1	H	310	ILE
2	L	95	LEU

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Mol	Chain	Res	Type
1	J	127	HIS
1	J	187	LEU
1	J	267	GLN
2	M	109	PHE
3	B	5	ILE
1	J	115	PRO
2	M	95	LEU
2	M	98	TYR
3	A	5	ILE
3	A	39	VAL
3	A	60	GLY
3	B	32	THR
1	J	155	GLY
1	J	310	ILE
1	H	196	PRO
2	L	114	GLY
1	H	115	PRO

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	H	264/264 (100%)	216 (82%)	48 (18%)	2	3
1	J	264/264 (100%)	215 (81%)	49 (19%)	1	3
2	L	99/99 (100%)	83 (84%)	16 (16%)	2	4
2	M	99/99 (100%)	83 (84%)	16 (16%)	2	4
3	A	83/83 (100%)	53 (64%)	30 (36%)	0	0
3	B	83/83 (100%)	54 (65%)	29 (35%)	0	0
All	All	892/892 (100%)	704 (79%)	188 (21%)	1	2

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU

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Mol	Chain	Res	Type
1	H	21	SER
1	H	37	THR
1	H	69	LEU
1	H	88	ARG
1	H	93	LYS
1	H	105	THR
1	H	122	VAL
1	H	131	ASN
1	H	142	LEU
1	H	182	SER
1	H	187	LEU
1	H	190	SER
1	H	192	LEU
1	H	202	VAL
1	H	205	GLN
1	H	207	THR
1	H	215	GLN
1	H	218	GLN
1	H	225	LEU
1	H	226	VAL
1	H	229	VAL
1	H	233	ILE
1	H	244	THR
1	H	249	ILE
1	H	250	ASP
1	H	253	GLU
1	H	263	SER
1	H	269	VAL
1	H	271	LYS
1	H	274	ASN
1	H	275	THR
1	H	278	ILE
1	H	287	ARG
1	H	290	LEU
1	H	302	SER
1	H	306	THR
1	H	310	ILE
1	H	311	SER
1	H	315	ASP
1	H	320	ILE
1	H	323	GLN
1	H	327	SER

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Mol	Chain	Res	Type
1	H	338	VAL
1	H	341	ILE
1	H	352	SER
1	H	362	LEU
1	H	365	GLN
2	L	12	LYS
2	L	14	GLN
2	L	34	ASN
2	L	43	LEU
2	L	50	THR
2	L	71	ILE
2	L	89	LEU
2	L	94	GLU
2	L	95	LEU
2	L	97	VAL
2	L	100	LYS
2	L	103	ASN
2	L	106	ILE
2	L	113	ASP
2	L	119	CYS
2	L	121	ILE
1	J	1	GLU
1	J	4	LYS
1	J	5	VAL
1	J	21	SER
1	J	38	LEU
1	J	45	THR
1	J	50	VAL
1	J	61	HIS
1	J	69	LEU
1	J	81	LEU
1	J	93	LYS
1	J	107	LEU
1	J	122	VAL
1	J	125	ARG
1	J	126	VAL
1	J	131	ASN
1	J	142	LEU
1	J	145	SER
1	J	151	LEU
1	J	153	VAL
1	J	187	LEU

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Mol	Chain	Res	Type
1	J	192	LEU
1	J	201	ILE
1	J	202	VAL
1	J	205	GLN
1	J	225	LEU
1	J	226	VAL
1	J	229	VAL
1	J	233	ILE
1	J	234	LEU
1	J	245	MET
1	J	269	VAL
1	J	271	LYS
1	J	273	LYS
1	J	278	ILE
1	J	287	ARG
1	J	290	LEU
1	J	295	ASN
1	J	303	VAL
1	J	307	SER
1	J	310	ILE
1	J	315	ASP
1	J	323	GLN
1	J	338	VAL
1	J	341	ILE
1	J	352	SER
1	J	357	LYS
1	J	362	LEU
1	J	365	GLN
2	M	12	LYS
2	M	14	GLN
2	M	34	ASN
2	M	43	LEU
2	M	50	THR
2	M	52	VAL
2	M	71	ILE
2	M	78	CYS
2	M	82	VAL
2	M	89	LEU
2	M	94	GLU
2	M	100	LYS
2	M	103	ASN
2	M	106	ILE

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Mol	Chain	Res	Type
2	M	119	CYS
2	M	121	ILE
3	A	4	THR
3	A	5	ILE
3	A	8	GLU
3	A	11	PHE
3	A	15	GLU
3	A	16	VAL
3	A	18	ASP
3	A	22	VAL
3	A	25	ILE
3	A	29	LYS
3	A	35	LEU
3	A	36	HIS
3	A	37	VAL
3	A	39	VAL
3	A	41	ASP
3	A	42	THR
3	A	43	VAL
3	A	46	ILE
3	A	51	MET
3	A	55	VAL
3	A	61	VAL
3	A	62	LEU
3	A	71	MET
3	A	81	THR
3	A	83	THR
3	A	87	THR
3	A	93	THR
3	A	95	HIS
3	A	98	MET
3	A	99	ARG
3	B	4	THR
3	B	5	ILE
3	B	8	GLU
3	B	11	PHE
3	B	15	GLU
3	B	16	VAL
3	B	18	ASP
3	B	22	VAL
3	B	24	ASP
3	B	25	ILE

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Mol	Chain	Res	Type
3	B	35	LEU
3	B	36	HIS
3	B	37	VAL
3	B	43	VAL
3	B	44	THR
3	B	46	ILE
3	B	51	MET
3	B	55	VAL
3	B	58	VAL
3	B	61	VAL
3	B	62	LEU
3	B	72	MET
3	B	73	LYS
3	B	74	LYS
3	B	81	THR
3	B	83	THR
3	B	87	THR
3	B	93	THR
3	B	95	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	35	HIS
1	H	61	HIS
1	H	171	HIS
1	H	205	GLN
1	H	210	GLN
1	H	215	GLN
1	H	218	GLN
1	H	260	ASN
1	H	267	GLN
1	H	305	GLN
1	H	312	ASN
1	H	323	GLN
2	L	14	GLN
2	L	81	ASN
2	L	103	ASN
1	J	25	HIS
1	J	35	HIS
1	J	131	ASN
1	J	160	GLN

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Mol	Chain	Res	Type
1	J	171	HIS
1	J	205	GLN
1	J	210	GLN
1	J	215	GLN
1	J	218	GLN
1	J	267	GLN
1	J	305	GLN
1	J	323	GLN
1	J	366	ASN
2	M	34	ASN
2	M	81	ASN
2	M	103	ASN
3	A	95	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRQ	L	57	2	16,17,18	1.54	4 (25%)	16,24,26	1.27	1 (6%)
2	TRQ	M	57	2	16,17,18	1.63	3 (18%)	16,24,26	1.11	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRQ	L	57	2	-	1/5/19/21	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRQ	M	57	2	-	0/5/19/21	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	57	TRQ	CH2-CZ2	-3.47	1.37	1.53
2	M	57	TRQ	CZ3-CH2	-3.43	1.36	1.45
2	L	57	TRQ	CE2-CZ2	-3.40	1.38	1.50
2	M	57	TRQ	CE2-CZ2	-3.00	1.39	1.50
2	L	57	TRQ	CH2-CZ2	-2.96	1.39	1.53
2	L	57	TRQ	CZ3-CH2	-2.62	1.38	1.45
2	L	57	TRQ	CD2-CG	2.04	1.46	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	57	TRQ	O7-CZ2-CH2	2.99	122.20	118.39
2	M	57	TRQ	O7-CZ2-CH2	2.34	121.37	118.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	57	TRQ	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	57	TRQ	2	0
2	M	57	TRQ	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.