Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 06:46 PM EDT

PDB ID	:	1MDA
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 (i) 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 (i)) were used in the production of this report:

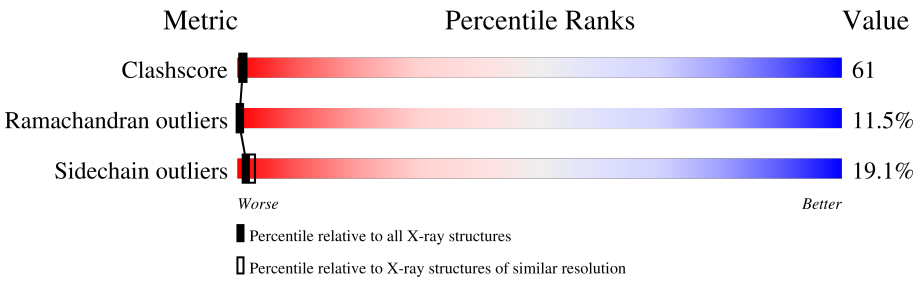
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	368	39% 42% 15% •
1	J	368	41% 40% 15% •
2	L	121	40% 43% 14% •
2	M	121	31% 50% 14% 5%
3	A	103	9% 36% 38% 17%
3	B	103	16% 38% 33% 14%

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 (i)

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
			Total	C	N	O	S			
1	H	368	2582	1585	451	532	14	0	0	0
1	J	368	2583	1585	451	533	14	0	0	0

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

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

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
			Total	C	N	O	S			
3	A	103	790	506	130	148	6	0	0	0
3	B	103	790	506	130	148	6	0	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

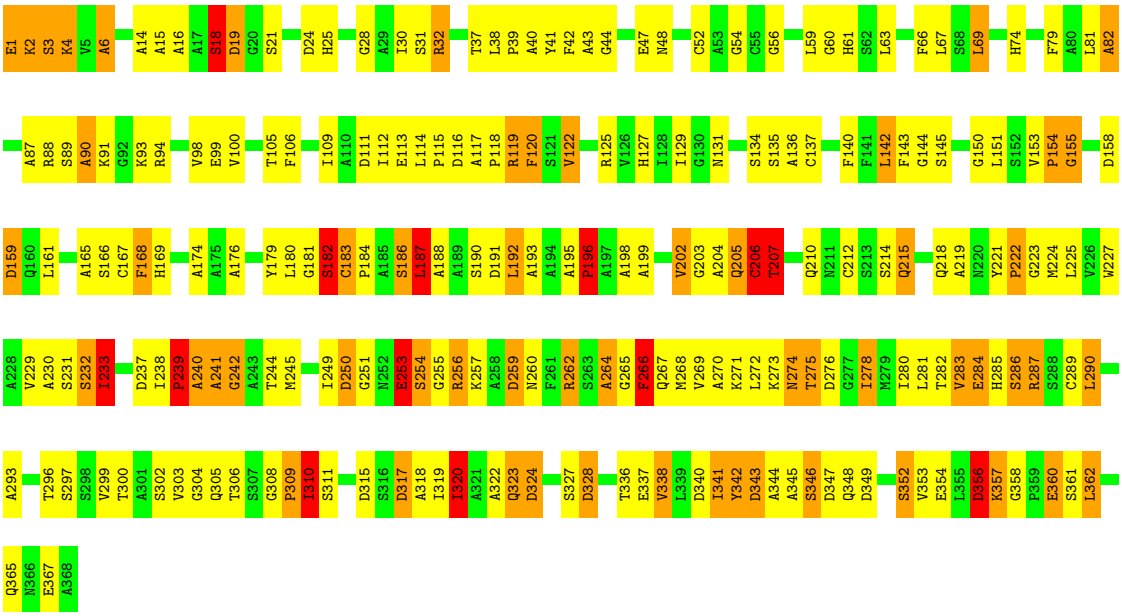
3 Residue-property plots (i)

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.

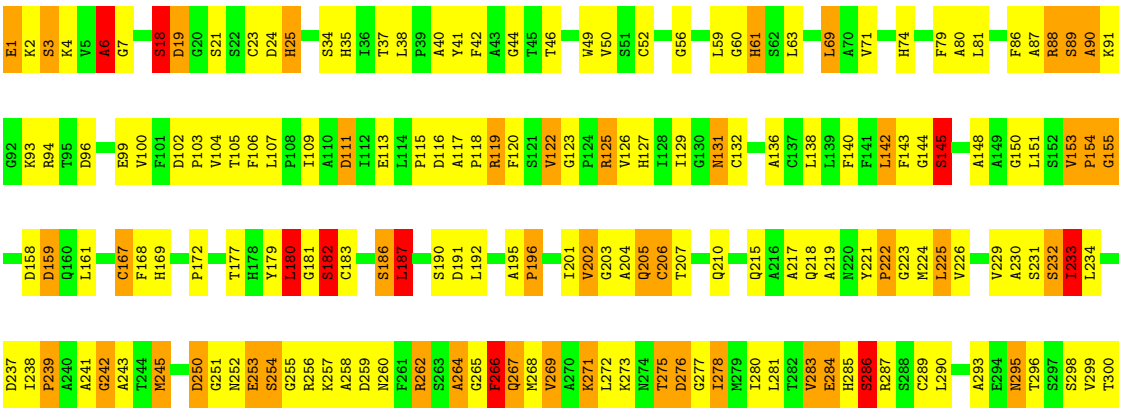
• Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

Chain H: 39% 42% 15% •



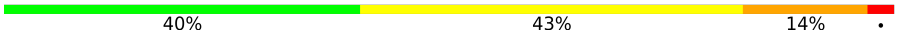
• Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

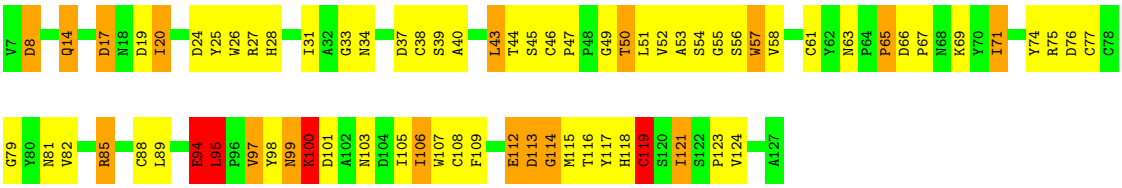
Chain J: 41% 40% 15% •



• Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

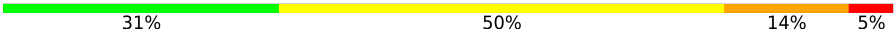
Chain L:

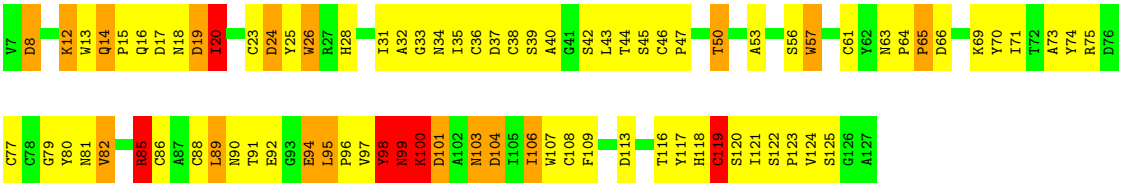




• Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

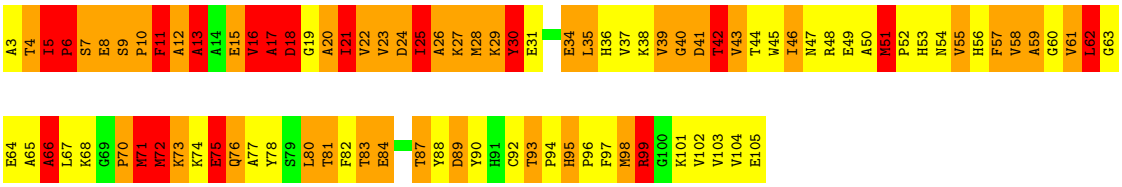
Chain M:





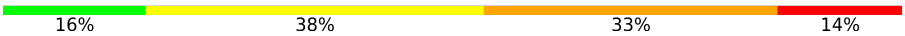
• Molecule 3: AMICYANIN

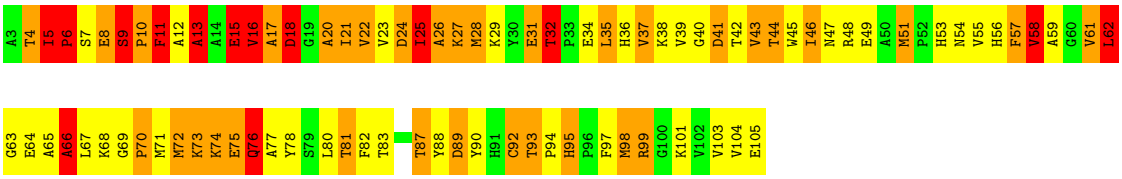
Chain A:



• Molecule 3: AMICYANIN

Chain B:





4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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	0.87	9/2629 (0.3%)	1.76	77/3577 (2.2%)
1	J	0.84	7/2630 (0.3%)	1.65	69/3577 (1.9%)
2	L	0.86	2/917 (0.2%)	1.59	21/1250 (1.7%)
2	M	0.84	2/917 (0.2%)	1.59	25/1250 (2.0%)
3	A	1.09	7/811 (0.9%)	1.99	32/1102 (2.9%)
3	B	1.08	4/811 (0.5%)	2.06	29/1102 (2.6%)
All	All	0.90	31/8715 (0.4%)	1.74	253/11858 (2.1%)

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 (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	253	GLU	CD-OE1	6.93	1.33	1.25
2	L	94	GLU	CD-OE1	6.83	1.33	1.25
1	J	113	GLU	CD-OE1	6.74	1.33	1.25
1	H	284	GLU	CD-OE2	6.46	1.32	1.25
1	H	47	GLU	CD-OE1	6.40	1.32	1.25
1	H	113	GLU	CD-OE1	6.39	1.32	1.25
3	A	84	GLU	CD-OE1	6.34	1.32	1.25
3	B	31	GLU	CD-OE2	6.24	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	64	GLU	CD-OE1	6.24	1.32	1.25
2	M	94	GLU	CD-OE1	6.19	1.32	1.25
1	J	337	GLU	CD-OE2	6.18	1.32	1.25
1	H	253	GLU	CD-OE1	6.05	1.32	1.25
1	H	367	GLU	CD-OE2	6.04	1.32	1.25
3	A	75	GLU	CD-OE2	6.03	1.32	1.25
3	A	49	GLU	CD-OE1	5.91	1.32	1.25
1	J	284	GLU	CD-OE1	5.85	1.32	1.25
3	A	31	GLU	CD-OE1	5.75	1.31	1.25
3	A	34	GLU	CD-OE1	5.74	1.31	1.25
3	B	105	GLU	CD-OE1	5.71	1.31	1.25
1	H	360	GLU	CD-OE2	5.62	1.31	1.25
3	B	64	GLU	CD-OE1	5.51	1.31	1.25
2	L	112	GLU	CD-OE1	5.41	1.31	1.25
1	H	99	GLU	CD-OE2	5.41	1.31	1.25
1	H	337	GLU	CD-OE2	5.39	1.31	1.25
2	M	92	GLU	CD-OE2	5.37	1.31	1.25
1	J	99	GLU	CD-OE2	5.29	1.31	1.25
1	J	367	GLU	CD-OE1	5.28	1.31	1.25
3	A	8	GLU	CD-OE1	5.25	1.31	1.25
1	H	1	GLU	CD-OE2	5.21	1.31	1.25
3	B	8	GLU	CD-OE1	5.12	1.31	1.25
1	J	360	GLU	CD-OE2	5.05	1.31	1.25

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	240	ALA	N-CA-CB	-14.04	90.45	110.10
3	B	9	SER	C-N-CD	-11.45	95.41	120.60
1	J	182	SER	N-CA-CB	10.74	126.61	110.50
3	B	10	PRO	N-CA-CB	10.64	116.06	103.30
1	H	182	SER	N-CA-CB	10.48	126.22	110.50
1	J	88	ARG	NE-CZ-NH1	-10.12	115.24	120.30
3	B	10	PRO	CA-N-CD	-9.82	97.75	111.50
1	H	191	ASP	CB-CG-OD2	-9.33	109.90	118.30
1	H	240	ALA	CA-C-N	-9.11	97.16	117.20
1	H	347	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	H	119	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	H	343	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	H	347	ASP	CB-CG-OD1	8.56	126.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	287	ARG	N-CA-CB	8.52	125.94	110.60
1	H	324	ASP	CB-CG-OD2	-8.42	110.72	118.30
1	H	61	HIS	CA-CB-CG	8.37	127.83	113.60
1	H	155	GLY	N-CA-C	-8.35	92.23	113.10
1	J	6	ALA	CA-C-N	-8.27	99.66	116.20
3	B	16	VAL	CA-CB-CG1	8.14	123.11	110.90
1	H	349	ASP	CB-CG-OD2	-8.14	110.98	118.30
2	L	37	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	J	155	GLY	N-CA-C	-8.10	92.86	113.10
2	L	119	CYS	CA-CB-SG	-8.06	99.48	114.00
3	A	16	VAL	CA-CB-CG1	8.04	122.96	110.90
1	H	320	ILE	N-CA-CB	8.04	129.29	110.80
1	J	167	CYS	N-CA-CB	-8.04	96.13	110.60
3	A	24	ASP	N-CA-CB	-8.03	96.14	110.60
3	A	30	TYR	CB-CG-CD2	-7.96	116.23	121.00
3	A	24	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	J	61	HIS	CA-CB-CG	7.89	127.01	113.60
1	H	4	LYS	N-CA-CB	-7.82	96.52	110.60
2	L	24	ASP	CB-CG-OD2	-7.78	111.30	118.30
3	A	11	PHE	CB-CA-C	-7.74	94.91	110.40
1	H	356	ASP	CB-CG-OD1	-7.74	111.34	118.30
1	J	259	ASP	CB-CG-OD1	-7.72	111.36	118.30
1	J	191	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	H	119	ARG	NE-CZ-NH2	-7.66	116.47	120.30
3	A	80	LEU	N-CA-CB	7.58	125.57	110.40
2	M	32	ALA	N-CA-CB	7.56	120.69	110.10
3	A	18	ASP	CB-CG-OD1	7.55	125.10	118.30
1	J	88	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	J	343	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	J	343	ASP	CB-CG-OD1	7.45	125.00	118.30
1	H	25	HIS	N-CA-CB	7.35	123.83	110.60
2	M	8	ASP	CB-CG-OD1	-7.32	111.71	118.30
3	B	41	ASP	CB-CG-OD1	7.28	124.85	118.30
1	J	6	ALA	C-N-CA	7.25	137.53	122.30
3	A	18	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	J	340	ASP	CB-CG-OD2	7.22	124.80	118.30
1	J	25	HIS	N-CA-CB	7.21	123.58	110.60
1	J	24	ASP	CB-CG-OD2	-7.21	111.81	118.30
2	M	8	ASP	CB-CG-OD2	7.19	124.78	118.30
1	H	340	ASP	CB-CG-OD2	7.18	124.76	118.30
3	A	23	VAL	CA-CB-CG2	-7.17	100.14	110.90
2	M	119	CYS	N-CA-CB	-7.17	97.70	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	262	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	J	116	ASP	CB-CG-OD1	-7.12	111.90	118.30
1	H	328	ASP	CB-CG-OD1	-7.09	111.92	118.30
3	B	10	PRO	N-CA-C	7.09	130.53	112.10
3	B	11	PHE	CB-CA-C	-7.08	96.25	110.40
3	B	11	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	J	347	ASP	CB-CG-OD1	6.99	124.59	118.30
1	H	24	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	H	18	SER	N-CA-C	6.98	129.84	111.00
1	J	18	SER	N-CA-CB	-6.97	100.04	110.50
3	B	9	SER	N-CA-CB	-6.94	100.09	110.50
3	A	12	ALA	CB-CA-C	6.94	120.51	110.10
1	J	356	ASP	CB-CG-OD1	-6.93	112.06	118.30
3	B	18	ASP	CB-CG-OD1	6.91	124.52	118.30
3	A	71	MET	N-CA-CB	-6.86	98.25	110.60
1	H	3	SER	CA-C-N	-6.82	102.19	117.20
1	H	191	ASP	CB-CG-OD1	6.77	124.39	118.30
1	J	183	CYS	CB-CA-C	-6.77	96.86	110.40
1	J	286	SER	N-CA-CB	-6.74	100.40	110.50
1	J	347	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	M	36	CYS	CA-CB-SG	-6.71	101.92	114.00
1	H	259	ASP	CB-CG-OD1	-6.69	112.28	118.30
2	M	85	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	M	104	ASP	CB-CG-OD1	-6.65	112.31	118.30
1	J	3	SER	CA-C-N	-6.61	102.65	117.20
1	H	240	ALA	CB-CA-C	-6.61	100.18	110.10
3	B	11	PHE	CB-CG-CD1	6.61	125.43	120.80
3	A	6	PRO	N-CA-CB	6.61	111.23	103.30
1	H	158	ASP	CB-CG-OD1	6.60	124.24	118.30
1	J	18	SER	N-CA-C	6.59	128.80	111.00
1	H	239	PRO	N-CA-CB	6.59	111.21	103.30
2	L	8	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	J	158	ASP	CB-CG-OD1	6.57	124.21	118.30
3	B	41	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	H	159	ASP	CB-CG-OD1	-6.56	112.40	118.30
2	L	76	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	J	81	LEU	CA-CB-CG	6.54	130.35	115.30
2	L	119	CYS	N-CA-CB	-6.51	98.88	110.60
1	J	154	PRO	C-N-CA	6.50	135.96	122.30
1	H	340	ASP	CB-CG-OD1	-6.47	112.47	118.30
1	J	324	ASP	CB-CG-OD1	6.47	124.13	118.30
1	J	324	ASP	CB-CG-OD2	-6.45	112.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	61	HIS	N-CA-CB	-6.40	99.08	110.60
2	L	8	ASP	CB-CG-OD2	6.37	124.04	118.30
3	A	13	ALA	N-CA-C	-6.37	93.81	111.00
1	J	340	ASP	CB-CG-OD1	-6.36	112.58	118.30
2	M	99	ASN	N-CA-C	6.36	128.18	111.00
1	J	116	ASP	CB-CG-OD2	6.36	124.02	118.30
1	H	266	PHE	N-CA-CB	6.35	122.03	110.60
3	B	13	ALA	N-CA-C	-6.35	93.87	111.00
3	B	66	ALA	CB-CA-C	-6.34	100.59	110.10
1	J	320	ILE	N-CA-CB	6.33	125.37	110.80
2	L	99	ASN	N-CA-C	6.32	128.07	111.00
1	J	183	CYS	CA-CB-SG	6.31	125.35	114.00
2	M	24	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	M	101	ASP	CB-CG-OD1	6.29	123.96	118.30
1	H	174	ALA	N-CA-CB	-6.27	101.33	110.10
1	H	19	ASP	N-CA-CB	6.26	121.87	110.60
3	B	99	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	B	58	VAL	CB-CA-C	6.23	123.24	111.40
3	A	10	PRO	N-CA-CB	6.22	110.77	103.30
1	H	158	ASP	CB-CG-OD2	-6.21	112.72	118.30
3	A	11	PHE	CB-CG-CD2	-6.21	116.45	120.80
1	J	310	ILE	N-CA-C	6.20	127.75	111.00
1	J	233	ILE	N-CA-C	6.20	127.74	111.00
1	H	183	CYS	CB-CA-C	-6.18	98.04	110.40
3	B	18	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	J	349	ASP	CB-CG-OD2	-6.17	112.75	118.30
3	B	6	PRO	N-CA-CB	6.17	110.70	103.30
2	M	119	CYS	CA-CB-SG	-6.16	102.91	114.00
2	L	24	ASP	CB-CG-OD1	6.14	123.82	118.30
1	J	191	ASP	CB-CG-OD1	6.13	123.82	118.30
1	H	3	SER	C-N-CA	6.13	137.02	121.70
2	L	98	TYR	C-N-CA	6.12	137.01	121.70
3	B	32	THR	C-N-CD	-6.10	107.18	120.60
1	J	275	THR	N-CA-CB	6.09	121.88	110.30
1	H	182	SER	CB-CA-C	6.09	121.66	110.10
1	J	182	SER	CB-CA-C	6.08	121.66	110.10
1	H	233	ILE	N-CA-C	6.06	127.37	111.00
2	M	17	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	H	6	ALA	N-CA-C	-6.03	94.72	111.00
1	J	232	SER	N-CA-C	6.02	127.26	111.00
2	L	17	ASP	CB-CG-OD1	6.02	123.71	118.30
2	L	98	TYR	CB-CA-C	6.02	122.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	237	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	J	111	ASP	CB-CG-OD2	5.98	123.68	118.30
3	A	66	ALA	N-CA-CB	-5.98	101.73	110.10
2	M	19	ASP	CB-CG-OD1	-5.94	112.95	118.30
2	L	17	ASP	CB-CG-OD2	-5.91	112.98	118.30
3	A	89	ASP	CB-CG-OD2	5.90	123.61	118.30
1	H	324	ASP	CB-CG-OD1	5.90	123.61	118.30
3	A	24	ASP	CB-CG-OD1	5.89	123.60	118.30
3	A	13	ALA	C-N-CA	-5.89	106.98	121.70
1	J	3	SER	C-N-CA	5.87	136.38	121.70
2	M	19	ASP	CB-CG-OD2	5.86	123.58	118.30
1	J	125	ARG	CD-NE-CZ	-5.86	115.40	123.60
3	A	66	ALA	CB-CA-C	-5.86	101.31	110.10
1	H	81	LEU	N-CA-CB	-5.85	98.69	110.40
3	A	89	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	H	237	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	H	19	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	H	342	TYR	CB-CA-C	-5.82	98.77	110.40
1	H	349	ASP	CB-CG-OD1	5.80	123.52	118.30
2	L	99	ASN	C-N-CA	5.79	136.19	121.70
2	M	37	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	H	18	SER	N-CA-CB	-5.79	101.82	110.50
1	H	310	ILE	N-CA-C	5.77	126.58	111.00
1	H	6	ALA	CA-C-N	-5.77	104.66	116.20
1	H	154	PRO	N-CA-CB	5.76	110.21	103.30
3	B	13	ALA	C-N-CA	-5.75	107.32	121.70
1	J	3	SER	N-CA-C	-5.74	95.50	111.00
3	B	58	VAL	N-CA-CB	5.74	124.13	111.50
2	L	100	LYS	N-CA-C	5.73	126.47	111.00
1	H	79	PHE	N-CA-CB	5.73	120.91	110.60
2	L	37	ASP	CB-CG-OD1	5.72	123.45	118.30
1	H	317	ASP	CB-CG-OD2	-5.71	113.16	118.30
3	A	49	GLU	CA-C-N	-5.70	104.67	117.20
1	J	19	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	H	207	THR	CA-CB-CG2	-5.68	104.45	112.40
1	J	125	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	J	356	ASP	CB-CG-OD2	5.67	123.40	118.30
1	J	250	ASP	CB-CG-OD2	5.67	123.40	118.30
1	H	256	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	J	159	ASP	CB-CG-OD1	-5.66	113.20	118.30
1	J	346	SER	N-CA-C	5.64	126.23	111.00
1	H	4	LYS	CA-CB-CG	5.62	125.77	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	232	SER	N-CA-C	5.62	126.18	111.00
1	J	102	ASP	CB-CG-OD1	-5.62	113.24	118.30
3	B	11	PHE	N-CA-CB	-5.61	100.50	110.60
2	M	99	ASN	C-N-CA	5.61	135.71	121.70
3	A	99	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	L	101	ASP	CB-CG-OD1	5.59	123.33	118.30
1	J	262	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	H	32	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	H	168	PHE	N-CA-C	5.57	126.03	111.00
1	H	24	ASP	CB-CG-OD1	5.54	123.28	118.30
1	H	259	ASP	CB-CG-OD2	5.53	123.28	118.30
3	A	11	PHE	N-CA-CB	-5.53	100.65	110.60
1	J	259	ASP	CB-CG-OD2	5.52	123.27	118.30
1	H	343	ASP	CB-CG-OD1	5.52	123.27	118.30
1	H	241	ALA	CB-CA-C	5.51	118.37	110.10
3	A	21	ILE	C-N-CA	-5.50	107.94	121.70
3	B	68	LYS	N-CA-CB	5.50	120.50	110.60
1	J	365	GLN	N-CA-CB	5.50	120.50	110.60
1	J	356	ASP	N-CA-C	5.48	125.79	111.00
1	J	309	PRO	C-N-CA	5.47	135.37	121.70
2	M	98	TYR	CB-CA-C	5.47	121.34	110.40
1	H	116	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	H	119	ARG	N-CA-C	5.46	125.76	111.00
2	M	17	ASP	CB-CG-OD1	5.46	123.22	118.30
1	J	237	ASP	CB-CG-OD1	5.45	123.21	118.30
1	H	196	PRO	N-CA-C	5.45	126.26	112.10
1	J	7	GLY	N-CA-C	-5.45	99.49	113.10
3	A	11	PHE	CB-CG-CD1	5.42	124.59	120.80
1	J	34	SER	N-CA-CB	5.41	118.62	110.50
1	J	6	ALA	N-CA-C	-5.41	96.40	111.00
1	H	15	ALA	N-CA-CB	5.39	117.65	110.10
1	J	119	ARG	N-CA-C	5.38	125.52	111.00
2	M	104	ASP	CB-CG-OD2	5.36	123.13	118.30
2	M	20	ILE	N-CA-CB	5.36	123.13	110.80
1	H	82	ALA	N-CA-CB	5.36	117.60	110.10
1	H	74	HIS	CA-CB-CG	-5.35	104.50	113.60
3	A	10	PRO	N-CA-C	5.35	126.01	112.10
3	A	13	ALA	N-CA-CB	-5.34	102.62	110.10
1	H	238	ILE	C-N-CD	-5.33	108.86	120.60
2	L	88	CYS	CA-CB-SG	5.33	123.60	114.00
1	H	232	SER	C-N-CA	5.33	135.03	121.70
2	M	98	TYR	C-N-CA	5.32	135.00	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	101	ASP	CB-CG-OD2	-5.31	113.52	118.30
3	A	72	MET	N-CA-CB	5.29	120.13	110.60
1	J	123	GLY	N-CA-C	-5.26	99.94	113.10
3	B	15	GLU	CG-CD-OE2	-5.25	107.79	118.30
1	J	276	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	J	180	LEU	N-CA-C	-5.25	96.84	111.00
1	H	154	PRO	C-N-CA	5.21	133.23	122.30
1	H	174	ALA	CB-CA-C	-5.20	102.30	110.10
2	L	94	GLU	N-CA-CB	5.19	119.95	110.60
2	M	100	LYS	N-CA-C	5.17	124.97	111.00
2	M	99	ASN	O-C-N	5.15	130.93	122.70
1	H	54	GLY	N-CA-C	-5.14	100.24	113.10
2	L	76	ASP	CB-CG-OD2	5.13	122.92	118.30
2	M	98	TYR	CA-C-N	-5.11	105.97	117.20
1	J	328	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	J	266	PHE	N-CA-CB	5.09	119.76	110.60
3	A	17	ALA	N-CA-C	-5.08	97.28	111.00
3	B	76	GLN	O-C-N	-5.08	114.57	122.70
1	H	187	LEU	N-CA-C	5.08	124.72	111.00
1	H	61	HIS	CB-CA-C	-5.08	100.25	110.40
3	A	64	GLU	N-CA-CB	5.07	119.72	110.60
2	M	94	GLU	N-CA-CB	5.05	119.70	110.60
3	B	8	GLU	N-CA-CB	5.05	119.69	110.60
3	B	89	ASP	CB-CG-OD2	5.05	122.84	118.30
1	H	159	ASP	CB-CG-OD2	5.04	122.84	118.30
1	H	79	PHE	CB-CA-C	5.01	120.42	110.40
1	H	237	ASP	CB-CG-OD1	5.01	122.81	118.30
3	B	8	GLU	N-CA-C	5.01	124.52	111.00

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

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Mol	Chain	Res	Type	Group
1	J	180	LEU	Mainchain
2	M	98	TYR	Mainchain

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	H	2582	0	2472	219	0
1	J	2583	0	2472	237	0
2	L	910	0	808	85	0
2	M	910	0	809	108	0
3	A	790	0	774	226	0
3	B	790	0	774	206	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8567	0	8109	1009	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 (1009) 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
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
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
3:A:54:ASN:HB3	3:A:71:MET:HE3	1.33	1.07
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:J:44:GLY:H	2:M:81:ASN:ND2	1.65	0.95
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:B:25:ILE:HG21	3:B:48:ARG:C	1.90	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: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: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:12:ALA:HB1	3:A:76:GLN:CD	1.94	0.87
3:A:39:VAL:HG12	3:A:104:VAL:HG12	1.56	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: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:J:205:GLN:HG2	1:J:245:MET:HE2	1.59	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
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
3:B:25:ILE:HG13	3:B:49:GLU:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:54:ASN:CB	3:A:71:MET:HE3	2.12	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
2:L:97:VAL:C	2:L:99:ASN:H	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:124:VAL:HG12	1:J:19:ASP:OD2	1.85	0.75
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
1:J:205:GLN:HG2	1:J:245:MET:HE1	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:253:GLU:H	1:J:256:ARG:HD2	1.56	0.71
2:L:58:VAL:HG21	3:A:51:MET:HE3	1.71	0.71
3:B:20:ALA:O	3:B:21:ILE:HB	1.91	0.71
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
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: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
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: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
3:A:25:ILE:HD11	3:A:98:MET:HE3	1.75	0.66
1:H:272:LEU:HD23	1:H:275:THR:H	1.61	0.66
3:B:10:PRO:C	3:B:11:PHE:HD1	1.98	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: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
3:A:70:PRO:C	3:A:71:MET:HG2	2.13	0.65
1:H:205:GLN:HG2	1:H:245:MET:HE2	1.79	0.65
2:L:100:LYS:HD2	3:A:28:MET:HE1	1.79	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
3:A:28:MET:O	3:A:29:LYS:HB3	1.97	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:B:54:ASN:HB3	3:B:71:MET:CE	2.26	0.64
3:A:7:SER:CB	3:A:81:THR:HG23	2.26	0.64
3:A:53:HIS:HD1	3:A:95:HIS:HE1	1.45	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: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
3:A:95:HIS:HB3	3:A:97:PHE:CE2	2.33	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
1:J:136:ALA:O	1:J:154:PRO:HD2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:21:ILE:HG21	3:B:42:THR:C	2.19	0.62
1:H:117:ALA:N	1:H:118:PRO:HD3	2.14	0.62
3:A:71:MET:O	3:A:72:MET:HB2	1.99	0.62
3:B:54:ASN:HB3	3:B:71:MET:HE2	1.80	0.62
1:J:283:VAL:HG12	1:J:293:ALA:HB1	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
3:A:54:ASN:HB3	3:A:71:MET:CE	2.21	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
1:H:343:ASP:C	1:H:345:ALA:H	2.03	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
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
1:J:38:LEU:HG	1:J:38:LEU:O	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:10:PRO:C	3:A:11:PHE:HD1	2.03	0.61
1:H:328:ASP:HB3	1:H:341:ILE:HD13	1.82	0.60
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: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
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
3:A:6:PRO:CB	3:A:82:PHE:HA	2.31	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:229:VAL:C	1:J:231:SER:H	2.04	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
2:M:97:VAL:C	2:M:99:ASN:H	2.02	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
3:A:45:TRP:C	3:A:46:ILE:HG22	2.22	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
3:A:15:GLU:O	3:A:16:VAL:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:43:VAL:CG2	3:B:82:PHE:HE1	2.15	0.59
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: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
2:M:99:ASN:C	2:M:100:LYS:HD3	2.23	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: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
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
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:B:28:MET:HE1	3:B:51:MET:HG2	1.86	0.57
3:B:95:HIS:C	3:B:97:PHE:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:M:12:LYS:HZ2	2:M:13:TRP:H	1.52	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
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
3:B:58:VAL:CG1	3:B:59:ALA:N	2.68	0.56
1:H:38:LEU:HD21	1:H:40:ALA:HB2	1.85	0.56
3:B:57:PHE:HE2	3:B:88:TYR:CB	2.18	0.56
3:A:50:ALA:C	3:A:73:LYS:HZ3	2.08	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
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
2:M:117:TYR:HE1	2:M:120:SER:HG	1.52	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
3:B:10:PRO:C	3:B:11:PHE:CD1	2.79	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:138:LEU:C	1:J:138:LEU:HD23	2.27	0.55
1:J:168:PHE:N	1:J:168:PHE:CD1	2.75	0.55
2:M:13:TRP:CH2	2:M:24:ASP:HA	2.41	0.55
3:A:29:LYS:O	3:A:30:TYR:C	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:361:SER:C	1:H:362:LEU:HD12	2.27	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:A:72:MET:HB3	3:A:76:GLN:CD	2.26	0.55
1:H:283:VAL:CG2	1:H:284:GLU:H	2.20	0.55
3:A:23:VAL:CG2	3:A:45:TRP:CD2	2.88	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
1:H:205:GLN:HG3	1:H:245:MET:HE1	1.90	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
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:25:ILE:HD11	3:A:98:MET:HE1	1.89	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:59:LEU:C	2:M:40:ALA:HB2	2.28	0.54
2:L:66:ASP:O	2:L:66:ASP:OD1	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:VAL:C	1:H:231:SER:H	2.10	0.53
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
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
3:A:87:THR:CB	3:A:103:VAL:HG22	2.38	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
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:B:24:ASP:O	3:B:25:ILE:O	2.28	0.52
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:VAL:O	1:J:231:SER:N	2.43	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:H:179:TYR:C	1:H:181:GLY:H	2.12	0.52
2:L:44:THR:C	2:L:121:ILE:HD11	2.29	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: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:J:343:ASP:C	1:J:345:ALA:H	2.13	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
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:341:ILE:HD12	1:H:341:ILE:C	2.30	0.51
2:M:14:GLN:H	2:M:14:GLN:CD	2.14	0.51
2:M:73:ALA:O	2:M:123:PRO:HD2	2.11	0.51
3:A:55:VAL:O	3:A:68:LYS:O	2.27	0.51
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:21:ILE:CG2	3:B:42:THR:O	2.47	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
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: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:H:205:GLN:HG2	1:H:245:MET:CE	2.41	0.50
1:J:232:SER:HB2	1:J:250:ASP:HA	1.92	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:5:ILE:O	3:B:5:ILE:CG1	2.60	0.50
3:B:5:ILE:CA	3:B:6:PRO:CG	2.89	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
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:A:35:LEU:HD13	3:A:35:LEU:C	2.32	0.50
3:B:37:VAL:HG12	3:B:41:ASP:CG	2.31	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
2:L:97:VAL:C	2:L:99:ASN:N	2.63	0.50
3:A:34:GLU:OE1	3:A:101:LYS:NZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
3:B:28:MET:HE3	3:B:53:HIS:HE1	1.75	0.49
1:H:111:ASP:CG	1:J:88:ARG:HH12	2.15	0.49
1:J:266:PHE:O	1:J:268:MET:N	2.45	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
3:A:16:VAL:O	3:A:17:ALA:HB2	2.11	0.49
1:H:192:LEU:C	1:H:192:LEU:HD22	2.32	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
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
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
1:H:354:GLU:C	1:H:356:ASP:H	2.15	0.49
1:J:71:VAL:HG23	1:J:80:ALA:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:21:ILE:C	3:B:22:VAL:HG12	2.33	0.49
3:B:43:VAL:HG21	3:B:82:PHE:HE1	1.78	0.49
2:L:40:ALA:HB2	1:J:59:LEU:C	2.33	0.48
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
1:J:229:VAL:C	1:J:231:SER:N	2.67	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
2:L:58:VAL:CG2	3:A:51:MET:HE3	2.41	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: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
2:M:14:GLN:CD	2:M:14:GLN:N	2.67	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
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
3:B:27:LYS:O	3:B:28:MET:C	2.51	0.48
1:H:343:ASP:OD2	1:H:345:ALA:HB3	2.14	0.47
3:A:95:HIS:C	3:A:97:PHE:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:47:ASN:HD21	3:B:53:HIS:CD2	2.23	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
2:L:40:ALA:CB	1:J:59:LEU:C	2.83	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
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:A:53:HIS:C	3:A:71:MET:HB3	2.36	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:231:SER:O	1:J:232:SER:OG	2.25	0.47
1:J:239:PRO:HG2	1:J:241:ALA:O	2.14	0.47
1:H:151:LEU:HD22	1:H:159:ASP:CB	2.44	0.47
1:H:179:TYR:C	1:H:181:GLY:N	2.67	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:A:45:TRP:C	3:A:46:ILE:CG2	2.82	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
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
1:H:100:VAL:O	1:H:109:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:VAL:C	1:H:231:SER:N	2.69	0.46
1:H:259:ASP:O	1:H:260:ASN:HB2	2.16	0.46
3:A:10:PRO:C	3:A:11:PHE:CD1	2.87	0.46
1:H:229:VAL:O	1:H:231:SER:N	2.48	0.46
1:J:303:VAL:C	1:J:305:GLN:H	2.16	0.46
3:A:47:ASN:O	3:A:75:GLU:HA	2.15	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
2:M:97:VAL:C	2:M:99:ASN:N	2.68	0.46
3:A:26:ALA:C	3:A:28:MET:N	2.67	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
1:J:276:ASP:CG	1:J:301:ALA:HB3	2.36	0.46
3:B:67:LEU:HD21	3:B:78:TYR:CZ	2.50	0.46
1:H:345:ALA:O	1:H:346:SER:HB2	2.15	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: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:J:267:GLN:CB	1:J:318:ALA:HB1	2.43	0.46
3:B:4:THR:C	3:B:5:ILE:HG23	2.36	0.46
1:J:125:ARG:HH11	1:J:125:ARG:HD3	1.48	0.45
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
1:J:341:ILE:HD12	1:J:341:ILE:C	2.37	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
1:H:69:LEU:CD2	1:H:129:ILE:HB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:100:LYS:CD	3:A:28:MET:HE1	2.47	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: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:103:ASN:HD22	2:M:103:ASN:C	2.20	0.45
2:M:106:ILE:CD1	2:M:108:CYS:HB2	2.47	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
1:J:167:CYS:HG	1:J:180:LEU:HG	1.82	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
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:H:167:CYS:HG	1:H:183:CYS:HG	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:H:151:LEU:O	1:H:159:ASP:N	2.48	0.44
1:J:229:VAL:HG23	1:J:230:ALA:N	2.33	0.44
3:A:22:VAL:HG12	3:A:44:THR:C	2.38	0.44
3:A:24:ASP:O	3:A:25:ILE:CB	2.66	0.44
3:B:6:PRO:CG	3:B:83:THR:N	2.72	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:2:LYS:O	1:H:2:LYS:HG3	2.18	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: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
1:J:144:GLY:O	1:J:145:SER:HB2	2.19	0.43
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
3:B:93:THR:C	3:B:95:HIS:H	2.21	0.43
1:H:60:GLY:HA2	2:M:40:ALA:CB	2.48	0.43
2:L:45:SER:N	2:L:121:ILE:HD11	2.32	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
2:M:90:ASN:C	2:M:91:THR:HG23	2.39	0.43
3:B:43:VAL:HG23	3:B:80:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:303:VAL:C	1:H:305:GLN:H	2.17	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
3:B:28:MET:HE1	3:B:53:HIS:CE1	2.53	0.43
1:H:151:LEU:HD23	1:H:151:LEU:C	2.38	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
1:H:63:LEU:CD1	2:M:80:TYR:HA	2.49	0.43
2:L:79:GLY:H	2:L:116:THR:HG23	1.83	0.43
3:A:41:ASP:C	3:A:42:THR:HG22	2.37	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:H:205:GLN:CG	1:H:245:MET:CE	2.96	0.42
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
2:M:25:TYR:HB3	2:M:28:HIS:CD2	2.53	0.42
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:4:THR:C	3:A:5:ILE:HG23	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:20:ALA:O	3:A:21:ILE:CB	2.59	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: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
1:J:119:ARG:O	1:J:120:PHE:HB3	2.19	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:H:150:GLY:HA2	1:H:161:LEU:HD13	2.01	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
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:28:MET:C	3:B:98:MET:SD	2.97	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
1:H:38:LEU:HD12	1:H:358:GLY:C	2.41	0.41
3:B:51:MET:HE3	3:B:51:MET:HB2	1.85	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: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:95:HIS:C	3:A:97:PHE:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:71:MET:C	3:B:72:MET:CG	2.85	0.41
1:H:69:LEU:HD12	1:H:69:LEU:C	2.40	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: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:14:ALA:C	1:H:16:ALA:H	2.24	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: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
3:B:95:HIS:C	3:B:97:PHE:N	2.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:CYS:C	1:H:168:PHE:CD1	2.94	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:73:LYS:C	3:A:75:GLU:N	2.75	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%)	1	1
1	J	366/368 (100%)	291 (80%)	42 (12%)	33 (9%)	1	0
2	L	118/121 (98%)	98 (83%)	12 (10%)	8 (7%)	1	1
2	M	118/121 (98%)	94 (80%)	14 (12%)	10 (8%)	1	1
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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%)	219 (83%)	45 (17%)	2	3
1	J	264/264 (100%)	225 (85%)	39 (15%)	3	5
2	L	99/99 (100%)	83 (84%)	16 (16%)	2	4
2	M	99/99 (100%)	85 (86%)	14 (14%)	3	6
3	A	83/83 (100%)	54 (65%)	29 (35%)	0	0
3	B	83/83 (100%)	56 (68%)	27 (32%)	0	0
All	All	892/892 (100%)	722 (81%)	170 (19%)	1	2

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	21	SER
1	H	37	THR
1	H	48	ASN
1	H	69	LEU
1	H	93	LYS
1	H	105	THR
1	H	122	VAL
1	H	131	ASN
1	H	142	LEU
1	H	182	SER

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Mol	Chain	Res	Type
1	H	187	LEU
1	H	190	SER
1	H	192	LEU
1	H	202	VAL
1	H	205	GLN
1	H	206	CYS
1	H	207	THR
1	H	215	GLN
1	H	218	GLN
1	H	225	LEU
1	H	233	ILE
1	H	244	THR
1	H	250	ASP
1	H	253	GLU
1	H	262	ARG
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	323	GLN
1	H	327	SER
1	H	338	VAL
1	H	341	ILE
1	H	352	SER
1	H	362	LEU
1	H	365	GLN
2	L	14	GLN
2	L	26	TRP
2	L	34	ASN
2	L	43	LEU
2	L	50	THR
2	L	71	ILE
2	L	89	LEU
2	L	94	GLU

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Mol	Chain	Res	Type
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	21	SER
1	J	50	VAL
1	J	61	HIS
1	J	69	LEU
1	J	89	SER
1	J	122	VAL
1	J	126	VAL
1	J	131	ASN
1	J	132	CYS
1	J	142	LEU
1	J	145	SER
1	J	151	LEU
1	J	153	VAL
1	J	187	LEU
1	J	192	LEU
1	J	201	ILE
1	J	202	VAL
1	J	205	GLN
1	J	225	LEU
1	J	233	ILE
1	J	234	LEU
1	J	245	MET
1	J	269	VAL
1	J	271	LYS
1	J	278	ILE
1	J	287	ARG
1	J	290	LEU
1	J	295	ASN
1	J	307	SER
1	J	310	ILE
1	J	315	ASP
1	J	323	GLN
1	J	338	VAL

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Mol	Chain	Res	Type
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	26	TRP
2	M	34	ASN
2	M	43	LEU
2	M	50	THR
2	M	71	ILE
2	M	82	VAL
2	M	89	LEU
2	M	94	GLU
2	M	100	LYS
2	M	103	ASN
2	M	106	ILE
2	M	119	CYS
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	28	MET
3	A	29	LYS
3	A	35	LEU
3	A	37	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

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Mol	Chain	Res	Type
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	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
3	B	35	LEU
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	61	VAL
3	B	62	LEU
3	B	72	MET
3	B	73	LYS
3	B	74	LYS
3	B	81	THR
3	B	87	THR
3	B	92	CYS
3	B	93	THR
3	B	95	HIS
3	B	98	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	171	HIS
1	H	178	HIS
1	H	205	GLN
1	H	210	GLN
1	H	215	GLN

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Mol	Chain	Res	Type
1	H	260	ASN
1	H	267	GLN
1	H	305	GLN
1	H	323	GLN
2	L	34	ASN
2	L	81	ASN
2	L	103	ASN
1	J	25	HIS
1	J	35	HIS
1	J	48	ASN
1	J	131	ASN
1	J	160	GLN
1	J	205	GLN
1	J	210	GLN
1	J	215	GLN
1	J	218	GLN
1	J	267	GLN
1	J	295	ASN
1	J	305	GLN
1	J	323	GLN
1	J	365	GLN
2	M	34	ASN
2	M	81	ASN
2	M	103	ASN
3	A	95	HIS
3	B	95	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	M	57	2	13,17,18	4.85	5 (38%)	14,24,26	2.66	7 (50%)
2	TRQ	L	57	2	13,17,18	4.48	4 (30%)	14,24,26	2.79	5 (35%)

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	M	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	L	57	2	-	1/4/19/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	57	TRQ	CH2-CZ2	-14.82	1.37	1.54
2	L	57	TRQ	CH2-CZ2	-12.70	1.39	1.54
2	L	57	TRQ	CE2-CZ2	-8.99	1.38	1.50
2	M	57	TRQ	CE2-CZ2	-7.92	1.39	1.50
2	M	57	TRQ	CZ3-CH2	-3.42	1.36	1.45
2	L	57	TRQ	CZ3-CH2	-2.60	1.38	1.45
2	L	57	TRQ	CD2-CE3	-2.40	1.39	1.44
2	M	57	TRQ	CD2-CE3	-2.18	1.40	1.44
2	M	57	TRQ	CB-CG	-2.07	1.48	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	57	TRQ	CZ2-CE2-NE1	6.87	130.92	119.94
2	M	57	TRQ	CZ2-CE2-NE1	6.30	129.99	119.94
2	M	57	TRQ	O6-CH2-CZ2	4.43	121.52	118.51
2	L	57	TRQ	O6-CH2-CZ2	4.24	121.39	118.51
2	L	57	TRQ	O7-CZ2-CE2	-3.92	117.69	121.84
2	M	57	TRQ	CB-CG-CD1	-2.76	124.55	127.97
2	L	57	TRQ	O7-CZ2-CH2	2.72	122.20	119.00
2	M	57	TRQ	CG-CB-CA	-2.72	110.32	114.53
2	M	57	TRQ	CE3-CZ3-CH2	2.63	123.07	121.08
2	M	57	TRQ	CE2-CD2-CE3	-2.59	115.92	119.15
2	L	57	TRQ	CB-CG-CD1	-2.59	124.77	127.97
2	M	57	TRQ	O7-CZ2-CH2	2.02	121.37	119.00

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	M	57	TRQ	7	0
2	L	57	TRQ	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.