



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:47 PM UTC

PDB ID : 4K17 / pdb_00004k17
Title : Crystal Structure of mouse CARMIL residues 1-668
Authors : Zwolak, A.; Dominguez, R.
Deposited on : 2013-04-04
Resolution : 2.90 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

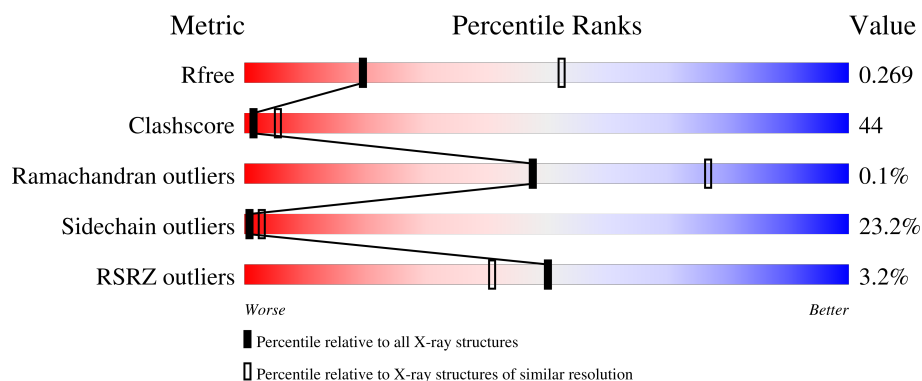
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	669	3% 41% 41% 14% ..
1	B	669	4% 42% 41% 14% ..
1	C	669	2% 37% 46% 12% ..
1	D	669	4% 38% 42% 16% ..

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	702	-	-	X	-
4	ABU	C	701	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20371 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.

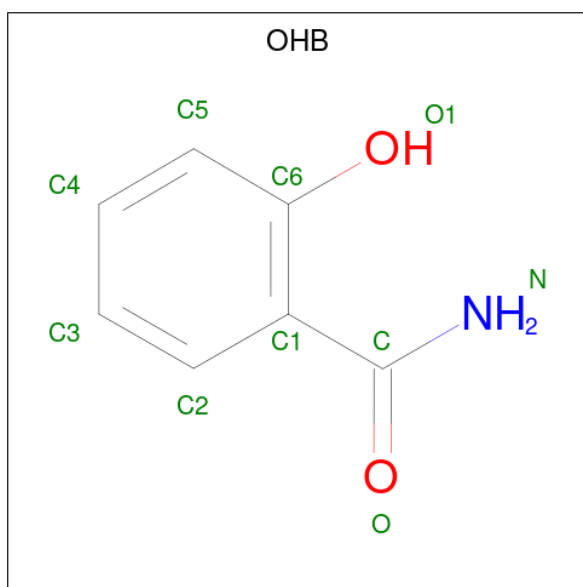
- Molecule 1 is a protein called Leucine-rich repeat-containing protein 16A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	Se	0	2	0
			5112	3220	888	969	17	18			
1	B	660	Total	C	N	O	S	Se	0	0	0
			5102	3211	884	973	16	18			
1	C	656	Total	C	N	O	S	Se	0	0	0
			5073	3196	880	963	16	18			
1	D	655	Total	C	N	O	S	Se	0	0	0
			5066	3191	879	962	16	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q6EDY6
B	0	SER	-	expression tag	UNP Q6EDY6
C	0	SER	-	expression tag	UNP Q6EDY6
D	0	SER	-	expression tag	UNP Q6EDY6

- Molecule 2 is salicylamide (CCD ID: OHB) (formula: C₇H₇NO₂).

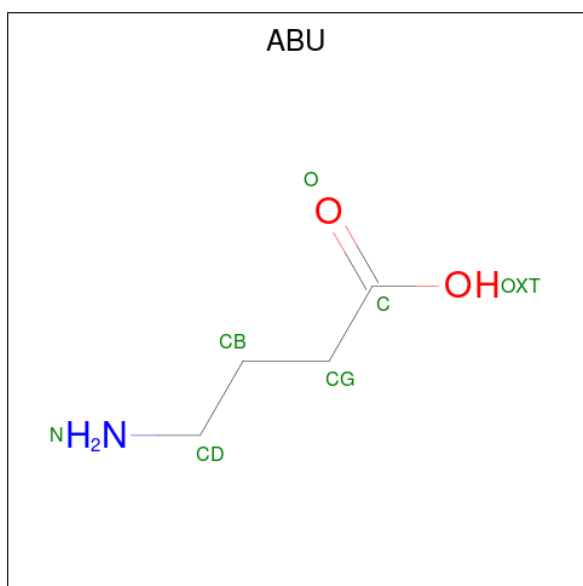


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: C₄H₉NO₂).

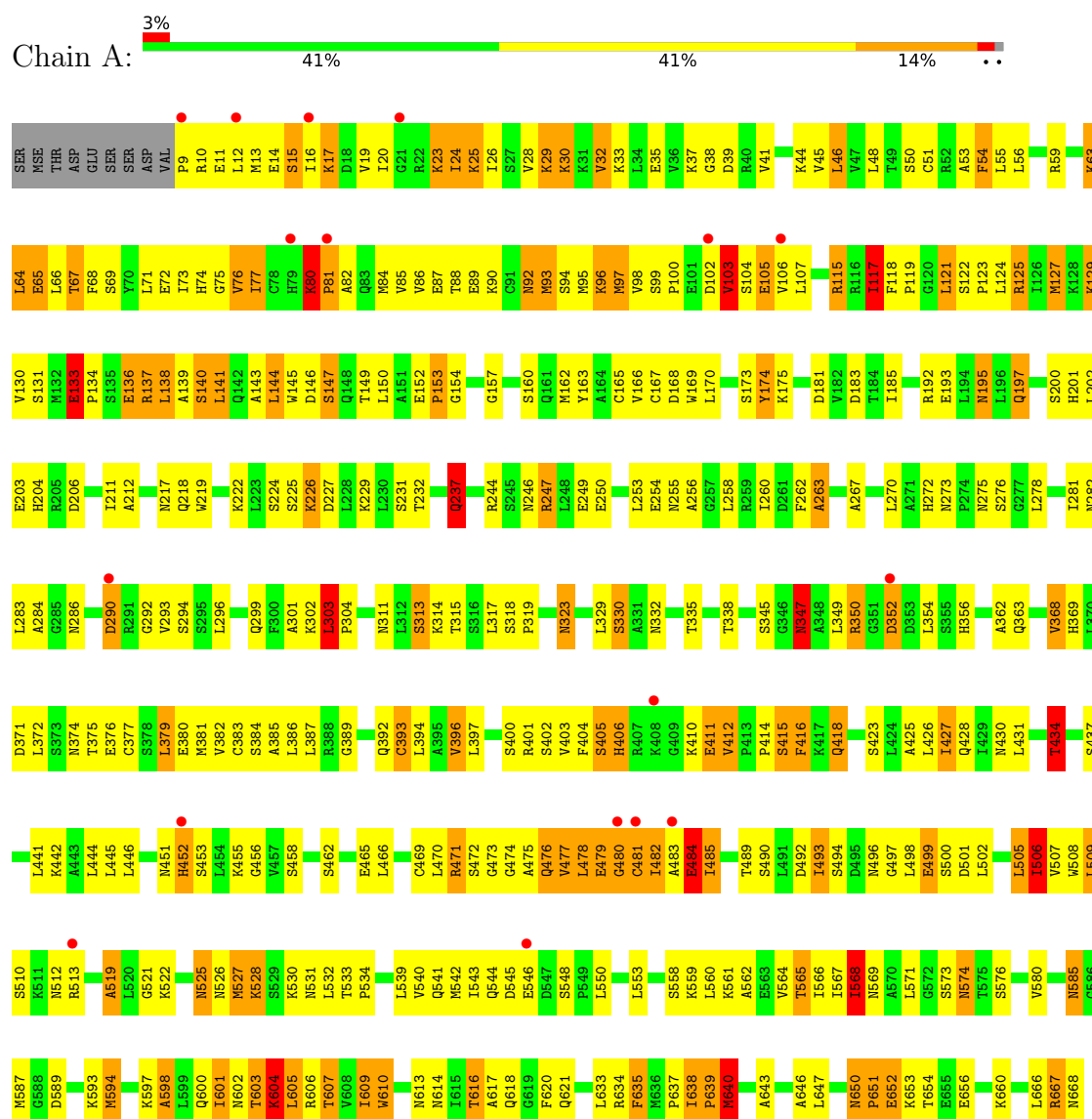


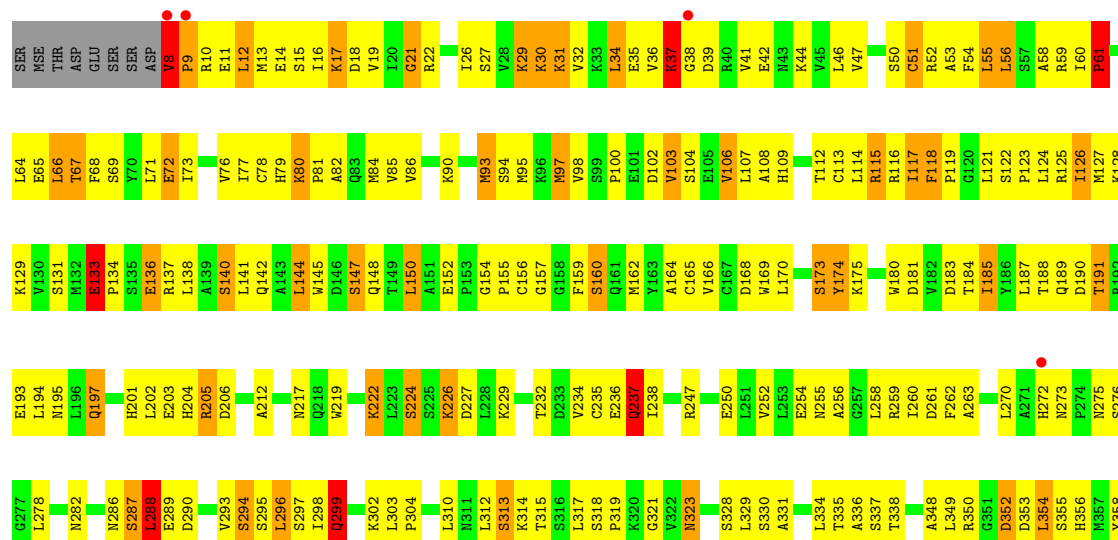
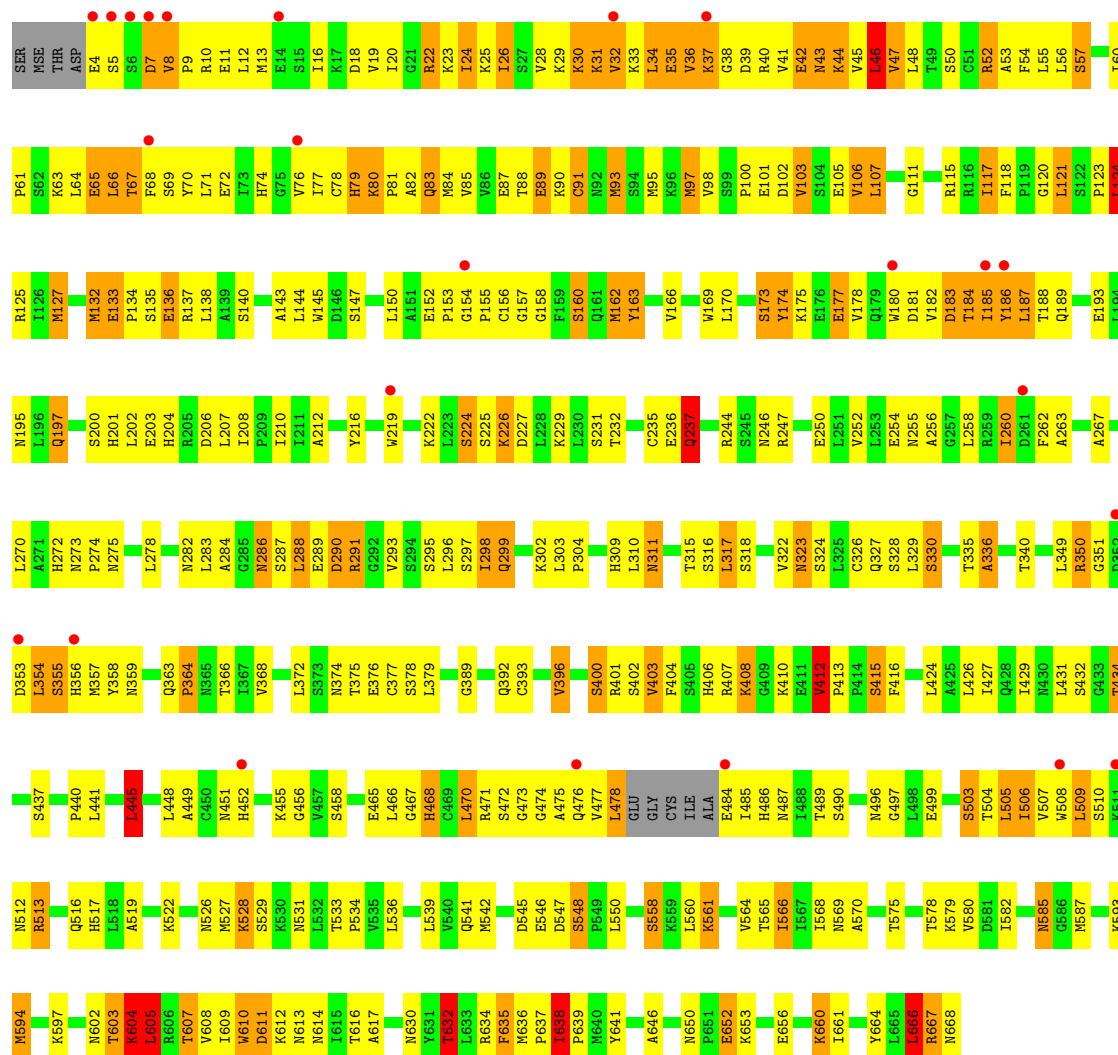
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			7	4	1	2		

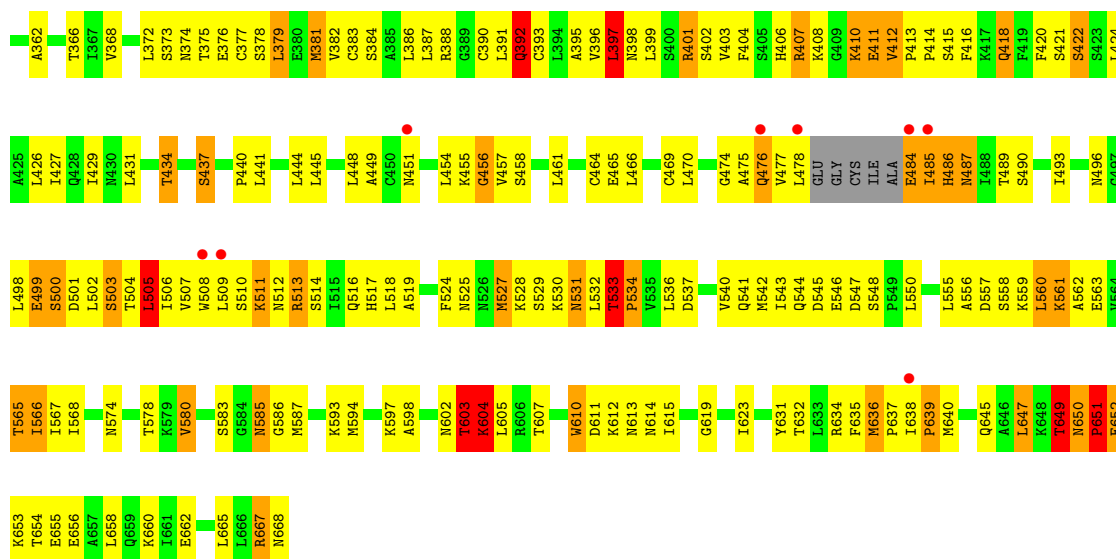
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Leucine-rich repeat-containing protein 16A

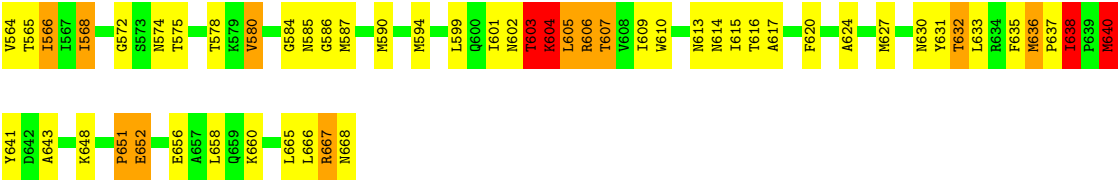






● Molecule 1: Leucine-rich repeat-containing protein 16A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.17Å 67.99Å 212.15Å 92.73° 96.95° 110.15°	Depositor
Resolution (Å)	49.76 – 2.90 49.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.4 (49.76-2.90) 67.1 (49.76-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.259 0.219 , 0.269	Depositor DCC
R_{free} test set	2001 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20371	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OHB, ABU, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.52	35/5179 (0.7%)	1.39	58/6967 (0.8%)
1	B	1.44	34/5160 (0.7%)	1.34	59/6941 (0.9%)
1	C	1.38	21/5131 (0.4%)	1.35	57/6902 (0.8%)
1	D	1.17	14/5124 (0.3%)	1.36	49/6891 (0.7%)
All	All	1.38	104/20594 (0.5%)	1.36	223/27701 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
All	All	0	6

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	ILE	CA-CB	-8.59	1.43	1.54
1	A	519	ALA	CA-CB	-8.58	1.40	1.53
1	A	540	VAL	CA-CB	-7.65	1.45	1.54
1	C	164	ALA	CA-CB	-7.33	1.41	1.53
1	B	133	GLU	C-N	7.07	1.41	1.33
1	B	666	LEU	CG-CD1	-7.02	1.29	1.52
1	A	237	GLN	CD-NE2	-6.80	1.19	1.33
1	D	384	SER	C-O	6.77	1.31	1.24
1	B	609	ILE	C-O	-6.72	1.16	1.24
1	C	412	VAL	N-CA	-6.67	1.41	1.46
1	A	406	HIS	CG-ND1	-6.66	1.30	1.38
1	B	605	LEU	CG-CD1	-6.62	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ILE	CA-CB	-6.55	1.46	1.54
1	B	400	SER	CA-C	-6.41	1.44	1.53
1	D	519	ALA	CA-CB	-6.39	1.43	1.53
1	C	222	LYS	C-O	-6.37	1.16	1.24
1	B	396	VAL	C-O	-6.36	1.17	1.24
1	A	452	HIS	CG-ND1	-6.29	1.31	1.38
1	B	336	ALA	CA-CB	-6.26	1.43	1.53
1	C	126	ILE	CA-CB	-6.19	1.46	1.54
1	C	397	LEU	C-O	-6.18	1.17	1.24
1	A	303	LEU	CA-C	-6.17	1.46	1.52
1	B	309	HIS	CG-ND1	-6.10	1.31	1.38
1	B	412	VAL	CA-C	-6.09	1.47	1.52
1	A	253	LEU	C-O	-6.05	1.17	1.24
1	B	605	LEU	CG-CD2	-5.88	1.33	1.52
1	A	452	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	211	ILE	CA-CB	-5.86	1.46	1.54
1	C	237	GLN	CD-NE2	-5.84	1.21	1.33
1	A	423	SER	CA-C	-5.83	1.45	1.52
1	B	641	TYR	C-O	-5.83	1.17	1.24
1	A	195	ASN	C-O	-5.82	1.17	1.24
1	C	299	GLN	CD-NE2	-5.79	1.21	1.33
1	C	636	MSE	C-N	5.77	1.40	1.33
1	B	154	GLY	C-N	5.75	1.40	1.33
1	B	8	VAL	C-N	5.67	1.41	1.33
1	C	429	ILE	C-O	-5.64	1.18	1.24
1	D	317	LEU	CG-CD1	-5.62	1.34	1.52
1	A	313	SER	CA-C	-5.62	1.45	1.52
1	B	570	ALA	CA-CB	-5.61	1.44	1.53
1	A	376	GLU	C-O	-5.61	1.16	1.23
1	A	263	ALA	CA-CB	-5.61	1.44	1.53
1	A	430	ASN	C-O	-5.58	1.17	1.24
1	B	311	ASN	C-O	-5.57	1.17	1.24
1	C	519	ALA	CA-CB	-5.56	1.45	1.53
1	B	611	ASP	CA-C	-5.56	1.45	1.53
1	D	384	SER	CA-C	5.55	1.60	1.52
1	B	317	LEU	CG-CD1	-5.53	1.34	1.52
1	B	309	HIS	CD2-NE2	-5.53	1.31	1.37
1	C	636	MSE	CA-C	-5.52	1.46	1.52
1	D	640	MSE	CA-C	-5.52	1.45	1.52
1	A	406	HIS	CD2-NE2	-5.50	1.31	1.37
1	C	154	GLY	C-N	5.50	1.40	1.33
1	B	445	LEU	CG-CD2	-5.49	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLY	C-N	5.49	1.40	1.33
1	A	347	ASN	C-O	-5.47	1.16	1.23
1	A	640	MSE	CG-SE	5.47	2.11	1.95
1	A	462	SER	C-O	-5.46	1.17	1.23
1	B	426	LEU	CA-C	-5.43	1.45	1.52
1	A	428	GLN	C-O	-5.40	1.17	1.24
1	C	61	PRO	N-CD	5.40	1.55	1.47
1	B	153	PRO	N-CD	5.38	1.55	1.47
1	A	639	PRO	N-CD	5.37	1.55	1.47
1	A	635	PHE	C-O	-5.35	1.17	1.24
1	B	310	LEU	C-O	-5.34	1.17	1.24
1	D	638	ILE	C-O	-5.34	1.18	1.25
1	B	561	LYS	C-O	-5.33	1.19	1.24
1	B	661	ILE	CA-CB	-5.32	1.47	1.54
1	D	123	PRO	N-CD	5.31	1.55	1.47
1	A	616	THR	CA-C	-5.31	1.46	1.52
1	D	118	PHE	C-N	5.31	1.40	1.33
1	B	237	GLN	CD-OE1	-5.30	1.13	1.23
1	B	652	GLU	C-O	-5.27	1.18	1.24
1	C	106	VAL	CA-CB	5.26	1.60	1.54
1	B	638	ILE	CA-C	-5.24	1.46	1.52
1	A	237	GLN	CD-OE1	-5.22	1.13	1.23
1	B	646	ALA	C-O	-5.19	1.17	1.24
1	D	237	GLN	CD-OE1	-5.18	1.13	1.23
1	B	636	MSE	C-N	5.18	1.40	1.33
1	D	119	PRO	N-CD	5.16	1.54	1.47
1	C	118	PHE	C-N	5.16	1.40	1.33
1	A	396	VAL	C-O	-5.16	1.18	1.24
1	D	651	PRO	N-CD	5.15	1.54	1.47
1	A	153	PRO	N-CD	5.15	1.54	1.47
1	B	610	TRP	NE1-CE2	-5.15	1.31	1.37
1	A	362	ALA	CA-CB	-5.15	1.44	1.53
1	D	643	ALA	CA-CB	-5.14	1.45	1.53
1	B	519	ALA	CA-CB	-5.13	1.45	1.53
1	A	574	ASN	CA-C	-5.11	1.46	1.52
1	A	605	LEU	CG-CD2	-5.08	1.35	1.52
1	A	118	PHE	C-N	5.08	1.40	1.33
1	A	598	ALA	CA-CB	-5.08	1.45	1.53
1	D	636	MSE	N-CA	-5.07	1.42	1.46
1	C	534	PRO	N-CD	5.06	1.54	1.47
1	C	362	ALA	CA-CB	-5.05	1.45	1.53
1	C	9	PRO	N-CD	5.05	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	ILE	C-O	-5.04	1.18	1.24
1	C	180	TRP	CA-C	-5.03	1.46	1.52
1	D	228	LEU	CA-C	-5.03	1.46	1.52
1	C	119	PRO	N-CD	5.02	1.54	1.47
1	A	80	LYS	C-N	5.02	1.40	1.34
1	B	582	ILE	CA-CB	-5.01	1.47	1.54
1	C	635	PHE	C-O	-5.01	1.18	1.24
1	B	432	SER	CA-C	-5.00	1.46	1.52

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	ARG	NE-CZ-NH2	-11.73	108.64	119.20
1	D	389	GLY	N-CA-C	11.60	126.53	112.49
1	A	389	GLY	N-CA-C	11.54	127.54	112.77
1	D	192	ARG	NE-CZ-NH2	11.35	129.42	119.20
1	A	604	LYS	N-CA-C	10.99	127.06	112.88
1	A	548	SER	CA-C-N	10.98	131.29	119.87
1	A	548	SER	C-N-CA	10.98	131.29	119.87
1	C	412	VAL	N-CA-C	-10.54	97.97	107.56
1	D	192	ARG	NE-CZ-NH1	-10.49	111.01	121.50
1	D	133	GLU	CA-C-N	-10.05	108.33	119.98
1	D	133	GLU	C-N-CA	-10.05	108.33	119.98
1	B	389	GLY	N-CA-C	9.09	124.40	112.77
1	C	392	GLN	N-CA-C	8.84	120.99	111.36
1	D	640	MSE	CB-CA-C	-8.80	97.07	110.88
1	A	527	MSE	N-CA-CB	-8.63	95.68	111.13
1	D	60	ILE	C-N-CD	8.61	139.55	120.60
1	B	604	LYS	N-CA-C	8.59	123.96	112.88
1	A	260	ILE	N-CA-C	8.46	120.26	110.62
1	D	632	THR	N-CA-C	8.45	120.57	111.36
1	B	132	MSE	N-CA-C	-8.21	95.53	109.24
1	D	548	SER	CA-C-N	8.21	128.40	119.87
1	D	548	SER	C-N-CA	8.21	128.40	119.87
1	A	416	PHE	N-CA-C	8.16	119.96	111.14
1	C	117	ILE	CB-CA-C	-8.13	100.00	111.38
1	C	60	ILE	C-N-CD	8.10	138.42	120.60
1	C	548	SER	CA-C-N	8.00	128.19	119.87
1	C	548	SER	C-N-CA	8.00	128.19	119.87
1	A	392	GLN	N-CA-C	7.82	119.58	111.14
1	C	603	THR	CA-C-N	-7.79	112.59	123.03
1	C	603	THR	C-N-CA	-7.79	112.59	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	LYS	N-CA-C	7.78	119.76	111.28
1	B	548	SER	CA-C-N	7.78	127.96	119.87
1	B	548	SER	C-N-CA	7.78	127.96	119.87
1	A	568	ILE	N-CA-C	-7.76	102.88	110.72
1	D	603	THR	CA-C-N	-7.56	111.99	122.87
1	D	603	THR	C-N-CA	-7.56	111.99	122.87
1	A	472	SER	N-CA-C	7.55	119.59	111.36
1	C	487	ASN	N-CA-C	7.53	119.49	111.28
1	D	604	LYS	N-CA-C	7.53	119.85	109.54
1	D	640	MSE	CB-CG-SE	-7.42	90.43	112.70
1	B	473	GLY	N-CA-C	-7.40	99.26	112.58
1	A	411	GLU	N-CA-C	-7.39	100.75	110.43
1	B	38	GLY	N-CA-C	-7.31	101.08	112.85
1	A	393	CYS	N-CA-C	7.29	124.54	113.61
1	D	192	ARG	CD-NE-CZ	7.26	134.56	124.40
1	B	585	ASN	N-CA-C	7.23	122.28	113.17
1	A	610	TRP	N-CA-C	7.23	122.98	113.30
1	A	303	LEU	N-CA-C	-7.19	97.85	109.58
1	B	117	ILE	CB-CA-C	-7.19	103.40	111.45
1	D	17	LYS	CG-CD-CE	7.19	127.84	111.30
1	B	410	LYS	N-CA-C	7.16	119.16	111.36
1	B	666	LEU	CD1-CG-CD2	-7.10	95.17	110.80
1	D	22	ARG	NE-CZ-NH1	7.05	128.55	121.50
1	A	480	GLY	N-CA-C	6.96	121.08	112.73
1	C	412	VAL	CA-C-N	-6.89	114.63	119.66
1	C	412	VAL	C-N-CA	-6.89	114.63	119.66
1	A	455	LYS	CG-CD-CE	6.88	127.13	111.30
1	A	652	GLU	N-CA-C	6.88	118.57	111.14
1	D	19	VAL	N-CA-C	6.85	116.97	110.53
1	C	127	MSE	N-CA-C	-6.85	98.45	109.96
1	B	154	GLY	CA-C-N	-6.85	113.25	120.03
1	B	154	GLY	C-N-CA	-6.85	113.25	120.03
1	A	479	GLU	N-CA-C	-6.84	98.51	109.39
1	B	392	GLN	N-CA-C	6.80	118.48	111.14
1	C	103	VAL	N-CA-CB	6.80	118.03	110.62
1	B	185	ILE	N-CA-C	6.80	116.92	110.53
1	B	452	HIS	N-CA-C	6.79	118.77	111.36
1	A	154	GLY	CA-C-N	-6.75	113.35	120.03
1	A	154	GLY	C-N-CA	-6.75	113.35	120.03
1	A	102	ASP	N-CA-C	6.66	119.53	111.40
1	C	585	ASN	N-CA-C	6.64	121.53	113.17
1	B	133	GLU	CA-C-N	-6.61	112.32	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	GLU	C-N-CA	-6.61	112.32	119.98
1	D	514	SER	N-CA-C	6.54	118.40	111.28
1	B	403	VAL	CB-CA-C	-6.52	104.41	111.59
1	B	8	VAL	CA-C-N	-6.50	113.06	119.76
1	B	8	VAL	C-N-CA	-6.50	113.06	119.76
1	B	605	LEU	CD1-CG-CD2	-6.48	96.54	110.80
1	C	604	LYS	N-CA-C	6.46	119.15	108.49
1	A	249	GLU	N-CA-C	6.45	120.35	112.23
1	B	127	MSE	N-CA-C	-6.45	98.68	108.67
1	A	601	ILE	N-CA-C	6.44	118.02	111.00
1	B	46	LEU	N-CA-C	-6.43	98.42	108.90
1	C	610	TRP	N-CA-C	6.43	121.05	112.30
1	C	636	MSE	CA-C-N	-6.41	112.90	119.83
1	C	636	MSE	C-N-CA	-6.41	112.90	119.83
1	A	654	THR	CB-CA-C	-6.39	100.84	110.88
1	C	38	GLY	N-CA-C	-6.37	100.42	112.27
1	C	154	GLY	CA-C-N	-6.36	113.73	120.03
1	C	154	GLY	C-N-CA	-6.36	113.73	120.03
1	B	267	ALA	N-CA-C	-6.35	103.65	111.33
1	B	326	CYS	N-CA-C	-6.33	104.48	111.82
1	D	318	SER	CA-C-N	-6.29	112.52	119.19
1	D	318	SER	C-N-CA	-6.29	112.52	119.19
1	A	385	ALA	N-CA-C	6.26	118.18	111.36
1	D	118	PHE	CA-C-N	-6.24	113.34	119.76
1	D	118	PHE	C-N-CA	-6.24	113.34	119.76
1	D	100	PRO	N-CA-C	-6.17	104.96	113.53
1	B	327	GLN	N-CA-C	-6.16	104.64	111.36
1	C	133	GLU	CA-C-N	-6.14	112.17	119.84
1	C	133	GLU	C-N-CA	-6.14	112.17	119.84
1	A	267	ALA	N-CA-C	-6.13	103.91	111.33
1	B	393	CYS	N-CA-C	6.13	122.22	114.31
1	A	118	PHE	CA-C-N	-6.12	113.48	119.78
1	A	118	PHE	C-N-CA	-6.12	113.48	119.78
1	C	103	VAL	N-CA-C	-6.12	104.37	110.30
1	A	585	ASN	N-CA-C	6.10	120.85	113.17
1	A	338	THR	N-CA-C	6.08	120.97	113.50
1	B	106	VAL	N-CA-C	6.08	116.19	110.30
1	C	651	PRO	N-CA-C	6.07	122.15	113.47
1	D	636	MSE	CA-C-N	-6.07	113.51	119.76
1	D	636	MSE	C-N-CA	-6.07	113.51	119.76
1	C	650	ASN	CA-C-N	-6.06	112.67	118.97
1	C	650	ASN	C-N-CA	-6.06	112.67	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	652	GLU	CA-C-N	6.05	128.39	120.28
1	C	652	GLU	C-N-CA	6.05	128.39	120.28
1	B	636	MSE	CA-C-N	-6.03	113.55	119.76
1	B	636	MSE	C-N-CA	-6.03	113.55	119.76
1	C	118	PHE	CA-C-N	-6.00	113.50	119.92
1	C	118	PHE	C-N-CA	-6.00	113.50	119.92
1	A	133	GLU	CA-C-N	-6.00	112.34	119.84
1	A	133	GLU	C-N-CA	-6.00	112.34	119.84
1	A	368	VAL	N-CA-C	5.98	120.78	112.35
1	D	24	ILE	N-CA-C	5.97	117.38	108.54
1	D	17	LYS	CD-CE-NZ	5.97	131.00	111.90
1	C	66	LEU	N-CA-C	5.92	118.07	109.07
1	B	351	GLY	N-CA-C	-5.88	96.25	113.30
1	B	52	ARG	N-CA-C	5.86	117.76	108.79
1	A	141	LEU	N-CA-C	5.83	117.31	111.07
1	B	638	ILE	CA-C-N	-5.78	112.62	119.84
1	B	638	ILE	C-N-CA	-5.78	112.62	119.84
1	D	487	ASN	N-CA-C	5.77	120.46	112.90
1	A	479	GLU	CA-C-N	5.76	126.38	119.98
1	A	479	GLU	C-N-CA	5.76	126.38	119.98
1	B	80	LYS	CA-C-N	-5.76	112.65	119.05
1	B	80	LYS	C-N-CA	-5.76	112.65	119.05
1	B	451	ASN	CA-C-N	5.76	128.47	120.29
1	B	451	ASN	C-N-CA	5.76	128.47	120.29
1	A	484	GLU	N-CA-C	5.76	117.15	108.46
1	A	103	VAL	N-CA-CB	5.75	117.27	110.55
1	D	361	LEU	N-CA-C	-5.74	105.10	111.36
1	D	474	GLY	N-CA-C	-5.70	105.38	111.93
1	D	392	GLN	N-CA-C	5.70	117.57	111.36
1	B	244	ARG	N-CA-C	5.68	120.21	113.28
1	D	241	VAL	CB-CA-C	-5.67	104.48	112.14
1	A	185	ILE	N-CA-C	5.67	115.86	110.53
1	C	437	SER	CA-C-N	-5.66	113.19	119.19
1	C	437	SER	C-N-CA	-5.66	113.19	119.19
1	D	640	MSE	CA-CB-CG	-5.66	102.78	114.10
1	C	338	THR	N-CA-C	5.64	120.44	113.50
1	C	567	ILE	CB-CA-C	-5.64	104.65	112.04
1	D	17	LYS	CB-CG-CD	5.63	124.25	111.30
1	A	434	THR	CB-CA-C	-5.63	99.41	109.71
1	D	22	ARG	CD-NE-CZ	5.62	132.27	124.40
1	D	206	ASP	N-CA-C	5.61	119.22	112.38
1	D	122	SER	CA-C-N	-5.59	113.14	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	SER	C-N-CA	-5.59	113.14	119.28
1	C	649	THR	N-CA-C	5.57	117.43	111.36
1	B	57	SER	N-CA-C	-5.56	102.79	110.35
1	A	303	LEU	CA-C-N	-5.55	112.89	119.05
1	A	303	LEU	C-N-CA	-5.55	112.89	119.05
1	B	413	PRO	CA-C-N	5.54	125.20	119.05
1	B	413	PRO	C-N-CA	5.54	125.20	119.05
1	C	653	LYS	N-CA-C	5.53	117.31	111.28
1	D	98	VAL	CB-CA-C	-5.48	104.74	112.14
1	A	117	ILE	N-CA-C	-5.46	97.98	109.34
1	B	632	THR	N-CA-C	5.46	120.04	112.45
1	A	638	ILE	CA-C-N	-5.46	113.02	119.84
1	A	638	ILE	C-N-CA	-5.46	113.02	119.84
1	A	513	ARG	N-CA-C	5.44	119.92	113.28
1	B	152	GLU	CA-C-N	-5.43	113.05	119.84
1	B	152	GLU	C-N-CA	-5.43	113.05	119.84
1	C	456	GLY	N-CA-C	5.43	123.53	113.76
1	A	506	ILE	N-CA-C	-5.42	105.44	110.53
1	B	638	ILE	CB-CA-C	-5.41	105.58	110.88
1	D	604	LYS	CA-CB-CG	5.40	124.91	114.10
1	A	451	ASN	O-C-N	-5.35	116.05	123.01
1	C	191	THR	CB-CA-C	-5.34	100.48	109.50
1	D	585	ASN	N-CA-C	5.33	119.89	113.17
1	B	124	LEU	N-CA-C	-5.32	105.48	111.28
1	B	445	LEU	CD1-CG-CD2	-5.32	99.10	110.80
1	C	27	SER	N-CA-C	5.29	117.13	111.36
1	B	260	ILE	N-CA-C	5.28	120.31	109.34
1	A	540	VAL	CB-CA-C	-5.27	105.23	111.97
1	A	415	SER	N-CA-C	-5.26	105.54	111.28
1	C	117	ILE	N-CA-C	-5.26	101.07	109.17
1	A	455	LYS	CD-CE-NZ	5.24	128.67	111.90
1	C	415	SER	N-CA-C	-5.23	105.58	111.28
1	B	79	HIS	N-CA-C	5.22	116.65	111.07
1	C	238	ILE	N-CA-C	-5.21	105.41	110.42
1	C	505	LEU	N-CA-C	-5.21	105.71	111.71
1	D	386	LEU	N-CA-C	-5.21	106.18	112.54
1	C	31	LYS	N-CA-C	-5.19	100.84	109.46
1	D	31	LYS	N-CA-C	-5.19	101.23	109.59
1	C	533	THR	CA-C-N	-5.18	113.30	119.05
1	C	533	THR	C-N-CA	-5.18	113.30	119.05
1	A	260	ILE	N-CA-CB	-5.17	104.01	110.47
1	D	624	ALA	N-CA-C	-5.17	106.23	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	VAL	N-CA-C	-5.15	99.57	107.71
1	B	186	TYR	N-CA-C	5.14	116.97	111.36
1	C	8	VAL	CA-C-N	-5.14	113.41	119.84
1	C	8	VAL	C-N-CA	-5.14	113.41	119.84
1	C	185	ILE	N-CA-C	5.14	115.36	110.53
1	B	650	ASN	CA-C-N	-5.13	113.35	119.05
1	B	650	ASN	C-N-CA	-5.13	113.35	119.05
1	C	288	LEU	N-CA-C	-5.13	100.95	109.46
1	B	641	TYR	N-CA-C	5.12	116.67	111.14
1	C	159	PHE	CA-C-N	-5.11	113.80	120.44
1	C	159	PHE	C-N-CA	-5.11	113.80	120.44
1	A	473	GLY	N-CA-C	-5.11	101.07	113.18
1	B	28	VAL	N-CA-C	5.11	115.62	108.17
1	A	81	PRO	N-CA-C	5.09	120.61	113.53
1	D	101	GLU	N-CA-C	-5.06	105.76	111.28
1	B	163	TYR	N-CA-C	-5.06	105.77	111.28
1	C	21	GLY	N-CA-C	-5.05	106.08	112.65
1	C	358	TYR	N-CA-C	-5.04	105.97	111.82
1	B	526	ASN	N-CA-C	5.04	118.35	111.39
1	A	80	LYS	CA-C-N	-5.03	113.47	119.05
1	A	80	LYS	C-N-CA	-5.03	113.47	119.05
1	A	651	PRO	CA-N-CD	-5.03	104.96	112.00
1	A	567	ILE	CB-CA-C	-5.02	105.51	112.24
1	D	437	SER	CA-C-N	-5.00	113.89	119.19
1	D	437	SER	C-N-CA	-5.00	113.89	119.19

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	LYS	Peptide
1	A	481	CYS	Peptide
1	A	525	ASN	Peptide
1	C	410	LYS	Peptide
1	C	604	LYS	Mainchain
1	C	651	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5112	0	5253	428	1
1	B	5102	0	5239	383	1
1	C	5073	0	5217	475	3
1	D	5066	0	5213	534	3
2	B	10	0	7	2	0
3	B	1	0	0	3	1
4	C	7	0	0	0	0
All	All	20371	0	20929	1801	5

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 44.

All (1801) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:LEU:HG	1:C:508:TRP:CZ2	1.28	1.59
1:B:350:ARG:HG3	1:B:406:HIS:CE1	1.35	1.57
1:D:258:LEU:HD23	1:D:262:PHE:CE2	1.44	1.53
1:B:54:PHE:CD1	1:B:67:THR:HG21	1.46	1.49
1:A:474:GLY:HA2	1:A:477:VAL:CG1	1.43	1.46
1:B:350:ARG:CG	1:B:406:HIS:CE1	1.97	1.46
1:C:478:LEU:CG	1:C:508:TRP:CZ2	1.97	1.45
1:C:350:ARG:HD3	1:C:406:HIS:CE1	1.53	1.41
1:B:484:GLU:HG2	1:B:508:TRP:NE1	1.23	1.40
1:C:350:ARG:HD3	1:C:406:HIS:ND1	1.41	1.35
1:A:319:PRO:HB2	1:A:352:ASP:CB	1.56	1.35
1:A:319:PRO:CG	1:A:352:ASP:HB2	1.56	1.33
1:C:478:LEU:HG	1:C:508:TRP:CH2	1.62	1.33
1:D:499:GLU:C	1:D:527:MSE:CE	2.01	1.33
1:C:65:GLU:O	1:C:66:LEU:HD23	1.21	1.31
1:B:54:PHE:CD1	1:B:67:THR:CG2	2.15	1.28
1:A:319:PRO:CB	1:A:352:ASP:HB3	1.64	1.28
1:C:44:LYS:NZ	1:C:65:GLU:CD	1.92	1.27
1:A:374:ASN:OD1	1:A:401:ARG:HD2	1.34	1.27
1:D:258:LEU:CD2	1:D:262:PHE:CE2	2.19	1.26
1:C:55:LEU:HD11	1:C:95:MSE:CE	1.66	1.25
1:D:145:TRP:HA	1:D:148:GLN:OE1	1.37	1.24
1:A:319:PRO:CB	1:A:352:ASP:CB	2.14	1.24
1:B:484:GLU:HG2	1:B:508:TRP:CD1	1.70	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:GLU:OE2	1:C:511:LYS:HB3	1.38	1.23
1:A:9:PRO:CB	1:A:12:LEU:HD21	1.68	1.22
1:A:402:SER:O	1:A:434:THR:CG2	1.86	1.22
1:A:474:GLY:CA	1:A:477:VAL:HG12	1.69	1.22
1:C:477:VAL:O	1:C:508:TRP:CZ3	1.90	1.21
1:C:374:ASN:OD1	1:C:401:ARG:HG3	1.36	1.21
1:C:448:LEU:O	1:C:487:ASN:ND2	1.70	1.21
1:D:258:LEU:HD23	1:D:262:PHE:CD2	1.75	1.21
1:C:478:LEU:CB	1:C:508:TRP:CZ2	2.19	1.20
1:C:504:THR:O	1:C:507:VAL:HG22	1.41	1.20
1:B:484:GLU:OE2	1:B:508:TRP:O	1.57	1.19
1:C:350:ARG:CD	1:C:406:HIS:CE1	2.22	1.19
1:C:484:GLU:OE2	1:C:511:LYS:CB	1.88	1.19
1:B:484:GLU:CG	1:B:508:TRP:NE1	2.07	1.18
1:B:36:VAL:HG21	1:B:42:GLU:CG	1.72	1.17
1:A:9:PRO:HB2	1:A:12:LEU:HD21	1.17	1.17
1:A:349:LEU:HG	1:A:375:THR:OG1	1.44	1.16
1:A:484:GLU:HG3	1:A:508:TRP:NE1	1.59	1.16
1:D:136:GLU:O	1:D:140:SER:OG	1.63	1.16
1:C:478:LEU:CG	1:C:508:TRP:HZ2	1.46	1.14
1:D:349:LEU:CD1	1:D:357:MSE:HE1	1.76	1.13
1:D:499:GLU:HA	1:D:527:MSE:HE3	1.28	1.13
1:D:118:PHE:CD2	1:D:126:ILE:CD1	2.32	1.12
1:B:24:ILE:HD12	1:B:25:LYS:H	1.14	1.12
1:A:402:SER:O	1:A:434:THR:HG23	1.43	1.12
1:D:349:LEU:HB3	1:D:354:LEU:HD21	1.33	1.11
1:D:499:GLU:C	1:D:527:MSE:HE1	1.75	1.11
1:A:484:GLU:CG	1:A:508:TRP:HE1	1.62	1.11
1:A:485:ILE:HG22	1:A:512:ASN:HD22	1.12	1.11
1:A:493:ILE:O	1:A:496:ASN:ND2	1.83	1.10
1:A:374:ASN:OD1	1:A:401:ARG:CD	1.99	1.09
1:A:484:GLU:HG3	1:A:508:TRP:HE1	0.95	1.09
1:D:144:LEU:O	1:D:148:GLN:OE1	1.71	1.09
1:C:474:GLY:HA2	1:C:475:ALA:CB	1.82	1.09
1:D:474:GLY:HA2	1:D:475:ALA:HB3	1.29	1.09
1:C:349:LEU:HG	1:C:375:THR:OG1	1.50	1.09
1:B:323:ASN:ND2	1:B:356:HIS:ND1	2.01	1.08
1:C:36:VAL:HG12	1:C:37:LYS:HD2	1.32	1.08
1:A:652:GLU:HG2	1:A:653:LYS:H	1.17	1.08
1:D:118:PHE:HD2	1:D:126:ILE:CD1	1.67	1.08
1:A:485:ILE:CG2	1:A:512:ASN:ND2	2.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LYS:NZ	1:C:65:GLU:OE1	1.85	1.06
1:C:44:LYS:HZ2	1:C:65:GLU:CD	1.52	1.06
1:B:36:VAL:HG21	1:B:42:GLU:HG3	1.07	1.06
1:B:354:LEU:HB3	1:B:358:TYR:CE2	1.90	1.06
1:A:498:LEU:HD12	1:A:502:LEU:HD13	1.32	1.06
1:B:54:PHE:HD1	1:B:67:THR:CG2	1.58	1.06
1:C:68:PHE:CD2	1:C:93:MSE:CE	2.39	1.06
1:D:411:GLU:OE2	1:D:412:VAL:N	1.88	1.06
1:A:485:ILE:HG22	1:A:512:ASN:ND2	1.69	1.06
1:B:448:LEU:O	1:B:487:ASN:ND2	1.89	1.06
1:D:322:VAL:HG11	1:D:357:MSE:HE3	1.37	1.06
1:B:182:VAL:O	1:B:186:TYR:HB2	1.55	1.05
1:D:145:TRP:CA	1:D:148:GLN:OE1	2.04	1.05
1:A:638:ILE:HD12	1:B:638:ILE:HG12	1.34	1.05
1:D:349:LEU:HD11	1:D:357:MSE:HE1	1.34	1.05
1:B:374:ASN:OD1	1:B:401:ARG:HD3	1.55	1.05
1:D:513:ARG:HH21	1:D:513:ARG:HG3	1.22	1.05
1:B:350:ARG:HG2	1:B:406:HIS:CE1	1.87	1.05
1:C:44:LYS:NZ	1:C:65:GLU:OE2	1.89	1.04
1:C:562:ALA:O	1:C:565:THR:OG1	1.76	1.04
1:C:610:TRP:CE2	1:C:636:MSE:HE2	1.91	1.04
1:C:68:PHE:CD2	1:C:93:MSE:HE2	1.93	1.04
1:C:474:GLY:HA3	1:C:476:GLN:H	1.21	1.04
1:B:74:HIS:CE1	1:B:89:GLU:HB2	1.93	1.04
1:C:474:GLY:CA	1:C:475:ALA:HB3	1.87	1.03
1:B:349:LEU:HG	1:B:375:THR:OG1	1.57	1.03
1:C:478:LEU:HB2	1:C:508:TRP:CZ2	1.90	1.02
1:C:113:CYS:O	1:C:117:ILE:HD12	1.59	1.02
1:B:177:GLU:OE1	1:B:177:GLU:N	1.91	1.02
1:C:36:VAL:CG1	1:C:37:LYS:HD2	1.89	1.02
1:B:402:SER:O	1:B:434:THR:HB	1.58	1.01
1:B:484:GLU:CD	1:B:508:TRP:O	2.02	1.01
1:C:36:VAL:HG12	1:C:37:LYS:H	1.20	1.01
1:B:78:CYS:HB2	1:B:132:MSE:HA	1.43	1.01
1:C:350:ARG:HG2	1:C:406:HIS:HE1	1.26	1.01
1:C:402:SER:O	1:C:434:THR:HB	1.60	1.01
1:D:499:GLU:CA	1:D:527:MSE:HE3	1.89	1.01
1:A:303:LEU:HD23	1:A:304:PRO:HD2	1.39	1.00
1:B:484:GLU:CG	1:B:508:TRP:CD1	2.41	1.00
1:C:478:LEU:CB	1:C:508:TRP:HZ2	1.67	0.99
1:B:88:THR:HG23	1:B:91:CYS:H	1.23	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:LEU:O	1:C:402:SER:OG	1.81	0.99
1:B:80:LYS:CE	1:B:81:PRO:HD2	1.92	0.99
1:C:350:ARG:CG	1:C:406:HIS:HE1	1.76	0.99
1:C:474:GLY:HA2	1:C:475:ALA:HB3	1.02	0.99
1:A:24:ILE:HD12	1:A:25:LYS:H	1.24	0.98
1:D:37:LYS:HA	1:D:39:ASP:H	1.25	0.98
1:C:114:LEU:O	1:C:117:ILE:O	1.81	0.98
1:D:291:ARG:HB3	1:D:291:ARG:HH21	1.29	0.98
1:D:118:PHE:CD2	1:D:126:ILE:HD13	1.98	0.97
1:C:474:GLY:CA	1:C:476:GLN:H	1.77	0.97
1:A:652:GLU:HG2	1:A:653:LYS:N	1.71	0.97
1:C:478:LEU:CG	1:C:508:TRP:CH2	2.23	0.97
1:D:322:VAL:CG1	1:D:357:MSE:HE3	1.94	0.97
1:A:369:HIS:CD2	1:A:396:VAL:HG21	2.00	0.96
1:A:319:PRO:CB	1:A:352:ASP:HB2	1.87	0.96
1:D:26:ILE:HD12	1:D:47:VAL:CG2	1.94	0.96
1:A:319:PRO:CG	1:A:352:ASP:CB	2.41	0.96
1:C:353:ASP:OD1	1:C:355:SER:OG	1.83	0.96
1:D:78:CYS:SG	1:D:103:VAL:HG11	2.04	0.96
1:C:431:LEU:O	1:C:434:THR:HG23	1.66	0.96
1:D:638:ILE:H	1:D:638:ILE:HD12	1.28	0.96
1:A:319:PRO:HG2	1:A:352:ASP:HB2	0.99	0.96
1:B:66:LEU:HD12	1:B:93:MSE:HE1	1.46	0.95
1:B:456:GLY:HA2	1:B:489:THR:HG23	1.48	0.95
1:B:36:VAL:CG2	1:B:42:GLU:HG3	1.95	0.95
1:C:68:PHE:CE2	1:C:93:MSE:HE2	2.01	0.95
1:A:290:ASP:O	1:A:294:SER:N	1.99	0.95
1:C:55:LEU:HD21	1:C:95:MSE:HE2	1.47	0.95
1:D:13:MSE:HE1	1:D:26:ILE:HD11	1.46	0.95
1:B:66:LEU:CD1	1:B:93:MSE:HE1	1.97	0.95
1:A:474:GLY:CA	1:A:477:VAL:CG1	2.36	0.95
1:A:293:VAL:HG21	1:A:317:LEU:HD11	1.46	0.94
1:A:9:PRO:CB	1:A:12:LEU:CD2	2.46	0.94
1:D:507:VAL:O	1:D:510:SER:OG	1.85	0.94
1:B:611:ASP:OD1	1:B:612:LYS:N	2.00	0.94
1:D:258:LEU:HD23	1:D:262:PHE:HE2	1.32	0.94
1:C:350:ARG:CD	1:C:406:HIS:ND1	2.30	0.94
1:D:467:GLY:CA	1:D:498:LEU:HD23	1.98	0.94
1:C:543:ILE:CG2	1:C:574:ASN:ND2	2.31	0.93
1:D:18:ASP:OD1	1:D:22:ARG:NH2	2.02	0.93
1:A:9:PRO:HB2	1:A:12:LEU:CD2	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:O	1:D:347:ASN:ND2	2.00	0.93
2:B:701:OHB:O	3:B:702:CL:CL	2.24	0.93
1:B:88:THR:HG23	1:B:91:CYS:N	1.84	0.93
1:B:54:PHE:CE1	1:B:67:THR:HG21	2.04	0.92
1:C:68:PHE:CE2	1:C:93:MSE:CE	2.52	0.92
1:D:512:ASN:OD1	1:D:515:ILE:HG13	1.68	0.92
1:B:80:LYS:HE3	1:B:81:PRO:HD2	1.48	0.92
1:C:381:MSE:HA	1:C:381:MSE:HE3	1.51	0.92
1:B:178:VAL:O	1:B:182:VAL:HG23	1.68	0.92
1:C:610:TRP:NE1	1:C:636:MSE:HE2	1.84	0.91
1:A:319:PRO:HG2	1:A:352:ASP:CB	1.96	0.91
1:C:256:ALA:HB3	1:C:258:LEU:HD13	1.51	0.91
1:B:180:TRP:O	1:B:184:THR:OG1	1.88	0.91
1:B:185:ILE:O	1:B:189:GLN:HG3	1.71	0.91
1:C:55:LEU:HD11	1:C:95:MSE:HE3	1.53	0.90
1:C:350:ARG:HG2	1:C:406:HIS:CE1	2.05	0.90
1:D:13:MSE:CE	1:D:26:ILE:HD11	2.01	0.90
1:C:68:PHE:HD2	1:C:93:MSE:HE1	1.33	0.90
1:D:322:VAL:HG11	1:D:357:MSE:CE	2.01	0.90
1:C:506:ILE:HG23	1:C:542:MSE:CE	2.03	0.89
1:B:484:GLU:OE2	1:B:508:TRP:CD1	2.26	0.89
1:D:34:LEU:CD2	1:D:42:GLU:HB2	2.02	0.89
1:C:350:ARG:CG	1:C:406:HIS:CE1	2.54	0.89
1:C:509:LEU:CD2	1:C:518:LEU:HD22	2.03	0.89
1:C:528:LYS:O	1:C:531:ASN:ND2	2.04	0.89
1:C:484:GLU:OE1	1:C:484:GLU:N	2.06	0.89
1:D:64:LEU:HD23	1:D:65:GLU:N	1.88	0.89
1:B:449:ALA:O	1:B:486:HIS:HE1	1.56	0.89
1:D:499:GLU:O	1:D:527:MSE:HE1	1.71	0.89
1:B:7:ASP:O	1:B:31:LYS:HG3	1.72	0.89
1:C:134:PRO:HD2	1:C:137:ARG:HH21	1.37	0.88
1:D:431:LEU:O	1:D:434:THR:HG23	1.73	0.88
1:C:55:LEU:HD11	1:C:95:MSE:HE1	1.54	0.88
1:C:8:VAL:HG12	1:C:9:PRO:CD	2.04	0.88
1:D:423:SER:OG	1:D:426:LEU:HD13	1.73	0.88
1:A:605:LEU:O	1:A:633:LEU:HD12	1.74	0.88
1:B:484:GLU:CD	1:B:508:TRP:CD1	2.51	0.88
1:C:117:ILE:HB	1:C:118:PHE:CD2	2.09	0.88
1:D:499:GLU:C	1:D:527:MSE:HE3	1.93	0.88
1:C:115:ARG:HB3	1:C:115:ARG:HH21	1.36	0.88
1:A:319:PRO:HB2	1:A:352:ASP:HB3	0.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:VAL:O	1:C:508:TRP:HZ3	1.03	0.87
1:C:115:ARG:HH21	1:C:115:ARG:CB	1.88	0.87
1:D:350:ARG:H	1:D:350:ARG:HD3	1.37	0.87
1:A:402:SER:O	1:A:434:THR:HG22	1.75	0.86
1:B:24:ILE:HD12	1:B:25:LYS:N	1.88	0.86
1:B:350:ARG:HG2	1:B:406:HIS:NE2	1.90	0.86
1:D:543:ILE:HG22	1:D:574:ASN:ND2	1.90	0.86
1:A:374:ASN:HD21	1:A:401:ARG:HH21	1.20	0.86
1:C:193:GLU:HG3	1:C:222:LYS:HD3	1.54	0.86
1:C:531:ASN:O	1:C:534:PRO:HD2	1.76	0.86
1:C:65:GLU:C	1:C:66:LEU:HD23	1.99	0.86
1:D:32:VAL:HG23	1:D:96:LYS:O	1.76	0.86
1:D:143:ALA:O	1:D:147:SER:OG	1.93	0.86
1:A:24:ILE:HD12	1:A:25:LYS:N	1.91	0.85
1:A:138:LEU:HD23	1:A:139:ALA:N	1.91	0.85
1:C:68:PHE:CD2	1:C:93:MSE:HE1	2.08	0.85
1:C:543:ILE:CG2	1:C:574:ASN:HD22	1.90	0.85
1:C:12:LEU:HD12	1:C:12:LEU:O	1.77	0.85
1:C:113:CYS:O	1:C:117:ILE:CD1	2.24	0.85
1:A:258:LEU:HD23	1:A:262:PHE:CE2	2.12	0.85
1:A:372:LEU:O	1:A:375:THR:CG2	2.25	0.85
1:A:562:ALA:O	1:A:565:THR:OG1	1.95	0.85
1:B:484:GLU:HG2	1:B:508:TRP:HE1	1.04	0.84
1:C:484:GLU:OE1	1:C:508:TRP:CD1	2.30	0.84
1:C:504:THR:O	1:C:507:VAL:CG2	2.24	0.84
1:D:26:ILE:HD12	1:D:47:VAL:HG21	1.58	0.84
1:A:258:LEU:HD23	1:A:262:PHE:CD2	2.13	0.84
1:C:555:LEU:O	1:C:558:SER:OG	1.94	0.84
1:D:467:GLY:HA2	1:D:498:LEU:CD2	2.08	0.84
1:B:162:MSE:O	1:B:166:VAL:HG23	1.78	0.84
1:D:46:LEU:HD13	1:D:95:MSE:HE1	1.60	0.84
1:C:349:LEU:HG	1:C:375:THR:HG1	1.38	0.84
1:B:431:LEU:O	1:B:434:THR:HG23	1.78	0.83
1:A:117:ILE:CD1	1:A:165:CYS:SG	2.66	0.83
1:A:121:LEU:HD22	1:A:125:ARG:NH1	1.92	0.83
1:D:118:PHE:CD2	1:D:126:ILE:HD11	2.10	0.83
1:D:496:ASN:O	1:D:523:ASN:OD1	1.94	0.83
1:A:9:PRO:HB3	1:A:12:LEU:HD21	1.56	0.83
1:A:474:GLY:HA2	1:A:477:VAL:HG11	1.54	0.83
1:A:474:GLY:HA2	1:A:477:VAL:HG12	0.84	0.83
1:B:74:HIS:ND1	1:B:89:GLU:HB2	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:VAL:HG12	1:C:9:PRO:HD2	1.59	0.83
1:A:256:ALA:HB3	1:A:258:LEU:HD13	1.61	0.83
1:D:117:ILE:HD13	1:D:165:CYS:SG	2.18	0.83
1:C:26:ILE:HG23	1:C:47:VAL:CG1	2.08	0.83
1:D:610:TRP:CZ3	1:D:615:ILE:HD12	2.14	0.82
1:C:374:ASN:OD1	1:C:401:ARG:CG	2.23	0.82
1:C:65:GLU:O	1:C:66:LEU:CD2	2.17	0.82
1:A:44:LYS:NZ	1:A:65:GLU:OE2	2.12	0.82
1:A:372:LEU:O	1:A:375:THR:HG22	1.78	0.82
1:D:325:LEU:HD12	1:D:325:LEU:O	1.79	0.82
1:A:68:PHE:CD1	1:A:93:MSE:CE	2.62	0.82
1:D:404:PHE:CE1	1:D:440:PRO:HB3	2.14	0.82
1:A:374:ASN:HD21	1:A:401:ARG:NH2	1.76	0.81
1:C:353:ASP:OD1	1:C:355:SER:N	2.12	0.81
1:D:610:TRP:CZ3	1:D:615:ILE:CD1	2.62	0.81
1:C:407:ARG:HH21	1:C:407:ARG:HG3	1.43	0.81
1:D:318:SER:O	1:D:322:VAL:HG23	1.79	0.81
1:D:504:THR:O	1:D:507:VAL:HG22	1.81	0.81
1:B:65:GLU:C	1:B:66:LEU:HD23	2.04	0.81
1:C:373:SER:HB3	1:C:398:ASN:OD1	1.80	0.81
1:D:467:GLY:HA3	1:D:498:LEU:HD23	1.63	0.81
1:C:505:LEU:O	1:C:509:LEU:HD12	1.81	0.81
1:D:117:ILE:CD1	1:D:165:CYS:SG	2.68	0.81
1:D:318:SER:OG	1:D:320:LYS:N	2.14	0.81
1:D:467:GLY:CA	1:D:498:LEU:CD2	2.58	0.81
1:A:485:ILE:HG23	1:A:512:ASN:ND2	1.94	0.81
1:B:65:GLU:O	1:B:66:LEU:HD23	1.79	0.80
1:D:474:GLY:HA2	1:D:475:ALA:CB	2.11	0.80
1:C:474:GLY:O	1:C:477:VAL:HG12	1.81	0.80
1:D:172:PHE:CD2	1:D:209:PRO:HD3	2.16	0.80
1:A:485:ILE:HG23	1:A:512:ASN:HD21	1.44	0.80
1:B:124:LEU:O	1:B:127:MSE:O	2.00	0.80
1:D:34:LEU:HD22	1:D:42:GLU:HB2	1.62	0.80
1:A:484:GLU:CG	1:A:508:TRP:NE1	2.30	0.80
1:B:456:GLY:HA2	1:B:489:THR:CG2	2.11	0.80
1:C:258:LEU:HD23	1:C:262:PHE:CE2	2.17	0.80
1:D:37:LYS:HA	1:D:39:ASP:N	1.96	0.80
1:B:256:ALA:HB3	1:B:258:LEU:HD13	1.62	0.80
1:D:349:LEU:HD13	1:D:357:MSE:HE1	1.63	0.80
1:B:54:PHE:HD1	1:B:67:THR:HG21	0.97	0.79
1:D:44:LYS:NZ	1:D:65:GLU:OE2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:GLU:CA	1:D:527:MSE:CE	2.55	0.79
1:D:500:SER:N	1:D:527:MSE:CE	2.45	0.79
1:B:484:GLU:OE2	1:B:508:TRP:C	2.26	0.79
1:C:475:ALA:C	1:C:476:GLN:HE21	1.90	0.79
1:B:258:LEU:HD23	1:B:262:PHE:CE2	2.18	0.79
1:D:142:GLN:O	1:D:146:ASP:OD1	2.00	0.79
1:D:99:SER:HB2	1:D:101:GLU:HG3	1.63	0.78
1:D:500:SER:N	1:D:527:MSE:HE2	1.98	0.78
1:D:36:VAL:HG12	1:D:37:LYS:O	1.83	0.78
1:A:283:LEU:O	1:A:286:ASN:ND2	2.16	0.78
1:D:117:ILE:HG22	1:D:118:PHE:CD1	2.18	0.78
1:A:638:ILE:HD13	1:A:640:MSE:HE1	1.64	0.78
1:B:283:LEU:O	1:B:286:ASN:ND2	2.15	0.78
1:C:51:CYS:HB3	1:C:165:CYS:SG	2.24	0.78
1:A:16:ILE:O	1:A:19:VAL:HG12	1.83	0.78
1:C:509:LEU:CD2	1:C:518:LEU:CD2	2.62	0.78
1:C:418:GLN:O	1:C:422:SER:OG	2.02	0.77
1:D:116:ARG:HH21	1:D:116:ARG:HB2	1.49	0.77
1:D:468:HIS:O	1:D:472:SER:HB3	1.84	0.77
1:A:638:ILE:HD13	1:A:640:MSE:CE	2.13	0.77
1:A:13:MSE:SE	1:A:29:LYS:HD2	2.34	0.77
1:A:484:GLU:HG3	1:A:508:TRP:CE2	2.19	0.77
1:A:638:ILE:CD1	1:B:638:ILE:HG12	2.14	0.77
1:B:7:ASP:O	1:B:31:LYS:CG	2.31	0.77
1:D:256:ALA:HB3	1:D:258:LEU:HD13	1.64	0.77
1:D:610:TRP:CE2	1:D:636:MSE:HE2	2.19	0.77
1:B:350:ARG:CG	1:B:406:HIS:NE2	2.47	0.77
1:A:374:ASN:ND2	1:A:401:ARG:HH21	1.81	0.77
1:D:26:ILE:HD12	1:D:47:VAL:HG23	1.67	0.77
1:A:666:LEU:HD22	1:B:666:LEU:CD1	2.15	0.77
1:B:258:LEU:HD23	1:B:262:PHE:CD2	2.18	0.77
1:D:478:LEU:HB3	1:D:508:TRP:NE1	1.98	0.77
1:B:115:ARG:NH2	1:B:150:LEU:HD11	1.99	0.77
1:C:476:GLN:HE21	1:C:476:GLN:N	1.82	0.76
1:A:160:SER:OG	1:A:183:ASP:OD1	2.02	0.76
1:B:183:ASP:O	1:B:187:LEU:HB3	1.86	0.76
1:B:354:LEU:CB	1:B:358:TYR:CE2	2.66	0.76
1:C:77:ILE:HB	1:C:85:VAL:HG22	1.67	0.76
1:C:372:LEU:O	1:C:375:THR:CG2	2.34	0.76
1:D:499:GLU:C	1:D:527:MSE:HE2	2.07	0.76
1:C:407:ARG:HG3	1:C:407:ARG:NH2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ARG:HG3	1:B:406:HIS:HE1	0.93	0.76
1:D:288:LEU:HD12	1:D:288:LEU:O	1.86	0.76
1:B:372:LEU:O	1:B:375:THR:CG2	2.33	0.76
1:B:353:ASP:OD1	1:B:355:SER:OG	2.02	0.76
1:C:379:LEU:HD13	1:C:402:SER:CB	2.16	0.76
1:A:23:LYS:HA	1:A:23:LYS:HE3	1.68	0.76
1:C:543:ILE:HG23	1:C:574:ASN:ND2	2.00	0.75
1:A:143:ALA:O	1:A:147:SER:N	2.19	0.75
1:C:350:ARG:CD	1:C:406:HIS:HE1	1.90	0.75
1:C:474:GLY:HA3	1:C:476:GLN:HG2	1.67	0.75
1:A:498:LEU:CD1	1:A:502:LEU:HD13	2.15	0.75
1:B:136:GLU:N	1:B:136:GLU:OE2	2.20	0.75
1:C:411:GLU:HA	1:C:411:GLU:OE2	1.87	0.75
1:C:610:TRP:CE2	1:C:636:MSE:CE	2.70	0.75
1:D:114:LEU:HD23	1:D:123:PRO:HB3	1.69	0.75
1:C:485:ILE:HG22	1:C:487:ASN:HB2	1.68	0.74
1:B:32:VAL:HG21	1:B:95:MSE:HB3	1.70	0.74
1:B:513:ARG:CB	1:B:513:ARG:HH11	2.00	0.74
1:D:372:LEU:O	1:D:375:THR:CG2	2.36	0.74
1:A:73:ILE:HG21	1:A:127:MSE:HE2	1.68	0.74
1:A:618:GLN:HE21	1:A:618:GLN:C	1.95	0.74
1:B:54:PHE:HA	1:B:67:THR:HG22	1.67	0.74
1:C:456:GLY:HA2	1:C:489:THR:HG23	1.68	0.74
1:D:258:LEU:HD21	1:D:262:PHE:CE2	2.22	0.74
1:B:484:GLU:OE1	1:B:508:TRP:O	2.04	0.74
1:C:640:MSE:SE	1:D:640:MSE:HG3	2.38	0.74
1:D:54:PHE:CD1	1:D:67:THR:HG23	2.22	0.74
1:A:13:MSE:HG3	1:A:17:LYS:CE	2.18	0.74
1:A:121:LEU:CD2	1:A:125:ARG:NH1	2.49	0.74
1:C:420:PHE:CZ	1:C:444:LEU:HD13	2.23	0.74
1:B:66:LEU:HD12	1:B:93:MSE:CE	2.18	0.74
1:B:449:ALA:O	1:B:486:HIS:CE1	2.40	0.74
1:B:604:LYS:HG3	1:B:604:LYS:O	1.88	0.74
1:D:63:LYS:HG3	1:D:63:LYS:O	1.88	0.74
1:D:82:ALA:HB1	1:D:97:MSE:O	1.85	0.74
1:C:26:ILE:HG23	1:C:47:VAL:HG12	1.69	0.73
1:D:564:VAL:HG13	1:D:568:ILE:HD12	1.69	0.73
1:A:104:SER:OG	1:A:137:ARG:NH1	2.20	0.73
1:C:133:GLU:HA	1:C:133:GLU:OE1	1.87	0.73
1:A:76:VAL:HG23	1:A:130:VAL:HG12	1.71	0.73
1:B:115:ARG:HG3	1:B:123:PRO:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:PRO:HD2	1:B:137:ARG:HH21	1.53	0.73
1:C:509:LEU:HD22	1:C:518:LEU:CD2	2.18	0.73
1:D:13:MSE:HE1	1:D:26:ILE:CD1	2.19	0.73
1:A:498:LEU:HD12	1:A:502:LEU:CD1	2.15	0.73
1:B:115:ARG:CZ	1:B:150:LEU:HD11	2.17	0.73
1:D:323:ASN:ND2	1:D:356:HIS:HB2	2.03	0.73
1:D:349:LEU:N	1:D:349:LEU:HD23	2.04	0.73
1:D:315:THR:OG1	1:D:317:LEU:CD1	2.36	0.73
1:C:604:LYS:O	1:C:604:LYS:HG3	1.89	0.73
1:D:68:PHE:CE2	1:D:86:VAL:HG11	2.24	0.73
1:A:12:LEU:C	1:A:12:LEU:HD12	2.14	0.73
1:A:68:PHE:CD1	1:A:93:MSE:HE2	2.24	0.73
1:B:638:ILE:HD12	1:B:638:ILE:N	2.03	0.73
1:B:293:VAL:HG21	1:B:317:LEU:HD11	1.71	0.73
1:A:369:HIS:CD2	1:A:396:VAL:CG2	2.72	0.73
1:D:485:ILE:O	1:D:512:ASN:ND2	2.21	0.73
1:A:638:ILE:CG2	1:A:640:MSE:HE3	2.19	0.72
1:D:114:LEU:O	1:D:117:ILE:O	2.06	0.72
1:B:134:PRO:HB2	1:B:137:ARG:HB2	1.71	0.72
1:D:144:LEU:C	1:D:148:GLN:OE1	2.31	0.72
1:B:80:LYS:HG2	1:B:81:PRO:CD	2.19	0.72
1:B:132:MSE:SE	1:B:138:LEU:HD13	2.39	0.72
1:C:509:LEU:HD23	1:C:518:LEU:HD22	1.71	0.72
1:D:349:LEU:HG	1:D:375:THR:OG1	1.89	0.72
1:D:474:GLY:HA3	1:D:476:GLN:CG	2.20	0.72
1:D:604:LYS:HG3	1:D:604:LYS:O	1.89	0.72
1:B:115:ARG:HG3	1:B:123:PRO:CG	2.19	0.72
1:C:498:LEU:HD13	1:C:505:LEU:HD12	1.71	0.72
1:B:64:LEU:HD11	1:B:66:LEU:O	1.90	0.72
1:B:66:LEU:CD1	1:B:93:MSE:CE	2.68	0.72
1:D:478:LEU:HB3	1:D:508:TRP:HE1	1.52	0.72
1:A:13:MSE:HG3	1:A:17:LYS:HE2	1.70	0.72
1:D:329:LEU:HD23	1:D:335:THR:HG21	1.71	0.72
1:C:503:SER:O	1:C:506:ILE:HB	1.90	0.71
1:D:118:PHE:CE2	1:D:126:ILE:HD13	2.24	0.71
1:C:505:LEU:O	1:C:509:LEU:CD1	2.38	0.71
1:D:77:ILE:O	1:D:85:VAL:HG12	1.90	0.71
1:B:177:GLU:O	1:B:181:ASP:HB2	1.90	0.71
1:C:498:LEU:HD11	1:C:505:LEU:HD13	1.72	0.71
1:D:64:LEU:HD23	1:D:65:GLU:H	1.53	0.71
1:B:484:GLU:CG	1:B:508:TRP:HE1	1.86	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ALA:O	1:C:427:ILE:HG22	1.90	0.71
1:A:124:LEU:HD22	1:A:130:VAL:HG21	1.72	0.71
1:C:77:ILE:HB	1:C:85:VAL:CG2	2.20	0.71
1:D:54:PHE:CD1	1:D:67:THR:CG2	2.74	0.71
1:D:580:VAL:CG1	1:D:605:LEU:HD21	2.21	0.71
1:C:352:ASP:N	1:C:352:ASP:OD1	2.20	0.71
1:D:507:VAL:HG23	1:D:508:TRP:N	2.05	0.71
1:B:32:VAL:CG2	1:B:95:MSE:HB3	2.21	0.71
1:C:484:GLU:CD	1:C:511:LYS:HB3	2.16	0.71
1:C:506:ILE:HG23	1:C:542:MSE:HE1	1.72	0.71
1:C:543:ILE:HG23	1:C:574:ASN:HD21	1.56	0.71
1:C:478:LEU:HB2	1:C:508:TRP:HZ2	1.39	0.70
1:D:34:LEU:HD21	1:D:42:GLU:OE2	1.91	0.70
1:A:73:ILE:HD13	1:A:127:MSE:CE	2.21	0.70
1:A:479:GLU:HA	1:A:481:CYS:SG	2.31	0.70
1:C:543:ILE:HG22	1:C:574:ASN:ND2	2.04	0.70
1:C:117:ILE:HB	1:C:118:PHE:HD2	1.55	0.70
1:A:480:GLY:N	1:A:481:CYS:HA	2.06	0.70
1:D:349:LEU:CB	1:D:354:LEU:HD21	2.16	0.70
1:A:134:PRO:O	1:A:137:ARG:HG3	1.92	0.70
1:B:54:PHE:CD1	1:B:67:THR:HG22	2.24	0.70
1:B:80:LYS:CD	1:B:81:PRO:HD2	2.22	0.70
1:D:99:SER:HB3	1:D:100:PRO:HD2	1.73	0.70
1:B:652:GLU:HG2	1:B:653:LYS:N	2.05	0.70
1:C:502:LEU:HD12	1:C:502:LEU:O	1.91	0.70
1:D:291:ARG:HB3	1:D:291:ARG:NH2	2.05	0.70
1:D:563:GLU:O	1:D:564:VAL:C	2.30	0.70
1:A:76:VAL:HG13	1:A:86:VAL:HG22	1.74	0.70
1:C:256:ALA:HB3	1:C:258:LEU:CD1	2.19	0.70
1:C:610:TRP:CZ3	1:C:615:ILE:HD13	2.26	0.70
1:A:323:ASN:OD1	1:A:354:LEU:HA	1.91	0.70
1:C:543:ILE:HG22	1:C:574:ASN:HD22	1.54	0.70
1:D:616:THR:HG22	1:D:617:ALA:N	2.07	0.70
1:B:36:VAL:HG21	1:B:42:GLU:HG2	1.71	0.69
1:C:484:GLU:OE2	1:C:511:LYS:CG	2.39	0.69
1:D:77:ILE:HD12	1:D:85:VAL:HG11	1.73	0.69
1:D:513:ARG:HG3	1:D:513:ARG:NH2	1.94	0.69
1:A:138:LEU:HD23	1:A:138:LEU:C	2.16	0.69
1:B:4:GLU:HG2	1:B:5:SER:N	2.07	0.69
1:C:55:LEU:CD1	1:C:95:MSE:CE	2.59	0.69
1:C:530:LYS:O	1:C:534:PRO:HD3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LEU:CD2	1:D:262:PHE:CD2	2.61	0.69
1:A:568:ILE:O	1:A:571:LEU:HB2	1.93	0.69
1:B:80:LYS:HG2	1:B:81:PRO:HD3	1.74	0.69
1:C:603:THR:O	1:C:603:THR:OG1	2.10	0.69
1:A:9:PRO:O	1:A:12:LEU:HG	1.92	0.69
1:B:323:ASN:ND2	1:B:356:HIS:CG	2.61	0.69
1:A:77:ILE:O	1:A:85:VAL:HG12	1.92	0.69
1:B:156:CYS:HA	1:B:219:TRP:CD1	2.28	0.69
1:C:610:TRP:NE1	1:C:636:MSE:CE	2.56	0.69
1:D:377:CYS:O	1:D:403:VAL:HG22	1.92	0.69
1:A:349:LEU:HG	1:A:375:THR:HG1	1.54	0.69
1:B:36:VAL:HB	1:B:41:VAL:HA	1.74	0.69
1:C:379:LEU:HD13	1:C:402:SER:HB3	1.74	0.69
1:A:470:LEU:CD2	1:A:477:VAL:HG11	2.23	0.69
1:D:30:LYS:HE3	1:D:102:ASP:OD1	1.93	0.69
1:D:53:ALA:HB3	1:D:68:PHE:CE1	2.28	0.69
1:D:506:ILE:HG21	1:D:538:ASN:HB3	1.74	0.69
1:A:414:PRO:O	1:A:418:GLN:HB2	1.93	0.68
1:B:8:VAL:HA	1:B:31:LYS:HD2	1.75	0.68
1:B:135:SER:HB3	1:B:136:GLU:OE2	1.93	0.68
1:C:290:ASP:OD2	1:C:321:GLY:N	2.26	0.68
1:A:117:ILE:HD13	1:A:165:CYS:SG	2.33	0.68
1:A:618:GLN:O	1:A:618:GLN:NE2	2.15	0.68
1:D:43:ASN:O	1:D:44:LYS:CE	2.41	0.68
1:A:73:ILE:CD1	1:A:127:MSE:HE3	2.23	0.68
1:A:638:ILE:HG21	1:A:640:MSE:HE3	1.75	0.68
1:D:507:VAL:HG23	1:D:508:TRP:H	1.58	0.68
1:B:78:CYS:HB2	1:B:132:MSE:CA	2.21	0.68
1:C:98:VAL:HG22	1:C:102:ASP:OD2	1.94	0.68
1:B:54:PHE:HA	1:B:67:THR:CG2	2.23	0.68
1:D:638:ILE:HD12	1:D:638:ILE:N	2.04	0.68
1:D:651:PRO:HG2	1:D:652:GLU:N	2.09	0.68
1:A:73:ILE:HG21	1:A:127:MSE:CE	2.24	0.68
1:B:36:VAL:HB	1:B:40:ARG:O	1.93	0.68
1:A:374:ASN:OD1	1:A:401:ARG:HD3	1.89	0.67
1:B:513:ARG:HH11	1:B:513:ARG:CG	2.07	0.67
1:C:256:ALA:CB	1:C:258:LEU:HD13	2.24	0.67
1:C:12:LEU:HD12	1:C:12:LEU:C	2.19	0.67
1:D:34:LEU:HD21	1:D:36:VAL:HG21	1.75	0.67
1:C:36:VAL:HG12	1:C:37:LYS:CD	2.18	0.67
1:D:144:LEU:C	1:D:144:LEU:HD13	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:ILE:CG2	1:D:574:ASN:ND2	2.57	0.67
1:A:95:MSE:HB2	1:A:97:MSE:CE	2.25	0.67
1:A:452:HIS:H	1:A:452:HIS:CD2	2.11	0.67
1:B:56:LEU:HD23	1:B:64:LEU:HB2	1.76	0.67
1:C:478:LEU:CD2	1:C:508:TRP:CH2	2.77	0.67
1:C:563:GLU:O	1:C:566:ILE:HG23	1.94	0.67
1:C:578:THR:HG22	1:C:604:LYS:HD2	1.75	0.67
1:D:46:LEU:CD1	1:D:95:MSE:HE1	2.25	0.67
1:D:80:LYS:HD2	1:D:81:PRO:HD2	1.77	0.67
1:A:80:LYS:HD2	1:A:81:PRO:N	2.10	0.67
1:D:610:TRP:CE3	1:D:615:ILE:HD12	2.29	0.67
1:A:141:LEU:HD23	1:A:144:LEU:HD23	1.77	0.67
1:A:143:ALA:HA	1:A:146:ASP:HB2	1.77	0.67
1:B:143:ALA:O	1:B:147:SER:HB3	1.95	0.67
1:C:185:ILE:HA	1:D:601:ILE:HD11	1.76	0.67
1:C:217:ASN:OD1	1:C:219:TRP:N	2.19	0.67
1:D:349:LEU:CD1	1:D:357:MSE:CE	2.64	0.67
1:B:52:ARG:HD3	1:B:67:THR:HB	1.76	0.66
1:C:378:SER:O	1:C:382:VAL:HG23	1.95	0.66
1:A:98:VAL:HG23	1:A:99:SER:N	2.09	0.66
1:C:478:LEU:HD23	1:C:508:TRP:HH2	1.58	0.66
1:D:46:LEU:HD13	1:D:95:MSE:CE	2.24	0.66
1:D:318:SER:HG	1:D:320:LYS:HG3	1.60	0.66
1:B:18:ASP:OD1	1:B:22:ARG:NH2	2.29	0.66
1:B:372:LEU:O	1:B:375:THR:HG22	1.94	0.66
1:B:496:ASN:O	1:B:497:GLY:C	2.37	0.66
1:C:134:PRO:CD	1:C:137:ARG:HH21	2.07	0.66
1:A:597:LYS:HE3	1:B:201:HIS:CE1	2.31	0.66
1:B:212:ALA:HB2	1:B:237:GLN:CG	2.25	0.66
1:B:478:LEU:HB3	1:B:508:TRP:CZ3	2.31	0.66
1:C:372:LEU:O	1:C:375:THR:HG22	1.94	0.66
1:C:527:MSE:CE	1:C:532:LEU:HG	2.25	0.66
1:D:100:PRO:CD	1:D:101:GLU:H	2.08	0.66
1:D:348:ALA:C	1:D:349:LEU:HD23	2.20	0.66
1:C:636:MSE:HB3	1:C:665:LEU:HD11	1.78	0.66
1:D:46:LEU:HD22	1:D:95:MSE:CE	2.25	0.66
1:A:13:MSE:CE	1:A:26:ILE:CD1	2.73	0.66
1:B:485:ILE:HG22	1:B:512:ASN:ND2	2.10	0.66
1:D:99:SER:CB	1:D:100:PRO:HD2	2.26	0.66
1:D:474:GLY:CA	1:D:475:ALA:HB3	2.16	0.66
1:B:7:ASP:N	1:B:7:ASP:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:NH2	1:C:150:LEU:HD21	2.09	0.66
1:C:484:GLU:OE2	1:C:511:LYS:HB2	1.89	0.66
1:A:35:GLU:HB2	1:A:94:SER:HB3	1.78	0.66
1:D:160:SER:OG	1:D:183:ASP:OD1	2.13	0.66
1:D:427:ILE:O	1:D:427:ILE:HD13	1.94	0.66
1:A:13:MSE:CE	1:A:26:ILE:HD12	2.25	0.65
1:A:97:MSE:SE	1:A:103:VAL:HG12	2.46	0.65
1:A:479:GLU:C	1:A:481:CYS:HB2	2.21	0.65
1:B:355:SER:O	1:B:359:ASN:HB2	1.97	0.65
1:C:478:LEU:CD2	1:C:508:TRP:HH2	2.09	0.65
1:C:478:LEU:CD1	1:C:508:TRP:HZ2	2.09	0.65
1:B:478:LEU:HB3	1:B:508:TRP:CE3	2.32	0.65
1:C:193:GLU:CG	1:C:222:LYS:HD3	2.27	0.65
1:D:117:ILE:HG22	1:D:118:PHE:CE1	2.31	0.65
1:C:256:ALA:CB	1:C:258:LEU:CD1	2.74	0.65
1:C:315:THR:OG1	1:C:317:LEU:HD13	1.95	0.65
1:A:89:GLU:HA	1:A:89:GLU:OE2	1.96	0.65
1:D:478:LEU:CB	1:D:508:TRP:HE1	2.10	0.65
1:A:119:PRO:HG2	1:A:153:PRO:HB3	1.79	0.65
1:C:503:SER:HA	1:C:506:ILE:HG13	1.77	0.65
1:D:172:PHE:CE2	1:D:209:PRO:HD3	2.32	0.65
1:D:117:ILE:HD11	1:D:165:CYS:SG	2.37	0.65
1:D:448:LEU:O	1:D:487:ASN:ND2	2.30	0.65
1:D:474:GLY:HA3	1:D:476:GLN:HG2	1.79	0.65
1:D:499:GLU:HA	1:D:527:MSE:CE	2.16	0.65
1:D:34:LEU:O	1:D:36:VAL:HG23	1.97	0.65
1:D:84:MSE:SE	1:D:107:LEU:CD1	2.95	0.65
1:C:474:GLY:CA	1:C:476:GLN:N	2.57	0.65
1:A:138:LEU:HD23	1:A:139:ALA:CA	2.27	0.64
1:A:254:GLU:O	1:A:255:ASN:C	2.38	0.64
1:B:52:ARG:HG3	1:B:68:PHE:O	1.97	0.64
1:C:160:SER:OG	1:C:183:ASP:OD1	2.13	0.64
1:A:394:LEU:HD21	1:A:397:LEU:HD13	1.78	0.64
1:D:437:SER:O	1:D:440:PRO:HD2	1.98	0.64
1:D:610:TRP:CE3	1:D:615:ILE:CD1	2.81	0.64
1:D:146:ASP:OD1	1:D:146:ASP:N	2.31	0.64
1:B:136:GLU:H	1:B:136:GLU:CD	2.04	0.64
1:B:256:ALA:HB3	1:B:258:LEU:CD1	2.27	0.64
1:D:113:CYS:O	1:D:116:ARG:HB3	1.98	0.64
1:D:40:ARG:HH21	1:D:40:ARG:CG	2.10	0.64
1:D:76:VAL:O	1:D:130:VAL:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:N	1:A:23:LYS:HD2	2.12	0.64
1:D:78:CYS:SG	1:D:103:VAL:CG1	2.83	0.64
1:D:110:ILE:HG21	1:D:127:MSE:HE1	1.80	0.64
1:A:593:LYS:HE2	1:B:200:SER:OG	1.98	0.64
1:D:37:LYS:CA	1:D:39:ASP:H	2.06	0.64
1:D:408:LYS:HE3	1:D:408:LYS:HA	1.79	0.64
1:A:258:LEU:CD2	1:A:262:PHE:CE2	2.81	0.64
1:B:8:VAL:HG22	1:B:31:LYS:HG2	1.80	0.64
1:C:193:GLU:HG3	1:C:222:LYS:CD	2.28	0.64
1:C:381:MSE:HA	1:C:381:MSE:CE	2.27	0.64
1:B:32:VAL:CG2	1:B:95:MSE:HG2	2.28	0.63
1:A:84:MSE:HE1	1:A:106:VAL:HG11	1.80	0.63
1:C:290:ASP:O	1:C:294:SER:OG	2.16	0.63
1:C:484:GLU:N	1:C:508:TRP:HE1	1.96	0.63
1:D:53:ALA:O	1:D:67:THR:HG22	1.99	0.63
1:D:115:ARG:HH11	1:D:115:ARG:HG3	1.62	0.63
1:B:174:TYR:CD1	1:B:174:TYR:C	2.76	0.63
1:C:602:ASN:ND2	1:C:605:LEU:HD23	2.13	0.63
1:D:144:LEU:O	1:D:148:GLN:CD	2.40	0.63
1:A:601:ILE:HD11	1:B:184:THR:O	1.97	0.63
1:C:404:PHE:CE1	1:C:440:PRO:HB3	2.32	0.63
1:C:449:ALA:HA	1:C:485:ILE:HG23	1.80	0.63
1:D:36:VAL:O	1:D:39:ASP:N	2.32	0.63
1:A:117:ILE:HD11	1:A:165:CYS:SG	2.37	0.63
1:D:70:TYR:CD1	1:D:110:ILE:HG23	2.32	0.63
1:A:543:ILE:CG2	1:A:574:ASN:ND2	2.61	0.63
1:C:611:ASP:OD1	1:C:612:LYS:N	2.31	0.63
1:A:143:ALA:O	1:A:146:ASP:HB2	1.98	0.63
1:A:290:ASP:HA	1:A:293:VAL:HB	1.81	0.63
1:A:638:ILE:CD1	1:A:640:MSE:HE1	2.27	0.63
1:B:288:LEU:O	1:B:289:GLU:HB2	1.97	0.63
1:C:55:LEU:CD2	1:C:95:MSE:HE2	2.27	0.63
1:D:477:VAL:C	1:D:478:LEU:HG	2.23	0.63
1:B:115:ARG:HG3	1:B:123:PRO:CD	2.29	0.63
1:B:580:VAL:HG12	1:B:608:VAL:HG22	1.81	0.63
1:C:134:PRO:HD2	1:C:137:ARG:HD3	1.81	0.63
1:C:441:LEU:HD11	1:C:445:LEU:HD11	1.81	0.63
1:B:8:VAL:HG21	1:B:45:VAL:HG13	1.81	0.62
1:B:115:ARG:HG3	1:B:123:PRO:HD3	1.80	0.62
1:D:48:LEU:HD11	1:D:106:VAL:HG13	1.80	0.62
1:B:80:LYS:HB3	1:B:83:GLN:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:LEU:HD11	1:C:505:LEU:HD11	1.81	0.62
1:D:174:TYR:HD1	1:D:174:TYR:C	2.08	0.62
1:D:43:ASN:O	1:D:44:LYS:HE2	1.97	0.62
1:A:301:ALA:O	1:A:332:ASN:HB2	1.99	0.62
1:B:503:SER:O	1:B:504:THR:C	2.42	0.62
1:B:513:ARG:HH11	1:B:513:ARG:CA	2.12	0.62
1:D:174:TYR:C	1:D:174:TYR:CD1	2.76	0.62
1:B:484:GLU:OE2	1:B:508:TRP:CA	2.48	0.62
1:C:474:GLY:HA3	1:C:476:GLN:N	2.05	0.62
1:A:617:ALA:O	1:A:621:GLN:HG3	2.00	0.62
1:C:532:LEU:CD2	1:C:536:LEU:HG	2.29	0.62
1:D:379:LEU:HD13	1:D:402:SER:OG	2.00	0.62
1:A:68:PHE:CD1	1:A:93:MSE:HE1	2.34	0.62
1:A:380:GLU:CD	1:A:405:SER:OG	2.43	0.62
1:C:509:LEU:HD22	1:C:518:LEU:HD22	1.77	0.62
1:A:133:GLU:OE1	1:A:133:GLU:HA	1.98	0.61
1:B:349:LEU:HG	1:B:375:THR:HG1	1.63	0.61
1:B:638:ILE:HD12	1:B:638:ILE:H	1.65	0.61
1:D:43:ASN:O	1:D:44:LYS:CD	2.48	0.61
1:D:378:SER:HB2	1:D:406:HIS:CD2	2.35	0.61
1:A:493:ILE:C	1:A:496:ASN:ND2	2.58	0.61
1:D:26:ILE:CD1	1:D:47:VAL:HG21	2.29	0.61
1:D:256:ALA:HB3	1:D:258:LEU:CD1	2.30	0.61
1:D:470:LEU:O	1:D:473:GLY:O	2.18	0.61
1:A:349:LEU:CG	1:A:375:THR:OG1	2.35	0.61
1:A:589:ASP:OD1	1:A:616:THR:OG1	2.18	0.61
1:C:587:MSE:HG2	1:C:613:ASN:CG	2.25	0.61
1:D:313:SER:HA	1:D:345:SER:O	2.01	0.61
1:B:115:ARG:NH1	1:B:150:LEU:HD11	2.16	0.61
1:B:157:GLY:O	1:B:162:MSE:HE3	2.00	0.61
1:B:477:VAL:HG23	1:B:478:LEU:HG	1.81	0.61
1:C:477:VAL:O	1:C:477:VAL:HG13	2.00	0.61
1:D:477:VAL:O	1:D:478:LEU:HD23	2.00	0.61
1:A:482:ILE:HG23	1:A:483:ALA:N	2.15	0.61
1:B:298:ILE:HG22	1:B:299:GLN:N	2.15	0.61
1:C:387:LEU:O	1:C:391:LEU:HD21	2.01	0.61
1:D:39:ASP:N	1:D:39:ASP:OD1	2.29	0.61
1:D:372:LEU:O	1:D:375:THR:HB	2.01	0.61
1:C:54:PHE:CD1	1:C:67:THR:HG23	2.35	0.61
1:D:180:TRP:CD1	1:D:184:THR:HG1	2.18	0.61
1:D:325:LEU:HD12	1:D:325:LEU:C	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LEU:CD1	1:C:505:LEU:CD1	2.79	0.61
1:D:516:GLN:C	1:D:517:HIS:CD2	2.78	0.61
1:A:76:VAL:HG12	1:A:85:VAL:O	2.01	0.61
1:C:80:LYS:HG2	1:C:81:PRO:HD2	1.82	0.61
1:D:318:SER:OG	1:D:320:LYS:HG3	2.01	0.61
1:D:34:LEU:O	1:D:34:LEU:HD23	2.00	0.61
1:D:82:ALA:O	1:D:97:MSE:N	2.25	0.61
1:D:322:VAL:HG12	1:D:357:MSE:HE3	1.83	0.61
1:A:478:LEU:HD13	1:A:508:TRP:CB	2.31	0.60
1:A:602:ASN:ND2	1:A:605:LEU:HD23	2.16	0.60
1:D:54:PHE:CE1	1:D:67:THR:HG21	2.36	0.60
1:D:284:ALA:HB1	1:D:313:SER:HB3	1.84	0.60
1:B:349:LEU:CG	1:B:375:THR:OG1	2.44	0.60
1:D:97:MSE:HE2	1:D:103:VAL:HA	1.83	0.60
1:D:474:GLY:HA3	1:D:476:GLN:HG3	1.83	0.60
1:A:431:LEU:O	1:A:434:THR:OG1	2.18	0.60
1:B:36:VAL:CG2	1:B:42:GLU:CG	2.65	0.60
1:A:65:GLU:O	1:A:66:LEU:HD23	2.02	0.60
1:A:666:LEU:HD22	1:B:666:LEU:HD11	1.83	0.60
1:B:474:GLY:O	1:B:475:ALA:HB3	2.00	0.60
1:C:185:ILE:O	1:C:189:GLN:HG3	2.01	0.60
1:C:509:LEU:HD22	1:C:518:LEU:HD21	1.84	0.60
1:C:650:ASN:O	1:C:652:GLU:HB3	2.00	0.60
1:D:325:LEU:HD11	1:D:329:LEU:HD11	1.84	0.60
1:D:355:SER:O	1:D:359:ASN:N	2.30	0.60
1:A:601:ILE:HD11	1:B:184:THR:C	2.27	0.60
1:B:182:VAL:O	1:B:186:TYR:CB	2.43	0.60
1:C:115:ARG:HH21	1:C:115:ARG:CG	2.14	0.60
1:D:586:GLY:HA2	1:D:614:ASN:HD22	1.65	0.60
1:A:263:ALA:CB	1:A:292:GLY:HA3	2.32	0.60
1:D:115:ARG:HH11	1:D:115:ARG:CG	2.14	0.60
1:D:638:ILE:H	1:D:638:ILE:CD1	1.99	0.60
1:A:303:LEU:HD23	1:A:304:PRO:CD	2.23	0.59
1:A:506:ILE:HG23	1:A:542:MSE:HE3	1.83	0.59
1:C:122:SER:O	1:C:125:ARG:N	2.35	0.59
1:C:169:TRP:CZ3	1:C:170:LEU:HD21	2.36	0.59
1:A:256:ALA:HB3	1:A:258:LEU:CD1	2.29	0.59
1:A:483:ALA:O	1:A:484:GLU:HB3	2.02	0.59
1:B:66:LEU:HD13	1:B:93:MSE:HE1	1.81	0.59
1:C:350:ARG:HG3	1:C:376:GLU:HG2	1.83	0.59
1:D:314:LYS:HG3	1:D:346:GLY:HA3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD23	1:A:63:LYS:O	2.01	0.59
1:B:84:MSE:HE1	1:B:106:VAL:HB	1.84	0.59
1:C:117:ILE:CG2	1:C:118:PHE:CE2	2.85	0.59
1:C:474:GLY:C	1:C:476:GLN:H	2.10	0.59
1:C:651:PRO:N	1:C:652:GLU:HB2	2.16	0.59
1:A:9:PRO:HB3	1:A:12:LEU:CD2	2.26	0.59
1:A:162:MSE:O	1:A:166:VAL:HG23	2.02	0.59
1:A:506:ILE:HG23	1:A:542:MSE:CE	2.32	0.59
1:B:374:ASN:OD1	1:B:401:ARG:CD	2.43	0.59
1:D:117:ILE:HG22	1:D:118:PHE:CG	2.38	0.59
1:D:142:GLN:OE1	1:D:146:ASP:OD1	2.20	0.59
1:B:44:LYS:HB3	1:B:56:LEU:O	2.02	0.59
1:C:414:PRO:O	1:C:418:GLN:HB2	2.02	0.59
1:A:652:GLU:CG	1:A:653:LYS:H	2.05	0.59
1:B:354:LEU:HD23	1:B:358:TYR:OH	2.03	0.59
1:D:16:ILE:HG23	1:D:56:LEU:HD13	1.83	0.59
1:A:32:VAL:HG21	1:A:95:MSE:HB3	1.85	0.59
1:A:174:TYR:C	1:A:174:TYR:CD1	2.81	0.59
1:A:528:LYS:O	1:A:531:ASN:HB2	2.02	0.59
1:A:574:ASN:OD1	1:A:576:SER:N	2.31	0.59
1:D:34:LEU:HD21	1:D:36:VAL:CG2	2.33	0.59
1:D:422:SER:O	1:D:424:LEU:CD1	2.51	0.59
1:D:620:PHE:CD1	1:D:658:LEU:HD21	2.38	0.59
1:B:76:VAL:HG11	1:B:107:LEU:HD21	1.85	0.59
1:C:36:VAL:HG21	1:C:42:GLU:HG3	1.85	0.59
1:D:616:THR:CG2	1:D:617:ALA:N	2.66	0.59
1:A:28:VAL:HB	1:A:48:LEU:HB2	1.85	0.59
1:A:121:LEU:HD22	1:A:125:ARG:HH11	1.66	0.59
1:B:56:LEU:CD2	1:B:64:LEU:HB2	2.33	0.59
1:D:372:LEU:O	1:D:375:THR:HG22	2.01	0.59
1:B:558:SER:HB2	1:B:560:LEU:HG	1.84	0.58
1:D:64:LEU:CD2	1:D:65:GLU:N	2.64	0.58
1:C:498:LEU:CD1	1:C:505:LEU:HD13	2.33	0.58
1:C:536:LEU:O	1:C:540:VAL:HG23	2.02	0.58
1:D:117:ILE:CG2	1:D:118:PHE:CE1	2.86	0.58
1:A:403:VAL:HG23	1:A:403:VAL:O	2.04	0.58
1:A:470:LEU:CD2	1:A:477:VAL:CG1	2.81	0.58
1:B:54:PHE:CA	1:B:67:THR:HG22	2.34	0.58
1:B:564:VAL:O	1:B:564:VAL:HG22	2.03	0.58
1:C:53:ALA:O	1:C:67:THR:HG22	2.02	0.58
1:C:387:LEU:O	1:C:391:LEU:HD11	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:LEU:HD12	1:C:509:LEU:H	1.68	0.58
1:C:647:LEU:HD23	1:C:654:THR:HB	1.83	0.58
1:A:13:MSE:O	1:A:16:ILE:HB	2.02	0.58
1:A:610:TRP:O	1:A:613:ASN:ND2	2.28	0.58
1:A:667:ARG:HG3	1:A:668:ASN:N	2.19	0.58
1:D:397:LEU:HD11	1:D:399:LEU:HD11	1.84	0.58
1:D:504:THR:O	1:D:507:VAL:CG2	2.51	0.58
1:A:474:GLY:C	1:A:477:VAL:HG12	2.29	0.58
1:A:543:ILE:HG22	1:A:574:ASN:ND2	2.19	0.58
1:C:16:ILE:HA	1:C:19:VAL:HG12	1.86	0.58
1:D:51:CYS:C	1:D:70:TYR:CE2	2.82	0.58
1:D:208:ILE:HG23	1:D:237:GLN:HE21	1.68	0.58
1:D:563:GLU:O	1:D:566:ILE:HG23	2.04	0.58
1:A:222:LYS:HG3	1:A:250:GLU:HB2	1.84	0.58
1:B:53:ALA:O	1:B:67:THR:HG22	2.04	0.58
1:C:117:ILE:CB	1:C:118:PHE:CD2	2.85	0.58
1:D:336:ALA:O	1:D:366:THR:HG22	2.03	0.58
1:B:80:LYS:HD3	1:B:82:ALA:H	1.68	0.58
1:B:270:LEU:HD21	1:B:278:LEU:HD12	1.85	0.58
1:B:322:VAL:HG21	1:B:349:LEU:HD21	1.86	0.58
1:C:476:GLN:HE21	1:C:476:GLN:CA	2.16	0.58
1:D:80:LYS:HD2	1:D:81:PRO:CD	2.34	0.58
1:D:115:ARG:NH2	1:D:150:LEU:HD22	2.18	0.58
1:D:610:TRP:HZ3	1:D:615:ILE:CD1	2.17	0.58
1:A:23:LYS:HE3	1:A:23:LYS:CA	2.34	0.57
1:A:603:THR:O	1:A:603:THR:OG1	2.21	0.57
1:C:107:LEU:O	1:C:108:ALA:C	2.42	0.57
1:B:258:LEU:CD2	1:B:262:PHE:CE2	2.86	0.57
1:D:56:LEU:HD23	1:D:64:LEU:HA	1.85	0.57
1:C:69:SER:N	1:C:72:GLU:OE1	2.34	0.57
1:C:493:ILE:O	1:C:496:ASN:ND2	2.34	0.57
1:D:97:MSE:HG3	1:D:103:VAL:HG22	1.87	0.57
1:D:110:ILE:HG21	1:D:127:MSE:CE	2.34	0.57
1:D:110:ILE:CG2	1:D:127:MSE:HE1	2.34	0.57
1:A:212:ALA:HB2	1:A:237:GLN:CG	2.35	0.57
1:B:132:MSE:SE	1:B:138:LEU:CD1	3.02	0.57
1:C:510:SER:O	1:C:513:ARG:NH1	2.37	0.57
1:D:37:LYS:CD	1:D:37:LYS:H	2.18	0.57
1:D:145:TRP:C	1:D:148:GLN:OE1	2.47	0.57
1:A:99:SER:OG	1:A:100:PRO:HD2	2.05	0.57
1:C:407:ARG:HH21	1:C:407:ARG:CG	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG13	1:A:20:ILE:HG23	1.86	0.57
1:A:589:ASP:OD2	1:A:616:THR:OG1	2.22	0.57
1:A:638:ILE:HG23	1:A:640:MSE:CE	2.35	0.57
1:A:650:ASN:HB3	1:A:652:GLU:OE2	2.05	0.57
1:D:70:TYR:CE1	1:D:110:ILE:HG12	2.39	0.57
1:D:212:ALA:HB2	1:D:237:GLN:CG	2.35	0.57
1:D:290:ASP:OD2	1:D:321:GLY:N	2.38	0.57
1:A:290:ASP:OD1	1:A:317:LEU:HA	2.04	0.57
1:D:499:GLU:HA	1:D:499:GLU:OE2	2.04	0.57
1:C:26:ILE:CG2	1:C:47:VAL:CG1	2.81	0.57
1:C:486:HIS:HA	1:C:514:SER:HB3	1.87	0.57
1:D:114:LEU:HB3	1:D:123:PRO:HG3	1.87	0.57
1:A:13:MSE:HG3	1:A:17:LYS:HE3	1.86	0.57
1:C:524:PHE:N	1:C:524:PHE:CD1	2.73	0.57
1:D:196:LEU:HB2	1:D:225:SER:HB2	1.87	0.57
1:A:604:LYS:HG3	1:A:604:LYS:O	2.05	0.57
1:B:315:THR:OG1	1:B:317:LEU:HD13	2.05	0.57
1:B:485:ILE:HG22	1:B:512:ASN:HD22	1.70	0.57
1:C:610:TRP:CD1	1:C:636:MSE:HE3	2.40	0.57
1:D:66:LEU:HD13	1:D:93:MSE:HE2	1.87	0.57
1:A:471:ARG:HG3	1:A:471:ARG:NH2	2.19	0.56
1:B:174:TYR:C	1:B:174:TYR:HD1	2.10	0.56
1:B:468:HIS:O	1:B:472:SER:HB3	2.05	0.56
1:C:381:MSE:HE3	1:C:381:MSE:CA	2.27	0.56
1:C:420:PHE:CZ	1:C:444:LEU:CD1	2.87	0.56
1:C:461:LEU:O	1:C:464:CYS:SG	2.62	0.56
1:C:613:ASN:O	1:C:614:ASN:HB2	2.03	0.56
1:C:34:LEU:HD23	1:C:36:VAL:HG22	1.87	0.56
1:D:27:SER:HB2	1:D:109:HIS:HE1	1.70	0.56
1:D:466:LEU:O	1:D:469:CYS:HB3	2.06	0.56
1:A:174:TYR:C	1:A:174:TYR:HD1	2.13	0.56
1:A:323:ASN:ND2	1:A:356:HIS:HB2	2.20	0.56
1:B:46:LEU:HA	1:B:55:LEU:HD23	1.88	0.56
1:D:159:PHE:O	1:D:159:PHE:HD1	1.88	0.56
1:C:68:PHE:HD2	1:C:93:MSE:CE	1.92	0.56
1:A:479:GLU:CA	1:A:481:CYS:SG	2.93	0.56
1:C:545:ASP:OD1	1:C:546:GLU:N	2.38	0.56
1:D:506:ILE:HG23	1:D:542:MSE:HE3	1.88	0.56
1:A:369:HIS:CG	1:A:396:VAL:CG2	2.89	0.56
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.71	0.56
1:A:13:MSE:HE2	1:A:26:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:GLU:HG2	1:A:653:LYS:HG3	1.88	0.56
1:C:498:LEU:HD13	1:C:505:LEU:CD1	2.35	0.56
1:D:375:THR:HG23	1:D:377:CYS:HB3	1.88	0.56
1:A:46:LEU:HD23	1:A:55:LEU:HD23	1.86	0.56
1:A:558:SER:HB2	1:A:585:ASN:OD1	2.06	0.56
1:B:88:THR:HG23	1:B:91:CYS:CA	2.36	0.56
1:B:323:ASN:ND2	1:B:356:HIS:HB2	2.21	0.56
1:C:602:ASN:HD21	1:C:605:LEU:HD23	1.70	0.56
1:D:563:GLU:O	1:D:565:THR:N	2.39	0.56
1:A:13:MSE:HE2	1:A:26:ILE:CD1	2.36	0.56
1:A:369:HIS:HA	1:A:396:VAL:HG22	1.88	0.56
1:B:284:ALA:HB2	1:B:311:ASN:OD1	2.05	0.56
1:C:29:LYS:O	1:C:30:LYS:HD2	2.05	0.56
1:A:119:PRO:HG2	1:A:153:PRO:CB	2.36	0.56
1:B:183:ASP:OD1	1:B:183:ASP:N	2.38	0.56
1:D:512:ASN:OD1	1:D:514:SER:OG	2.24	0.56
1:A:115:ARG:NH2	1:A:145:TRP:O	2.39	0.55
1:C:36:VAL:HG12	1:C:37:LYS:N	2.01	0.55
1:C:586:GLY:N	1:C:613:ASN:OD1	2.38	0.55
1:D:72:GLU:CD	1:D:90:LYS:HE3	2.31	0.55
1:A:587:MSE:HG2	1:A:613:ASN:OD1	2.06	0.55
1:B:32:VAL:HG21	1:B:95:MSE:CG	2.37	0.55
1:B:32:VAL:HG22	1:B:95:MSE:HG2	1.88	0.55
1:B:184:THR:O	1:B:188:THR:OG1	2.16	0.55
1:C:323:ASN:ND2	1:C:356:HIS:ND1	2.54	0.55
1:D:390:CYS:HB3	1:D:394:LEU:HB2	1.87	0.55
1:B:77:ILE:HG23	1:B:79:HIS:CE1	2.40	0.55
1:D:159:PHE:HD2	1:D:220:PHE:CE2	2.24	0.55
1:D:383:CYS:O	1:D:384:SER:C	2.47	0.55
1:A:284:ALA:HB1	1:A:313:SER:HB3	1.88	0.55
1:A:471:ARG:HH21	1:A:471:ARG:CG	2.18	0.55
1:A:484:GLU:CD	1:A:508:TRP:HE1	2.11	0.55
1:C:36:VAL:CG1	1:C:37:LYS:H	2.05	0.55
1:C:270:LEU:HD21	1:C:278:LEU:HD12	1.88	0.55
1:C:368:VAL:O	1:C:368:VAL:HG12	2.04	0.55
1:A:589:ASP:CG	1:A:616:THR:OG1	2.50	0.55
1:B:84:MSE:HE3	1:B:103:VAL:HB	1.87	0.55
1:B:117:ILE:HG22	1:B:118:PHE:CD2	2.42	0.55
1:B:375:THR:HG23	1:B:377:CYS:H	1.71	0.55
1:C:174:TYR:C	1:C:174:TYR:CD1	2.84	0.55
1:D:100:PRO:HD2	1:D:101:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:ALA:C	1:D:476:GLN:HG2	2.31	0.55
1:C:84:MSE:HE1	1:C:106:VAL:HG11	1.88	0.55
1:C:531:ASN:C	1:C:534:PRO:HD2	2.32	0.55
1:D:16:ILE:HG23	1:D:56:LEU:CD1	2.36	0.55
1:B:174:TYR:HD1	1:B:175:LYS:N	2.05	0.55
1:C:174:TYR:HD1	1:C:175:LYS:N	2.05	0.55
1:C:197:GLN:OE1	1:C:226:LYS:N	2.32	0.55
1:C:561:LYS:O	1:C:562:ALA:HB3	2.07	0.55
1:B:561:LYS:O	1:B:564:VAL:HG12	2.06	0.55
1:D:651:PRO:HG2	1:D:652:GLU:H	1.71	0.55
1:A:32:VAL:HG23	1:A:96:LYS:O	2.05	0.55
1:C:55:LEU:HD11	1:C:95:MSE:HE2	1.79	0.55
1:C:80:LYS:C	1:C:80:LYS:HD3	2.32	0.55
1:C:422:SER:O	1:C:424:LEU:CD1	2.55	0.55
1:C:502:LEU:O	1:C:506:ILE:HG12	2.07	0.55
1:A:218:GLN:HA	1:A:247:ARG:HG3	1.89	0.55
1:A:456:GLY:HA2	1:A:489:THR:HG23	1.89	0.55
1:A:494:SER:HB2	1:A:521:GLY:O	2.07	0.55
1:D:408:LYS:CA	1:D:408:LYS:CE	2.85	0.55
1:B:88:THR:CG2	1:B:91:CYS:CB	2.86	0.54
1:D:84:MSE:SE	1:D:107:LEU:HD11	2.57	0.54
1:D:99:SER:CB	1:D:101:GLU:HG3	2.36	0.54
1:D:290:ASP:OD2	1:D:318:SER:HB3	2.08	0.54
1:B:513:ARG:HH11	1:B:513:ARG:HA	1.71	0.54
1:C:14:GLU:OE1	1:C:14:GLU:HA	2.06	0.54
1:C:531:ASN:ND2	1:C:531:ASN:H	2.05	0.54
1:D:34:LEU:CD2	1:D:36:VAL:CG2	2.85	0.54
1:D:372:LEU:O	1:D:375:THR:CB	2.55	0.54
1:B:134:PRO:CD	1:B:137:ARG:HH21	2.19	0.54
1:C:8:VAL:HG11	1:C:13:MSE:HE3	1.88	0.54
1:C:372:LEU:O	1:C:375:THR:HB	2.08	0.54
1:D:631:TYR:O	1:D:668:ASN:CG	2.50	0.54
1:C:610:TRP:CE3	1:C:615:ILE:CD1	2.90	0.54
1:D:118:PHE:HD2	1:D:126:ILE:HD12	1.66	0.54
1:A:394:LEU:O	1:A:425:ALA:HB3	2.06	0.54
1:A:471:ARG:NH1	1:A:497:GLY:O	2.41	0.54
1:B:9:PRO:HG2	1:B:12:LEU:HB3	1.90	0.54
1:B:80:LYS:CG	1:B:81:PRO:CD	2.86	0.54
1:D:43:ASN:O	1:D:44:LYS:HD3	2.08	0.54
1:D:408:LYS:HE3	1:D:408:LYS:CA	2.37	0.54
1:A:104:SER:HG	1:A:137:ARG:HH11	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:LEU:HD13	1:A:508:TRP:HB2	1.90	0.54
1:A:600:GLN:OE1	1:B:185:ILE:HD13	2.07	0.54
1:B:404:PHE:CE1	1:B:440:PRO:HB3	2.43	0.54
1:C:212:ALA:HB2	1:C:237:GLN:CG	2.38	0.54
1:C:484:GLU:OE1	1:C:508:TRP:HD1	1.89	0.54
1:D:314:LYS:N	1:D:345:SER:O	2.41	0.54
1:A:98:VAL:CG2	1:A:99:SER:N	2.71	0.54
1:A:200:SER:OG	1:B:593:LYS:HE2	2.08	0.54
1:A:290:ASP:OD1	1:A:290:ASP:N	2.40	0.54
1:B:415:SER:OG	3:B:702:CL:CL	2.60	0.54
1:B:477:VAL:HG23	1:B:478:LEU:N	2.22	0.54
1:C:381:MSE:CE	1:C:381:MSE:CA	2.85	0.54
1:D:315:THR:OG1	1:D:317:LEU:HD12	2.07	0.54
1:C:282:ASN:C	1:C:282:ASN:OD1	2.51	0.54
1:D:172:PHE:HE2	1:D:208:ILE:HB	1.72	0.54
1:D:222:LYS:HG3	1:D:250:GLU:HB2	1.90	0.54
1:D:289:GLU:O	1:D:293:VAL:HG23	2.06	0.54
1:B:24:ILE:CD1	1:B:25:LYS:N	2.68	0.54
1:C:54:PHE:CD1	1:C:67:THR:CG2	2.91	0.54
1:C:174:TYR:C	1:C:174:TYR:HD1	2.15	0.54
1:C:141:LEU:O	1:C:144:LEU:N	2.41	0.54
1:C:386:LEU:HD23	1:C:390:CYS:SG	2.47	0.54
1:C:639:PRO:O	1:C:639:PRO:HG2	2.07	0.54
1:A:485:ILE:CG2	1:A:512:ASN:HD22	1.90	0.53
1:B:607:THR:HB	1:B:635:PHE:HD2	1.73	0.53
1:C:329:LEU:HD23	1:C:335:THR:HG21	1.91	0.53
1:C:474:GLY:C	1:C:476:GLN:N	2.66	0.53
1:A:319:PRO:HD2	1:A:352:ASP:OD2	2.07	0.53
1:C:162:MSE:HE1	1:C:217:ASN:HA	1.91	0.53
1:C:348:ALA:C	1:C:349:LEU:HD23	2.33	0.53
1:D:442:LYS:HG3	1:D:477:VAL:HG13	1.91	0.53
1:D:578:THR:HG22	1:D:604:LYS:HD2	1.90	0.53
1:A:601:ILE:CD1	1:B:184:THR:O	2.57	0.53
1:B:80:LYS:CD	1:B:81:PRO:CD	2.85	0.53
1:B:484:GLU:OE2	1:B:508:TRP:HA	2.08	0.53
1:B:506:ILE:CD1	1:B:539:LEU:HD13	2.38	0.53
1:C:162:MSE:O	1:C:166:VAL:HG23	2.09	0.53
1:D:46:LEU:HD22	1:D:95:MSE:HE1	1.91	0.53
1:D:610:TRP:HZ3	1:D:615:ILE:HD13	1.74	0.53
1:A:638:ILE:CG2	1:A:640:MSE:CE	2.85	0.53
1:D:80:LYS:HE2	1:D:82:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:LYS:HA	1:D:408:LYS:CE	2.38	0.53
1:A:76:VAL:HG13	1:A:86:VAL:CG2	2.38	0.53
1:A:474:GLY:O	1:A:475:ALA:HB3	2.07	0.53
1:B:32:VAL:HG21	1:B:95:MSE:CB	2.36	0.53
1:B:197:GLN:OE1	1:B:226:LYS:N	2.36	0.53
1:B:336:ALA:O	1:B:366:THR:HG22	2.09	0.53
1:D:261:ASP:OD1	1:D:262:PHE:N	2.42	0.53
1:B:484:GLU:OE2	1:B:508:TRP:CG	2.62	0.53
1:D:99:SER:CB	1:D:100:PRO:CD	2.87	0.53
1:D:516:GLN:HB2	1:D:517:HIS:CD2	2.44	0.53
1:A:80:LYS:HD2	1:A:80:LYS:C	2.33	0.53
1:A:607:THR:HB	1:A:635:PHE:HB2	1.90	0.53
1:B:16:ILE:O	1:B:19:VAL:HG12	2.09	0.53
1:B:117:ILE:CG2	1:B:118:PHE:CD2	2.92	0.53
1:C:498:LEU:HD11	1:C:505:LEU:CD1	2.39	0.53
1:C:71:LEU:HD12	1:C:71:LEU:N	2.23	0.53
1:C:195:ASN:OD1	1:C:197:GLN:HG2	2.08	0.53
1:C:466:LEU:HA	1:C:469:CYS:HB3	1.91	0.53
1:D:74:HIS:N	1:D:87:GLU:O	2.42	0.53
1:A:543:ILE:HG22	1:A:574:ASN:HD22	1.74	0.53
1:B:74:HIS:CE1	1:B:89:GLU:CB	2.81	0.53
1:B:77:ILE:O	1:B:85:VAL:HG12	2.09	0.53
1:B:254:GLU:O	1:B:255:ASN:C	2.51	0.53
1:B:297:SER:HB2	1:B:328:SER:HB2	1.90	0.53
1:D:68:PHE:CE2	1:D:86:VAL:CG1	2.91	0.53
1:D:172:PHE:CE2	1:D:208:ILE:HB	2.44	0.53
1:D:256:ALA:N	1:D:286:ASN:OD1	2.42	0.53
1:B:46:LEU:HG	1:B:55:LEU:HD21	1.90	0.52
1:C:116:ARG:HG3	1:C:116:ARG:NH1	2.24	0.52
1:C:610:TRP:CD1	1:C:636:MSE:CE	2.92	0.52
1:A:169:TRP:CZ3	1:A:170:LEU:HD21	2.44	0.52
1:A:382:VAL:O	1:A:386:LEU:HG	2.08	0.52
1:C:456:GLY:HA2	1:C:489:THR:CG2	2.38	0.52
1:D:72:GLU:OE2	1:D:90:LYS:HE3	2.09	0.52
1:D:408:LYS:HE2	1:D:408:LYS:O	2.08	0.52
1:A:73:ILE:HD12	1:A:127:MSE:HE3	1.90	0.52
1:A:368:VAL:O	1:A:368:VAL:HG12	2.09	0.52
1:D:111:GLY:O	1:D:115:ARG:N	2.36	0.52
1:D:298:ILE:HG22	1:D:299:GLN:HE21	1.75	0.52
1:D:312:LEU:C	1:D:315:THR:HG23	2.34	0.52
1:A:602:ASN:HD21	1:A:605:LEU:CD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:LYS:O	1:B:604:LYS:CG	2.57	0.52
1:C:411:GLU:O	1:C:413:PRO:HD3	2.10	0.52
1:D:71:LEU:N	1:D:71:LEU:HD12	2.24	0.52
1:D:159:PHE:HD1	1:D:159:PHE:C	2.16	0.52
1:A:647:LEU:HD23	1:A:651:PRO:HA	1.92	0.52
1:B:71:LEU:HD21	1:B:118:PHE:CZ	2.44	0.52
1:D:79:HIS:HA	1:D:133:GLU:HB2	1.91	0.52
1:D:159:PHE:C	1:D:159:PHE:CD1	2.86	0.52
1:D:349:LEU:HD13	1:D:357:MSE:CE	2.33	0.52
1:A:480:GLY:N	1:A:481:CYS:CA	2.72	0.52
1:A:485:ILE:O	1:A:512:ASN:ND2	2.42	0.52
1:A:558:SER:O	1:A:559:LYS:HB2	2.10	0.52
1:A:640:MSE:HE2	1:A:640:MSE:HA	1.92	0.52
1:B:513:ARG:CG	1:B:513:ARG:NH1	2.72	0.52
1:C:16:ILE:O	1:C:19:VAL:HG12	2.10	0.52
1:C:117:ILE:HG21	1:C:118:PHE:CE2	2.45	0.52
1:C:155:PRO:HB3	1:C:187:LEU:HD13	1.91	0.52
1:C:478:LEU:CD1	1:C:508:TRP:CZ2	2.87	0.52
1:C:556:ALA:HA	1:C:583:SER:O	2.09	0.52
1:C:558:SER:HB2	1:C:585:ASN:OD1	2.09	0.52
1:C:610:TRP:CH2	1:C:623:ILE:HG13	2.45	0.52
1:D:72:GLU:HG2	1:D:89:GLU:CG	2.40	0.52
1:D:152:GLU:HG2	1:D:153:PRO:CD	2.40	0.52
1:B:195:ASN:OD1	1:B:197:GLN:HG2	2.10	0.52
1:C:58:ALA:C	1:C:59:ARG:HG3	2.34	0.52
1:D:52:ARG:N	1:D:70:TYR:CE2	2.78	0.52
1:D:424:LEU:CD1	1:D:424:LEU:N	2.72	0.52
1:A:330:SER:HB3	1:A:363:GLN:OE1	2.09	0.52
1:A:380:GLU:OE2	1:A:405:SER:OG	2.28	0.52
1:B:16:ILE:HG23	1:B:56:LEU:HD13	1.90	0.52
1:B:158:GLY:O	1:B:162:MSE:HG3	2.09	0.52
1:B:158:GLY:O	1:B:162:MSE:CG	2.58	0.52
1:C:655:GLU:HA	1:D:640:MSE:HE1	1.91	0.52
1:D:13:MSE:CE	1:D:26:ILE:CD1	2.82	0.52
1:D:85:VAL:HG13	1:D:85:VAL:O	2.09	0.52
1:D:384:SER:HA	1:D:415:SER:HB3	1.92	0.52
1:B:36:VAL:CG1	1:B:37:LYS:N	2.73	0.52
1:C:98:VAL:CG2	1:C:102:ASP:OD2	2.58	0.52
1:C:441:LEU:HD22	1:C:466:LEU:HD22	1.92	0.52
1:A:9:PRO:C	1:A:12:LEU:HG	2.33	0.52
1:C:115:ARG:NH1	1:C:145:TRP:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:GLN:OE1	1:C:645:GLN:HA	2.10	0.52
1:D:100:PRO:CG	1:D:101:GLU:N	2.73	0.52
1:D:150:LEU:N	1:D:150:LEU:HD23	2.24	0.52
1:D:208:ILE:CG2	1:D:237:GLN:HE21	2.23	0.52
1:D:397:LEU:HD11	1:D:399:LEU:CD1	2.40	0.52
1:A:323:ASN:OD1	1:A:354:LEU:CA	2.58	0.51
1:B:36:VAL:HG13	1:B:37:LYS:H	1.75	0.51
1:D:543:ILE:HG22	1:D:574:ASN:HD22	1.71	0.51
1:C:169:TRP:CE3	1:C:170:LEU:HD21	2.45	0.51
1:D:30:LYS:CE	1:D:102:ASP:OD1	2.57	0.51
1:D:54:PHE:CD1	1:D:67:THR:HG21	2.45	0.51
1:B:16:ILE:HD11	1:B:45:VAL:HG21	1.92	0.51
1:B:34:LEU:HD12	1:B:35:GLU:O	2.10	0.51
1:B:212:ALA:HB2	1:B:237:GLN:HG2	1.93	0.51
1:C:8:VAL:HG11	1:C:13:MSE:CE	2.39	0.51
1:C:503:SER:HA	1:C:506:ILE:CG1	2.40	0.51
1:C:513:ARG:HH21	1:C:547:ASP:HB3	1.76	0.51
1:C:662:GLU:OE1	1:D:638:ILE:HD11	2.09	0.51
1:D:603:THR:O	1:D:603:THR:OG1	2.26	0.51
1:A:14:GLU:O	1:A:15:SER:C	2.54	0.51
1:A:54:PHE:CD2	1:A:67:THR:CG2	2.93	0.51
1:D:616:THR:CG2	1:D:617:ALA:H	2.22	0.51
1:A:13:MSE:HE2	1:A:29:LYS:HD3	1.93	0.51
1:A:270:LEU:HD21	1:A:278:LEU:HD12	1.93	0.51
1:A:602:ASN:CG	1:A:605:LEU:HD23	2.35	0.51
1:B:74:HIS:HD1	1:B:89:GLU:HB2	1.70	0.51
1:D:115:ARG:CG	1:D:115:ARG:NH1	2.73	0.51
1:D:355:SER:O	1:D:359:ASN:HB2	2.11	0.51
1:A:138:LEU:HD23	1:A:139:ALA:HA	1.92	0.51
1:A:352:ASP:O	1:A:354:LEU:HG	2.10	0.51
1:C:293:VAL:HG21	1:C:317:LEU:HD11	1.91	0.51
1:C:476:GLN:CA	1:C:476:GLN:NE2	2.73	0.51
1:D:80:LYS:HD2	1:D:81:PRO:N	2.26	0.51
1:D:375:THR:CG2	1:D:377:CYS:HB3	2.41	0.51
1:A:470:LEU:HD23	1:A:477:VAL:HG11	1.93	0.51
1:A:478:LEU:HD13	1:A:508:TRP:CG	2.46	0.51
1:A:484:GLU:HG3	1:A:508:TRP:CZ2	2.45	0.51
1:A:638:ILE:HG23	1:A:640:MSE:HE3	1.89	0.51
1:C:512:ASN:OD1	1:C:514:SER:N	2.43	0.51
1:D:40:ARG:CG	1:D:40:ARG:NH2	2.72	0.51
1:D:44:LYS:NZ	1:D:65:GLU:CD	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HG21	1:B:95:MSE:HG2	1.91	0.51
1:B:484:GLU:OE1	1:B:512:ASN:HB2	2.10	0.51
1:C:144:LEU:O	1:C:147:SER:OG	2.28	0.51
1:C:203:GLU:O	1:C:206:ASP:HB2	2.11	0.51
1:C:310:LEU:HD11	1:C:312:LEU:HD11	1.93	0.51
1:D:115:ARG:CB	1:D:115:ARG:CZ	2.89	0.51
1:D:507:VAL:CG2	1:D:508:TRP:N	2.73	0.51
1:D:667:ARG:HG3	1:D:668:ASN:N	2.24	0.51
1:C:391:LEU:HD22	1:C:422:SER:HB2	1.92	0.51
1:D:64:LEU:HD21	1:D:66:LEU:O	2.10	0.51
1:C:636:MSE:HB3	1:C:665:LEU:CD1	2.41	0.51
1:D:99:SER:HB3	1:D:100:PRO:CD	2.40	0.51
1:D:197:GLN:OE1	1:D:226:LYS:N	2.42	0.51
1:A:23:LYS:N	1:A:23:LYS:CD	2.73	0.50
1:B:375:THR:HG23	1:B:377:CYS:N	2.27	0.50
1:B:478:LEU:HB2	1:B:508:TRP:CD2	2.46	0.50
1:B:652:GLU:HG2	1:B:653:LYS:H	1.74	0.50
1:D:437:SER:C	1:D:440:PRO:HD2	2.36	0.50
1:D:506:ILE:CD1	1:D:539:LEU:HD13	2.41	0.50
1:B:366:THR:OG1	1:B:366:THR:O	2.26	0.50
1:C:68:PHE:HE1	1:C:73:ILE:HD11	1.75	0.50
1:B:93:MSE:HG3	1:B:95:MSE:HE2	1.93	0.50
1:B:222:LYS:HG3	1:B:250:GLU:HB2	1.93	0.50
1:A:478:LEU:O	1:A:480:GLY:N	2.41	0.50
1:C:258:LEU:HD23	1:C:262:PHE:CD2	2.45	0.50
1:D:323:ASN:CG	1:D:356:HIS:HB2	2.36	0.50
1:A:143:ALA:O	1:A:146:ASP:N	2.45	0.50
1:B:78:CYS:CB	1:B:132:MSE:HA	2.28	0.50
1:C:478:LEU:HD23	1:C:508:TRP:CH2	2.42	0.50
1:D:68:PHE:CD1	1:D:68:PHE:N	2.80	0.50
1:D:355:SER:HA	1:D:358:TYR:CD2	2.46	0.50
1:D:355:SER:HA	1:D:358:TYR:HD2	1.76	0.50
1:B:561:LYS:HA	1:B:585:ASN:O	2.11	0.50
1:C:115:ARG:HB3	1:C:115:ARG:NH2	2.17	0.50
1:D:350:ARG:HD3	1:D:350:ARG:N	2.07	0.50
1:D:477:VAL:C	1:D:478:LEU:CG	2.85	0.50
1:A:192:ARG:NH1	1:A:219:TRP:CZ3	2.80	0.50
1:B:506:ILE:HG23	1:B:542:MSE:CE	2.42	0.50
1:C:498:LEU:CD1	1:C:505:LEU:HD12	2.41	0.50
1:D:208:ILE:N	1:D:209:PRO:HD2	2.26	0.50
1:A:23:LYS:N	1:A:24:ILE:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:HB3	1:A:68:PHE:CE1	2.47	0.50
1:A:92:ASN:OD1	1:A:92:ASN:N	2.44	0.50
1:C:650:ASN:C	1:C:652:GLU:CB	2.85	0.50
1:C:667:ARG:HG3	1:C:668:ASN:N	2.25	0.50
1:D:115:ARG:NH1	1:D:115:ARG:HB2	2.27	0.50
1:D:174:TYR:HD1	1:D:175:LYS:N	2.10	0.50
1:A:80:LYS:C	1:A:80:LYS:CD	2.85	0.50
1:A:638:ILE:HD13	1:A:640:MSE:HE3	1.91	0.50
1:B:7:ASP:O	1:B:31:LYS:CD	2.60	0.50
1:B:507:VAL:HG23	1:B:508:TRP:N	2.27	0.50
1:C:86:VAL:HB	1:C:93:MSE:HG3	1.94	0.50
1:C:117:ILE:CG2	1:C:118:PHE:CD2	2.95	0.50
1:C:461:LEU:C	1:C:464:CYS:HG	2.19	0.50
1:D:55:LEU:O	1:D:64:LEU:HD23	2.12	0.50
1:A:602:ASN:HD21	1:A:605:LEU:HD23	1.76	0.49
1:D:65:GLU:C	1:D:66:LEU:HG	2.37	0.49
1:D:313:SER:O	1:D:314:LYS:C	2.53	0.49
1:D:613:ASN:O	1:D:614:ASN:HB2	2.12	0.49
1:A:313:SER:O	1:A:314:LYS:C	2.54	0.49
1:B:569:ASN:OD1	1:B:594:MSE:HG3	2.12	0.49
1:C:173:SER:O	1:C:174:TYR:C	2.56	0.49
1:C:372:LEU:O	1:C:375:THR:CB	2.60	0.49
1:C:503:SER:O	1:C:506:ILE:CB	2.59	0.49
1:C:611:ASP:O	1:C:612:LYS:HB2	2.11	0.49
1:B:52:ARG:CG	1:B:53:ALA:N	2.75	0.49
1:B:484:GLU:CB	1:B:508:TRP:NE1	2.73	0.49
1:C:386:LEU:CD2	1:C:390:CYS:SG	3.00	0.49
1:A:73:ILE:HD13	1:A:127:MSE:HE1	1.94	0.49
1:A:212:ALA:HB2	1:A:237:GLN:HG2	1.94	0.49
1:A:479:GLU:C	1:A:481:CYS:CB	2.85	0.49
1:A:506:ILE:CD1	1:A:539:LEU:HD13	2.43	0.49
1:B:610:TRP:N	1:B:610:TRP:CD1	2.80	0.49
1:C:379:LEU:CD1	1:C:402:SER:CB	2.88	0.49
1:D:171:GLY:C	1:D:172:PHE:HD1	2.20	0.49
1:D:563:GLU:C	1:D:565:THR:N	2.64	0.49
1:A:602:ASN:ND2	1:A:605:LEU:CD2	2.76	0.49
1:B:667:ARG:HG3	1:B:668:ASN:N	2.27	0.49
1:C:387:LEU:O	1:C:387:LEU:HD12	2.13	0.49
1:C:536:LEU:CB	1:C:566:ILE:HD11	2.42	0.49
1:C:563:GLU:C	1:C:565:THR:H	2.21	0.49
1:D:54:PHE:HD1	1:D:64:LEU:HD11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:ASN:ND2	1:D:356:HIS:CB	2.75	0.49
1:A:197:GLN:OE1	1:A:226:LYS:N	2.39	0.49
1:A:506:ILE:HD13	1:A:539:LEU:HD13	1.95	0.49
1:B:69:SER:O	1:B:72:GLU:N	2.46	0.49
1:B:134:PRO:HD2	1:B:137:ARG:HD3	1.94	0.49
1:B:416:PHE:HE2	1:B:440:PRO:O	1.96	0.49
1:C:647:LEU:O	1:C:651:PRO:HB3	2.12	0.49
1:D:72:GLU:HG2	1:D:89:GLU:HG3	1.93	0.49
1:D:231:SER:OG	1:D:234:VAL:HG23	2.12	0.49
1:D:394:LEU:O	1:D:426:LEU:HD12	2.12	0.49
1:A:493:ILE:C	1:A:496:ASN:HD21	2.19	0.49
1:B:160:SER:O	1:B:163:TYR:HB3	2.11	0.49
1:C:69:SER:O	1:C:72:GLU:HB2	2.12	0.49
1:C:604:LYS:O	1:C:604:LYS:CG	2.60	0.49
1:D:412:VAL:O	1:D:412:VAL:HG23	2.12	0.49
1:D:636:MSE:HB3	1:D:665:LEU:HD11	1.92	0.49
1:A:12:LEU:O	1:A:16:ILE:HG13	2.11	0.49
1:A:500:SER:C	1:A:502:LEU:H	2.21	0.49
1:A:618:GLN:NE2	1:A:618:GLN:CA	2.76	0.49
1:C:379:LEU:HD13	1:C:402:SER:HB2	1.92	0.49
1:C:16:ILE:HG12	1:C:56:LEU:HD13	1.94	0.49
1:C:260:ILE:O	1:C:263:ALA:HB3	2.12	0.49
1:D:97:MSE:HG3	1:D:103:VAL:CG2	2.43	0.49
1:A:484:GLU:CG	1:A:508:TRP:CE2	2.89	0.49
1:A:640:MSE:CE	1:A:640:MSE:HA	2.40	0.49
1:B:290:ASP:N	1:B:290:ASP:OD1	2.43	0.49
1:C:431:LEU:O	1:C:434:THR:CG2	2.50	0.49
1:D:68:PHE:CZ	1:D:86:VAL:HG11	2.47	0.49
1:D:80:LYS:HG3	1:D:83:GLN:H	1.77	0.49
1:D:142:GLN:O	1:D:146:ASP:CG	2.56	0.49
1:D:145:TRP:N	1:D:148:GLN:OE1	2.46	0.49
1:D:297:SER:HB2	1:D:328:SER:HB2	1.95	0.49
1:D:303:LEU:HD23	1:D:304:PRO:HD2	1.95	0.49
1:A:136:GLU:CD	1:A:136:GLU:H	2.19	0.48
1:D:26:ILE:CD1	1:D:47:VAL:CG2	2.80	0.48
1:A:68:PHE:HD1	1:A:93:MSE:HE1	1.78	0.48
1:A:174:TYR:HD1	1:A:175:LYS:N	2.11	0.48
1:B:610:TRP:CD1	1:B:610:TRP:H	2.31	0.48
1:C:189:GLN:O	1:C:190:ASP:C	2.53	0.48
1:C:224:SER:HB2	1:C:252:VAL:HB	1.95	0.48
1:C:397:LEU:HD11	1:C:399:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:LEU:CD2	1:C:654:THR:HB	2.43	0.48
1:D:310:LEU:HD11	1:D:312:LEU:CD1	2.43	0.48
1:D:503:SER:O	1:D:504:THR:C	2.53	0.48
1:B:115:ARG:HH22	1:B:150:LEU:HD11	1.75	0.48
1:B:124:LEU:HD13	1:B:145:TRP:HZ3	1.78	0.48
1:B:506:ILE:HG23	1:B:542:MSE:HE3	1.94	0.48
1:D:354:LEU:O	1:D:357:MSE:HB3	2.13	0.48
1:D:507:VAL:CG2	1:D:508:TRP:H	2.23	0.48
1:A:14:GLU:O	1:A:16:ILE:N	2.46	0.48
1:B:474:GLY:HA2	1:B:477:VAL:HG13	1.95	0.48
1:C:610:TRP:CZ3	1:C:623:ILE:HG13	2.48	0.48
1:D:64:LEU:CD2	1:D:66:LEU:N	2.76	0.48
1:D:185:ILE:O	1:D:189:GLN:HG3	2.13	0.48
1:A:12:LEU:HD12	1:A:13:MSE:N	2.28	0.48
1:A:201:HIS:CE1	1:B:597:LYS:HE3	2.49	0.48
1:B:97:MSE:CG	1:B:103:VAL:HG12	2.43	0.48
1:D:330:SER:HB3	1:D:363:GLN:OE1	2.14	0.48
1:A:441:LEU:HD22	1:A:466:LEU:HD22	1.96	0.48
1:B:12:LEU:HD12	1:B:12:LEU:O	2.13	0.48
1:C:638:ILE:HG23	1:C:638:ILE:O	2.13	0.48
1:D:64:LEU:CD2	1:D:64:LEU:C	2.86	0.48
1:D:516:GLN:HB2	1:D:517:HIS:HD2	1.79	0.48
1:A:38:GLY:O	1:A:39:ASP:C	2.57	0.48
1:D:322:VAL:HG21	1:D:349:LEU:HD22	1.95	0.48
1:D:586:GLY:HA2	1:D:614:ASN:ND2	2.28	0.48
1:A:500:SER:C	1:A:502:LEU:N	2.71	0.48
1:D:51:CYS:C	1:D:70:TYR:CD2	2.92	0.48
1:D:73:ILE:CD1	1:D:127:MSE:HE2	2.43	0.48
1:D:310:LEU:HD11	1:D:312:LEU:HD11	1.96	0.48
1:D:478:LEU:CB	1:D:508:TRP:NE1	2.73	0.48
1:D:478:LEU:HA	1:D:508:TRP:CZ2	2.49	0.48
1:D:602:ASN:HD21	1:D:605:LEU:HD12	1.79	0.48
1:A:273:ASN:C	1:A:273:ASN:OD1	2.57	0.48
1:C:602:ASN:HD21	1:C:605:LEU:CD2	2.26	0.48
1:C:650:ASN:C	1:C:652:GLU:HB3	2.38	0.48
1:D:79:HIS:O	1:D:133:GLU:HB3	2.13	0.48
1:A:14:GLU:C	1:A:16:ILE:N	2.72	0.48
1:A:56:LEU:HD23	1:A:64:LEU:HA	1.96	0.48
1:B:528:LYS:O	1:B:531:ASN:HB2	2.14	0.48
1:C:254:GLU:O	1:C:255:ASN:C	2.54	0.48
1:A:558:SER:HB3	1:A:560:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ILE:HG12	1:B:26:ILE:O	2.14	0.47
1:B:118:PHE:CD1	1:B:216:TYR:HB2	2.49	0.47
1:B:368:VAL:O	1:B:368:VAL:HG12	2.13	0.47
1:C:81:PRO:O	1:C:100:PRO:HB3	2.13	0.47
1:C:375:THR:HG23	1:C:377:CYS:HB3	1.95	0.47
1:C:449:ALA:CA	1:C:485:ILE:HG23	2.43	0.47
1:D:111:GLY:O	1:D:115:ARG:CG	2.61	0.47
1:D:323:ASN:HD21	1:D:356:HIS:HB2	1.74	0.47
1:D:369:HIS:CD2	1:D:396:VAL:HG21	2.49	0.47
1:C:212:ALA:HB2	1:C:237:GLN:HE21	1.79	0.47
1:C:513:ARG:NH2	1:C:547:ASP:HB3	2.28	0.47
1:C:610:TRP:CZ3	1:C:615:ILE:CD1	2.97	0.47
1:A:141:LEU:CD2	1:A:144:LEU:HD23	2.44	0.47
1:A:666:LEU:HD22	1:B:666:LEU:HD13	1.94	0.47
1:B:474:GLY:O	1:B:475:ALA:CB	2.62	0.47
1:B:528:LYS:HE3	1:B:529:SER:H	1.80	0.47
1:B:580:VAL:CG1	1:B:608:VAL:HG22	2.44	0.47
1:C:35:GLU:C	1:C:36:VAL:HG23	2.40	0.47
1:C:68:PHE:HE2	1:C:93:MSE:CE	2.21	0.47
1:D:532:LEU:O	1:D:532:LEU:HD23	2.14	0.47
1:A:282:ASN:C	1:A:282:ASN:OD1	2.57	0.47
1:C:117:ILE:C	1:C:118:PHE:CD2	2.92	0.47
1:D:100:PRO:CG	1:D:101:GLU:H	2.26	0.47
1:D:460:ASP:OD1	1:D:460:ASP:C	2.57	0.47
1:D:506:ILE:HG21	1:D:538:ASN:CB	2.44	0.47
1:A:506:ILE:CG2	1:A:542:MSE:HE3	2.43	0.47
1:C:602:ASN:CG	1:C:605:LEU:HD23	2.39	0.47
1:D:616:THR:HG22	1:D:617:ALA:H	1.77	0.47
1:A:103:VAL:CG2	1:A:104:SER:N	2.78	0.47
1:B:36:VAL:HG13	1:B:37:LYS:N	2.30	0.47
1:B:262:PHE:O	1:B:263:ALA:C	2.57	0.47
1:C:297:SER:HB2	1:C:328:SER:HB2	1.95	0.47
1:C:353:ASP:OD1	1:C:355:SER:CB	2.62	0.47
1:C:441:LEU:HD11	1:C:445:LEU:CD1	2.44	0.47
1:D:152:GLU:HG2	1:D:153:PRO:HD3	1.97	0.47
1:B:32:VAL:CG2	1:B:95:MSE:CB	2.92	0.47
1:B:120:GLY:O	1:B:121:LEU:HD23	2.14	0.47
1:C:61:PRO:HG2	1:C:61:PRO:O	2.14	0.47
1:C:157:GLY:O	1:C:162:MSE:HE3	2.14	0.47
1:C:484:GLU:N	1:C:508:TRP:NE1	2.63	0.47
1:D:298:ILE:HG22	1:D:299:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:SER:O	1:D:387:LEU:HB3	2.15	0.47
1:D:414:PRO:O	1:D:418:GLN:HB2	2.14	0.47
1:A:80:LYS:CD	1:A:81:PRO:N	2.78	0.47
1:A:195:ASN:OD1	1:A:197:GLN:HG2	2.14	0.47
1:A:476:GLN:CD	1:A:476:GLN:N	2.72	0.47
1:A:498:LEU:CD1	1:A:502:LEU:CD1	2.84	0.47
1:B:613:ASN:O	1:B:614:ASN:HB2	2.13	0.47
1:C:563:GLU:C	1:C:565:THR:N	2.72	0.47
1:C:634:ARG:O	1:D:666:LEU:HD11	2.14	0.47
1:A:93:MSE:HG3	1:A:95:MSE:HE3	1.97	0.47
1:A:384:SER:HA	1:A:415:SER:HB3	1.97	0.47
1:B:401:ARG:N	1:B:434:THR:HG22	2.30	0.47
1:B:513:ARG:HA	1:B:513:ARG:NH1	2.30	0.47
1:D:442:LYS:HE2	1:D:446:LEU:CD1	2.45	0.47
1:A:144:LEU:HD12	1:A:144:LEU:O	2.15	0.47
1:B:10:ARG:O	1:B:13:MSE:HB2	2.15	0.47
1:D:115:ARG:NH1	1:D:115:ARG:CB	2.78	0.47
1:A:69:SER:HB3	1:A:169:TRP:CD1	2.49	0.46
1:A:643:ALA:O	1:A:646:ALA:N	2.48	0.46
1:B:57:SER:HB3	1:B:65:GLU:OE2	2.15	0.46
1:B:71:LEU:HD11	1:B:118:PHE:HZ	1.80	0.46
1:B:660:LYS:O	1:B:664:TYR:CD2	2.67	0.46
1:C:128:LYS:CD	1:C:128:LYS:N	2.78	0.46
1:C:128:LYS:N	1:C:128:LYS:HD2	2.30	0.46
1:C:261:ASP:OD1	1:C:262:PHE:N	2.48	0.46
1:A:103:VAL:HG23	1:A:104:SER:N	2.28	0.46
1:B:282:ASN:C	1:B:282:ASN:OD1	2.59	0.46
1:B:330:SER:HB3	1:B:363:GLN:OE1	2.14	0.46
1:B:568:ILE:HD11	1:B:587:MSE:SE	2.65	0.46
1:D:78:CYS:HB2	1:D:132:MSE:HG2	1.97	0.46
1:D:311:ASN:C	1:D:311:ASN:OD1	2.57	0.46
1:D:401:ARG:N	1:D:434:THR:HG22	2.31	0.46
1:B:118:PHE:HD1	1:B:216:TYR:CB	2.27	0.46
1:B:226:LYS:O	1:B:227:ASP:HB2	2.14	0.46
1:D:545:ASP:OD1	1:D:546:GLU:N	2.48	0.46
1:A:122:SER:HA	1:A:123:PRO:HD3	1.82	0.46
1:A:374:ASN:CG	1:A:401:ARG:HH21	2.22	0.46
1:A:427:ILE:O	1:A:427:ILE:HG12	2.14	0.46
1:A:476:GLN:NE2	1:A:476:GLN:C	2.73	0.46
1:B:354:LEU:HB3	1:B:358:TYR:CD2	2.45	0.46
1:D:100:PRO:CD	1:D:101:GLU:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LEU:CD2	1:D:262:PHE:HE2	1.99	0.46
1:B:610:TRP:H	1:B:610:TRP:HD1	1.63	0.46
1:C:155:PRO:O	1:C:156:CYS:HB2	2.16	0.46
1:C:336:ALA:O	1:C:366:THR:HG22	2.15	0.46
1:D:26:ILE:HB	1:D:47:VAL:CG2	2.46	0.46
1:D:30:LYS:HA	1:D:30:LYS:HD2	1.69	0.46
1:D:100:PRO:HG2	1:D:101:GLU:N	2.30	0.46
1:D:111:GLY:HA2	1:D:114:LEU:HB2	1.97	0.46
1:D:144:LEU:HA	1:D:147:SER:OG	2.15	0.46
1:D:254:GLU:HG3	1:D:284:ALA:O	2.15	0.46
1:D:284:ALA:CB	1:D:313:SER:HB3	2.44	0.46
1:D:311:ASN:C	1:D:312:LEU:HD12	2.41	0.46
1:D:325:LEU:CD1	1:D:329:LEU:CD1	2.93	0.46
1:D:441:LEU:HD11	1:D:445:LEU:HD11	1.97	0.46
1:B:88:THR:CG2	1:B:91:CYS:CA	2.93	0.46
1:B:117:ILE:HB	1:B:118:PHE:CD2	2.51	0.46
1:C:15:SER:O	1:C:18:ASP:HB2	2.16	0.46
1:C:112:THR:HG23	1:C:148:GLN:OE1	2.15	0.46
1:C:534:PRO:O	1:C:537:ASP:HB2	2.16	0.46
1:D:380:GLU:CD	1:D:405:SER:OG	2.58	0.46
1:D:599:LEU:HD22	1:D:633:LEU:HD22	1.97	0.46
1:A:138:LEU:O	1:A:141:LEU:HB2	2.16	0.46
1:B:98:VAL:HG22	1:B:102:ASP:OD2	2.14	0.46
1:B:207:LEU:HA	1:B:210:ILE:HD12	1.98	0.46
1:C:662:GLU:OE1	1:D:638:ILE:CD1	2.64	0.46
1:D:12:LEU:HD12	1:D:12:LEU:O	2.16	0.46
1:D:22:ARG:HA	1:D:22:ARG:HD3	1.49	0.46
1:D:27:SER:CB	1:D:109:HIS:CE1	2.98	0.46
1:D:493:ILE:HD11	1:D:520:LEU:CD2	2.44	0.46
1:D:575:THR:O	1:D:604:LYS:HG2	2.16	0.46
1:A:441:LEU:HD11	1:A:445:LEU:HD11	1.97	0.46
1:A:561:LYS:O	1:A:564:VAL:HG12	2.15	0.46
2:B:701:OHB:C	3:B:702:CL:CL	3.00	0.46
1:D:30:LYS:HE3	1:D:102:ASP:CG	2.41	0.46
1:D:516:GLN:CB	1:D:517:HIS:CD2	2.99	0.46
1:D:517:HIS:CD2	1:D:517:HIS:N	2.83	0.46
1:B:375:THR:HG23	1:B:377:CYS:HB3	1.98	0.46
1:C:477:VAL:CG2	1:C:478:LEU:HD23	2.46	0.46
1:D:312:LEU:O	1:D:315:THR:HG23	2.15	0.46
1:D:377:CYS:O	1:D:403:VAL:CG2	2.62	0.46
1:D:379:LEU:HB2	1:D:404:PHE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:ARG:HH21	1:D:513:ARG:CG	2.07	0.46
1:A:74:HIS:CE1	1:A:89:GLU:HG2	2.51	0.46
1:A:315:THR:OG1	1:A:317:LEU:HD13	2.15	0.46
1:A:329:LEU:HD23	1:A:335:THR:HG21	1.97	0.46
1:A:410:LYS:C	1:A:411:GLU:O	2.55	0.46
1:B:52:ARG:HG2	1:B:53:ALA:N	2.30	0.46
1:B:80:LYS:HE3	1:B:81:PRO:CD	2.34	0.46
1:B:117:ILE:HG22	1:B:118:PHE:N	2.31	0.46
1:B:208:ILE:HG23	1:B:237:GLN:HE21	1.81	0.46
1:B:260:ILE:HD11	1:B:291:ARG:HB3	1.98	0.46
1:B:513:ARG:HH11	1:B:513:ARG:HG2	1.80	0.46
1:C:226:LYS:O	1:C:227:ASP:HB2	2.16	0.46
1:C:448:LEU:C	1:C:487:ASN:HD22	2.11	0.46
1:D:77:ILE:HB	1:D:85:VAL:CG1	2.44	0.46
1:D:369:HIS:CD2	1:D:396:VAL:CG2	2.98	0.46
1:A:256:ALA:CB	1:A:258:LEU:CD1	2.93	0.45
1:A:476:GLN:CD	1:A:476:GLN:H	2.24	0.45
1:C:222:LYS:HG3	1:C:250:GLU:HB2	1.98	0.45
1:D:66:LEU:CD1	1:D:93:MSE:HE2	2.45	0.45
1:D:604:LYS:O	1:D:604:LYS:CG	2.58	0.45
1:D:605:LEU:O	1:D:633:LEU:HD12	2.16	0.45
1:A:485:ILE:HG23	1:A:485:ILE:O	2.16	0.45
1:A:528:LYS:HB2	1:A:531:ASN:ND2	2.31	0.45
1:B:372:LEU:O	1:B:375:THR:HB	2.16	0.45
1:D:68:PHE:N	1:D:68:PHE:HD1	2.13	0.45
1:D:205:ARG:O	1:D:208:ILE:HG13	2.16	0.45
1:D:254:GLU:O	1:D:255:ASN:C	2.58	0.45
1:A:68:PHE:HE2	1:A:73:ILE:HD11	1.82	0.45
1:C:193:GLU:HG3	1:C:222:LYS:CG	2.46	0.45
1:C:403:VAL:HG23	1:C:403:VAL:O	2.17	0.45
1:C:454:LEU:HD13	1:C:457:VAL:HG21	1.99	0.45
1:D:40:ARG:NH2	1:D:40:ARG:HG2	2.31	0.45
1:A:383:CYS:HG	1:A:416:PHE:HD1	1.58	0.45
1:A:543:ILE:CG2	1:A:574:ASN:HD22	2.28	0.45
1:A:618:GLN:HE21	1:A:618:GLN:CA	2.29	0.45
1:A:620:PHE:CE1	1:A:639:PRO:HG3	2.52	0.45
1:B:193:GLU:CD	1:B:222:LYS:HD3	2.41	0.45
1:B:507:VAL:CG2	1:B:508:TRP:N	2.79	0.45
1:C:10:ARG:C	1:C:12:LEU:N	2.73	0.45
1:C:610:TRP:CZ2	1:C:636:MSE:HE2	2.46	0.45
1:D:172:PHE:CD2	1:D:209:PRO:CD	2.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:THR:HB	1:D:635:PHE:HB2	1.98	0.45
1:A:32:VAL:CG2	1:A:95:MSE:HB3	2.45	0.45
1:A:138:LEU:C	1:A:138:LEU:CD2	2.85	0.45
1:A:157:GLY:O	1:A:162:MSE:HE3	2.17	0.45
1:A:484:GLU:CG	1:A:508:TRP:CZ2	2.99	0.45
1:B:43:ASN:C	1:B:44:LYS:HG2	2.42	0.45
1:B:616:THR:O	1:B:617:ALA:C	2.59	0.45
1:C:144:LEU:HA	1:C:147:SER:OG	2.17	0.45
1:C:201:HIS:HB2	1:D:590:MSE:HE1	1.99	0.45
1:C:258:LEU:HD12	1:C:258:LEU:N	2.32	0.45
1:A:137:ARG:HE	1:A:137:ARG:HB3	1.63	0.45
1:B:181:ASP:OD2	1:B:185:ILE:HD12	2.16	0.45
1:B:329:LEU:HD23	1:B:335:THR:HG21	1.99	0.45
1:B:527:MSE:CE	1:B:531:ASN:HB3	2.46	0.45
1:B:639:PRO:O	1:B:639:PRO:HG2	2.16	0.45
1:B:652:GLU:CG	1:B:653:LYS:N	2.79	0.45
1:C:26:ILE:CG2	1:C:47:VAL:HG13	2.46	0.45
1:C:313:SER:O	1:C:314:LYS:C	2.60	0.45
1:A:143:ALA:CA	1:A:146:ASP:HB2	2.45	0.45
1:A:204:HIS:CD2	1:A:231:SER:HB3	2.52	0.45
1:A:609:ILE:HG13	1:A:637:PRO:HG2	1.99	0.45
1:B:136:GLU:N	1:B:136:GLU:CD	2.73	0.45
1:B:315:THR:O	1:B:316:SER:HB2	2.17	0.45
1:B:587:MSE:HG2	1:B:613:ASN:CG	2.42	0.45
1:C:375:THR:HG23	1:C:377:CYS:H	1.82	0.45
1:D:20:ILE:HG13	1:D:21:GLY:N	2.31	0.45
1:D:54:PHE:HA	1:D:67:THR:HG23	1.99	0.45
1:D:71:LEU:HD12	1:D:71:LEU:H	1.81	0.45
1:D:410:LYS:H	1:D:410:LYS:HG2	1.56	0.45
1:A:466:LEU:HA	1:A:469:CYS:HB3	1.99	0.45
1:A:528:LYS:HD3	1:A:528:LYS:HA	1.61	0.45
1:C:13:MSE:O	1:C:17:LYS:HG2	2.17	0.45
1:C:26:ILE:HG23	1:C:47:VAL:HG13	1.97	0.45
1:C:117:ILE:HB	1:C:118:PHE:CE2	2.51	0.45
1:C:319:PRO:HB3	1:C:354:LEU:HD13	1.98	0.45
1:D:34:LEU:CD2	1:D:36:VAL:HG23	2.47	0.45
1:D:52:ARG:HG3	1:D:68:PHE:O	2.17	0.45
1:D:397:LEU:HD11	1:D:399:LEU:CG	2.47	0.45
1:A:263:ALA:HB3	1:A:292:GLY:HA3	1.99	0.45
1:B:603:THR:O	1:B:603:THR:OG1	2.34	0.45
1:C:54:PHE:CE1	1:C:67:THR:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:LEU:CB	1:D:566:ILE:HD11	2.47	0.45
1:A:545:ASP:OD1	1:A:546:GLU:N	2.50	0.45
1:B:77:ILE:CG2	1:B:79:HIS:CE1	3.00	0.45
1:B:408:LYS:HE2	1:B:408:LYS:HB3	1.61	0.45
1:C:288:LEU:H	1:C:288:LEU:HG	1.55	0.45
1:C:303:LEU:HD23	1:C:304:PRO:HD2	1.99	0.45
1:A:525:ASN:N	1:A:525:ASN:HD22	2.15	0.44
1:B:375:THR:CG2	1:B:377:CYS:HB3	2.46	0.44
1:D:111:GLY:O	1:D:115:ARG:HG3	2.17	0.44
1:B:115:ARG:NH1	1:B:150:LEU:CD1	2.79	0.44
1:B:219:TRP:O	1:B:219:TRP:CG	2.70	0.44
1:B:323:ASN:ND2	1:B:356:HIS:CB	2.81	0.44
1:B:603:THR:O	1:B:632:THR:HG21	2.17	0.44
1:C:9:PRO:HG2	1:C:12:LEU:HB3	2.00	0.44
1:C:115:ARG:NH2	1:C:115:ARG:CG	2.73	0.44
1:C:136:GLU:CD	1:C:136:GLU:N	2.76	0.44
1:C:137:ARG:HA	1:C:140:SER:OG	2.17	0.44
1:C:286:ASN:O	1:C:315:THR:HA	2.17	0.44
1:C:587:MSE:HG2	1:C:613:ASN:ND2	2.31	0.44
1:D:360:PHE:CD1	1:D:360:PHE:O	2.70	0.44
1:A:13:MSE:CE	1:A:26:ILE:HD11	2.44	0.44
1:B:48:LEU:HB3	1:B:70:TYR:OH	2.18	0.44
1:B:111:GLY:HA3	1:B:145:TRP:CZ2	2.51	0.44
1:C:395:ALA:O	1:C:427:ILE:CG2	2.63	0.44
1:D:151:ALA:O	1:D:152:GLU:C	2.60	0.44
1:D:463:ASN:CG	1:D:463:ASN:O	2.60	0.44
1:A:12:LEU:C	1:A:12:LEU:CD1	2.86	0.44
1:A:30:LYS:HE2	1:A:105:GLU:OE2	2.18	0.44
1:A:163:TYR:CE1	1:A:167:CYS:SG	3.10	0.44
1:A:452:HIS:O	1:A:453:SER:C	2.60	0.44
1:A:482:ILE:CG2	1:A:483:ALA:N	2.80	0.44
1:B:513:ARG:NH1	1:B:513:ARG:HG2	2.33	0.44
1:C:378:SER:HB2	1:C:406:HIS:CD2	2.52	0.44
1:D:34:LEU:CD2	1:D:42:GLU:CB	2.85	0.44
1:D:408:LYS:O	1:D:408:LYS:HD3	2.18	0.44
1:A:46:LEU:HD23	1:A:55:LEU:CD2	2.47	0.44
1:A:80:LYS:HD3	1:A:81:PRO:CD	2.48	0.44
1:A:169:TRP:CE3	1:A:170:LEU:HD21	2.52	0.44
1:B:173:SER:O	1:B:174:TYR:C	2.61	0.44
1:C:328:SER:O	1:C:331:ALA:HB3	2.18	0.44
1:D:26:ILE:HB	1:D:47:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:CD	1:A:222:LYS:HD3	2.42	0.44
1:A:387:LEU:HD21	1:A:418:GLN:OE1	2.18	0.44
1:C:310:LEU:HD11	1:C:312:LEU:CD1	2.47	0.44
1:C:353:ASP:CG	1:C:355:SER:OG	2.56	0.44
1:C:375:THR:CG2	1:C:377:CYS:HB3	2.48	0.44
1:C:387:LEU:HA	1:C:391:LEU:HD21	1.99	0.44
1:D:212:ALA:HB2	1:D:237:GLN:HG2	2.00	0.44
1:D:380:GLU:OE2	1:D:405:SER:OG	2.35	0.44
1:A:456:GLY:HA2	1:A:489:THR:CG2	2.47	0.44
1:A:509:LEU:O	1:A:512:ASN:HB3	2.18	0.44
1:A:543:ILE:HG23	1:A:574:ASN:ND2	2.33	0.44
1:B:478:LEU:CB	1:B:508:TRP:CD2	3.01	0.44
1:C:337:SER:C	1:C:366:THR:HG21	2.42	0.44
1:C:416:PHE:CE1	1:C:420:PHE:HE2	2.35	0.44
1:D:605:LEU:O	1:D:633:LEU:CD1	2.66	0.44
1:A:77:ILE:HD12	1:A:85:VAL:HG11	1.99	0.44
1:A:311:ASN:OD1	1:A:311:ASN:C	2.61	0.44
1:A:374:ASN:ND2	1:A:401:ARG:NH2	2.50	0.44
1:B:64:LEU:HD11	1:B:67:THR:HG23	1.99	0.44
1:B:503:SER:C	1:B:505:LEU:N	2.71	0.44
1:C:383:CYS:HA	1:C:386:LEU:HB2	2.00	0.44
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.83	0.44
1:C:513:ARG:NH2	1:C:547:ASP:CB	2.81	0.44
1:C:610:TRP:HZ3	1:C:615:ILE:HD13	1.80	0.44
1:D:73:ILE:HD13	1:D:127:MSE:HE2	1.99	0.44
1:A:26:ILE:O	1:A:26:ILE:HG13	2.17	0.44
1:A:412:VAL:O	1:A:412:VAL:HG22	2.18	0.44
1:A:471:ARG:HG3	1:A:471:ARG:HH21	1.82	0.44
1:C:334:LEU:O	1:C:335:THR:C	2.61	0.44
1:C:533:THR:N	1:C:534:PRO:CD	2.81	0.44
1:D:80:LYS:HG3	1:D:83:GLN:N	2.33	0.44
1:D:424:LEU:N	1:D:424:LEU:HD12	2.32	0.44
1:B:354:LEU:HB3	1:B:358:TYR:CZ	2.44	0.43
1:C:193:GLU:CD	1:C:222:LYS:HD3	2.43	0.43
1:D:97:MSE:HE3	1:D:97:MSE:HB3	1.78	0.43
1:D:602:ASN:ND2	1:D:605:LEU:CD1	2.81	0.43
1:A:93:MSE:HG3	1:A:95:MSE:CE	2.47	0.43
1:A:192:ARG:NH1	1:A:219:TRP:CE3	2.86	0.43
1:A:410:LYS:O	1:A:411:GLU:C	2.55	0.43
1:A:479:GLU:O	1:A:481:CYS:HB2	2.18	0.43
1:B:602:ASN:ND2	1:B:605:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLU:C	1:C:36:VAL:CG2	2.90	0.43
1:C:474:GLY:CA	1:C:476:GLN:HG2	2.43	0.43
1:B:666:LEU:HD12	1:B:666:LEU:HA	1.63	0.43
1:C:124:LEU:HD21	1:C:145:TRP:CZ3	2.53	0.43
1:C:150:LEU:N	1:C:150:LEU:HD12	2.33	0.43
1:C:536:LEU:HB3	1:C:566:ILE:HD11	1.99	0.43
1:D:533:THR:HB	1:D:534:PRO:HD3	1.98	0.43
1:A:533:THR:HB	1:A:534:PRO:HD3	2.01	0.43
1:C:136:GLU:O	1:C:140:SER:OG	2.36	0.43
1:C:258:LEU:CD1	1:C:258:LEU:N	2.81	0.43
1:C:259:ARG:HA	1:C:259:ARG:HD3	1.80	0.43
1:C:485:ILE:CG2	1:C:487:ASN:HB2	2.45	0.43
1:C:543:ILE:CG2	1:C:574:ASN:HD21	2.15	0.43
1:D:40:ARG:HH21	1:D:40:ARG:HG3	1.82	0.43
1:D:69:SER:O	1:D:72:GLU:HB2	2.18	0.43
1:D:271:ALA:HB2	1:D:299:GLN:OE1	2.19	0.43
1:A:226:LYS:O	1:A:227:ASP:HB2	2.17	0.43
1:A:452:HIS:CD2	1:A:452:HIS:N	2.84	0.43
1:A:470:LEU:HD22	1:A:477:VAL:CG1	2.49	0.43
1:B:203:GLU:O	1:B:206:ASP:HB2	2.19	0.43
1:C:8:VAL:CG1	1:C:9:PRO:CD	2.86	0.43
1:C:141:LEU:O	1:C:142:GLN:C	2.61	0.43
1:D:77:ILE:HB	1:D:85:VAL:HG11	2.00	0.43
1:D:379:LEU:CD1	1:D:402:SER:OG	2.67	0.43
1:A:442:LYS:HE2	1:A:446:LEU:CD1	2.49	0.43
1:B:297:SER:HB2	1:B:328:SER:CB	2.49	0.43
1:B:547:ASP:O	1:B:548:SER:C	2.60	0.43
1:C:376:GLU:HG2	1:C:376:GLU:O	2.19	0.43
1:C:498:LEU:HD12	1:C:502:LEU:HD13	2.01	0.43
1:D:34:LEU:HD21	1:D:42:GLU:CD	2.44	0.43
1:D:40:ARG:HH21	1:D:40:ARG:HG2	1.83	0.43
1:A:483:ALA:O	1:A:484:GLU:CB	2.66	0.43
1:B:441:LEU:CD1	1:B:445:LEU:CD1	2.96	0.43
1:B:539:LEU:HA	1:B:539:LEU:HD12	1.81	0.43
1:C:109:HIS:CE1	1:C:113:CYS:SG	3.12	0.43
1:D:16:ILE:CG2	1:D:56:LEU:HD13	2.46	0.43
1:D:325:LEU:HD11	1:D:329:LEU:CD1	2.47	0.43
1:D:404:PHE:CZ	1:D:440:PRO:HB3	2.51	0.43
1:A:383:CYS:SG	1:A:416:PHE:HD1	2.41	0.43
1:A:505:LEU:HD13	1:A:505:LEU:HA	1.85	0.43
1:B:323:ASN:O	1:B:324:SER:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ASN:C	1:C:273:ASN:OD1	2.62	0.43
1:C:375:THR:HG23	1:C:377:CYS:N	2.32	0.43
1:C:638:ILE:HD11	1:C:658:LEU:HB3	2.01	0.43
1:D:93:MSE:O	1:D:93:MSE:HG3	2.19	0.43
1:D:403:VAL:O	1:D:403:VAL:HG23	2.19	0.43
1:B:355:SER:O	1:B:359:ASN:CB	2.65	0.43
1:B:376:GLU:O	1:B:376:GLU:HG2	2.19	0.43
1:C:294:SER:O	1:C:295:SER:C	2.62	0.43
1:C:560:LEU:H	1:C:560:LEU:HG	1.68	0.43
1:C:631:TYR:N	1:C:631:TYR:CD1	2.87	0.43
1:D:46:LEU:CD2	1:D:95:MSE:HE1	2.49	0.43
1:D:403:VAL:HG21	1:D:406:HIS:CE1	2.53	0.43
1:A:80:LYS:HD2	1:A:82:ALA:H	1.84	0.43
1:A:84:MSE:HE2	1:A:97:MSE:HE1	2.00	0.43
1:A:613:ASN:O	1:A:614:ASN:HB2	2.17	0.43
1:A:638:ILE:HG23	1:A:638:ILE:O	2.18	0.43
1:B:32:VAL:CG2	1:B:95:MSE:CG	2.95	0.43
1:B:372:LEU:O	1:B:375:THR:CB	2.66	0.43
1:C:76:VAL:HG11	1:C:107:LEU:HD11	2.01	0.43
1:C:256:ALA:CB	1:C:258:LEU:HD11	2.48	0.43
1:A:9:PRO:HB2	1:A:12:LEU:CG	2.47	0.42
1:A:347:ASN:ND2	1:A:347:ASN:N	2.67	0.42
1:A:396:VAL:O	1:A:396:VAL:HG23	2.18	0.42
1:B:349:LEU:HD13	1:B:357:MSE:SE	2.69	0.42
1:B:561:LYS:N	1:B:585:ASN:O	2.52	0.42
1:C:212:ALA:HB2	1:C:237:GLN:HG2	2.01	0.42
1:C:499:GLU:HB3	1:C:500:SER:H	1.67	0.42
1:C:650:ASN:C	1:C:652:GLU:HB2	2.44	0.42
1:D:185:ILE:HG22	1:D:189:GLN:HE21	1.84	0.42
1:D:399:LEU:O	1:D:400:SER:C	2.60	0.42
1:D:533:THR:O	1:D:534:PRO:C	2.59	0.42
1:D:602:ASN:C	1:D:602:ASN:OD1	2.62	0.42
1:A:203:GLU:O	1:A:206:ASP:HB2	2.19	0.42
1:A:647:LEU:HD23	1:A:647:LEU:HA	1.77	0.42
1:C:17:LYS:O	1:C:21:GLY:N	2.52	0.42
1:C:296:LEU:O	1:C:297:SER:C	2.62	0.42
1:C:296:LEU:O	1:C:299:GLN:N	2.50	0.42
1:C:297:SER:HB2	1:C:328:SER:CB	2.49	0.42
1:D:59:ARG:H	1:D:59:ARG:HD2	1.84	0.42
1:D:587:MSE:HG2	1:D:613:ASN:CG	2.44	0.42
1:D:651:PRO:CG	1:D:652:GLU:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:CD2	1:A:139:ALA:N	2.73	0.42
1:A:569:ASN:OD1	1:A:594:MSE:HG3	2.19	0.42
1:B:88:THR:HG22	1:B:91:CYS:O	2.19	0.42
1:B:117:ILE:CG2	1:B:118:PHE:CE2	3.02	0.42
1:B:193:GLU:CG	1:B:222:LYS:HD3	2.50	0.42
1:B:478:LEU:CB	1:B:508:TRP:CE3	3.01	0.42
1:C:189:GLN:HB2	1:C:191:THR:HG23	2.00	0.42
1:C:256:ALA:O	1:C:258:LEU:HD12	2.18	0.42
1:C:416:PHE:CE1	1:C:420:PHE:CE2	3.07	0.42
1:C:602:ASN:ND2	1:C:605:LEU:CD2	2.81	0.42
1:D:350:ARG:NE	1:D:350:ARG:O	2.52	0.42
1:D:602:ASN:HD21	1:D:605:LEU:CD1	2.31	0.42
1:A:46:LEU:HD23	1:A:54:PHE:O	2.20	0.42
1:A:124:LEU:HD21	1:A:145:TRP:HZ3	1.83	0.42
1:A:481:CYS:SG	1:A:481:CYS:O	2.78	0.42
1:A:652:GLU:CG	1:A:653:LYS:HG3	2.48	0.42
1:B:81:PRO:O	1:B:100:PRO:HB3	2.20	0.42
1:B:516:GLN:HB2	1:B:517:HIS:CD2	2.54	0.42
1:C:80:LYS:CE	1:C:82:ALA:H	2.33	0.42
1:C:540:VAL:O	1:C:544:GLN:HG2	2.18	0.42
1:D:271:ALA:HA	1:D:299:GLN:OE1	2.19	0.42
1:D:368:VAL:O	1:D:368:VAL:HG12	2.18	0.42
1:D:375:THR:HG23	1:D:377:CYS:N	2.35	0.42
1:D:431:LEU:O	1:D:432:SER:C	2.62	0.42
1:A:54:PHE:CD1	1:A:54:PHE:N	2.87	0.42
1:A:87:GLU:CD	1:A:129:LYS:HZ1	2.26	0.42
1:A:568:ILE:HD11	1:A:587:MSE:SE	2.70	0.42
1:B:224:SER:HB2	1:B:252:VAL:HB	2.00	0.42
1:B:536:LEU:CB	1:B:566:ILE:HD11	2.50	0.42
1:D:270:LEU:HD21	1:D:278:LEU:HD12	2.02	0.42
1:D:297:SER:HB2	1:D:328:SER:CB	2.49	0.42
1:D:580:VAL:CG1	1:D:605:LEU:CD2	2.96	0.42
1:D:640:MSE:O	1:D:641:TYR:C	2.60	0.42
1:A:73:ILE:HD13	1:A:127:MSE:HE3	1.87	0.42
1:A:263:ALA:CB	1:A:292:GLY:CA	2.97	0.42
1:A:544:GLN:O	1:A:545:ASP:C	2.61	0.42
1:C:561:LYS:H	1:C:561:LYS:HG3	1.54	0.42
1:D:64:LEU:HD22	1:D:66:LEU:N	2.35	0.42
1:D:266:LEU:O	1:D:267:ALA:C	2.63	0.42
1:A:474:GLY:CA	1:A:477:VAL:HG11	2.26	0.42
1:A:602:ASN:C	1:A:602:ASN:OD1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:THR:CG2	1:B:91:CYS:HB3	2.49	0.42
1:C:34:LEU:O	1:C:36:VAL:HG23	2.19	0.42
1:C:507:VAL:HA	1:C:510:SER:OG	2.20	0.42
1:A:403:VAL:O	1:A:404:PHE:C	2.62	0.42
1:A:604:LYS:O	1:A:604:LYS:CG	2.68	0.42
1:A:620:PHE:HE1	1:A:639:PRO:HG3	1.84	0.42
1:D:312:LEU:HD12	1:D:312:LEU:N	2.35	0.42
1:D:315:THR:OG1	1:D:317:LEU:HD11	2.17	0.42
1:D:493:ILE:O	1:D:496:ASN:ND2	2.53	0.42
1:D:543:ILE:HG22	1:D:574:ASN:HD21	1.77	0.42
1:A:136:GLU:CD	1:A:136:GLU:N	2.78	0.42
1:B:155:PRO:O	1:B:156:CYS:HB2	2.19	0.42
1:C:235:CYS:O	1:C:236:GLU:C	2.62	0.42
1:D:322:VAL:CG1	1:D:357:MSE:CE	2.76	0.42
1:D:354:LEU:HB2	1:D:358:TYR:CZ	2.55	0.42
1:D:606:ARG:HD3	1:D:606:ARG:HA	1.83	0.42
1:A:75:GLY:H	1:A:87:GLU:HG3	1.85	0.42
1:A:375:THR:HG23	1:A:377:CYS:HB3	2.02	0.42
1:A:402:SER:H	1:A:434:THR:HG23	1.84	0.42
1:A:568:ILE:CD1	1:A:587:MSE:SE	3.17	0.42
1:B:477:VAL:CG2	1:B:478:LEU:HG	2.49	0.42
1:C:103:VAL:O	1:C:104:SER:C	2.63	0.42
1:C:256:ALA:HB1	1:C:258:LEU:HD11	2.02	0.42
1:C:529:SER:O	1:C:533:THR:OG1	2.37	0.42
1:C:597:LYS:O	1:C:598:ALA:C	2.62	0.42
1:D:127:MSE:O	1:D:128:LYS:HB2	2.20	0.42
1:D:518:LEU:HD21	1:D:520:LEU:HD21	2.01	0.42
1:A:84:MSE:HB3	1:A:97:MSE:HE3	2.01	0.41
1:A:136:GLU:O	1:A:140:SER:OG	2.38	0.41
1:A:507:VAL:CG2	1:A:508:TRP:N	2.83	0.41
1:A:638:ILE:HG23	1:A:640:MSE:HE2	2.02	0.41
1:B:30:LYS:HE2	1:B:105:GLU:OE2	2.19	0.41
1:B:363:GLN:O	1:B:364:PRO:C	2.60	0.41
1:C:36:VAL:CG1	1:C:37:LYS:N	2.73	0.41
1:D:572:GLY:O	1:D:601:ILE:HG22	2.20	0.41
1:A:71:LEU:N	1:A:71:LEU:HD12	2.34	0.41
1:A:87:GLU:C	1:A:88:THR:CG2	2.93	0.41
1:B:39:ASP:O	1:B:41:VAL:HG13	2.20	0.41
1:B:117:ILE:HG21	1:B:118:PHE:CE2	2.54	0.41
1:B:323:ASN:CG	1:B:356:HIS:HB2	2.45	0.41
1:B:412:VAL:O	1:B:412:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:VAL:C	1:C:77:ILE:HG13	2.45	0.41
1:C:368:VAL:O	1:C:368:VAL:CG1	2.67	0.41
1:D:122:SER:O	1:D:125:ARG:HB2	2.20	0.41
1:D:235:CYS:O	1:D:236:GLU:C	2.63	0.41
1:D:560:LEU:HD23	1:D:560:LEU:HA	1.83	0.41
1:A:345:SER:HB3	1:A:371:ASP:OD1	2.19	0.41
1:A:499:GLU:HB3	1:A:500:SER:H	1.59	0.41
1:B:273:ASN:HA	1:B:274:PRO:HD2	1.92	0.41
1:B:545:ASP:OD1	1:B:546:GLU:N	2.53	0.41
1:B:568:ILE:CD1	1:B:587:MSE:SE	3.18	0.41
1:C:58:ALA:O	1:C:59:ARG:HG3	2.20	0.41
1:C:386:LEU:HD23	1:C:386:LEU:HA	1.71	0.41
1:C:532:LEU:HD22	1:C:536:LEU:CD1	2.50	0.41
1:D:99:SER:O	1:D:102:ASP:N	2.54	0.41
1:A:77:ILE:O	1:A:85:VAL:CG1	2.63	0.41
1:A:350:ARG:HG2	1:A:406:HIS:CE1	2.56	0.41
1:B:65:GLU:C	1:B:66:LEU:CD2	2.86	0.41
1:C:556:ALA:O	1:C:557:ASP:HB2	2.20	0.41
1:D:317:LEU:HB2	1:D:347:ASN:HB3	2.02	0.41
1:D:565:THR:O	1:D:565:THR:HG22	2.21	0.41
1:A:500:SER:O	1:A:502:LEU:N	2.53	0.41
1:B:26:ILE:HB	1:B:47:VAL:HG12	2.01	0.41
1:C:42:GLU:HB2	1:C:44:LYS:HE2	2.02	0.41
1:C:77:ILE:O	1:C:85:VAL:HG22	2.20	0.41
1:C:169:TRP:CE3	1:C:170:LEU:CD2	3.03	0.41
1:C:287:SER:O	1:C:287:SER:OG	2.26	0.41
1:D:9:PRO:HG2	1:D:10:ARG:H	1.86	0.41
1:D:27:SER:HB2	1:D:109:HIS:CE1	2.52	0.41
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.76	0.41
1:D:500:SER:C	1:D:502:LEU:H	2.28	0.41
1:D:560:LEU:O	1:D:561:LYS:HB2	2.20	0.41
1:D:630:ASN:OD1	1:D:630:ASN:C	2.63	0.41
1:C:509:LEU:HD21	1:C:518:LEU:CD1	2.51	0.41
1:C:593:LYS:HE2	1:D:200:SER:OG	2.21	0.41
1:D:75:GLY:HA2	1:D:129:LYS:O	2.21	0.41
1:D:298:ILE:HG22	1:D:299:GLN:NE2	2.36	0.41
1:D:400:SER:HB3	1:D:432:SER:OG	2.21	0.41
1:A:258:LEU:CD2	1:A:262:PHE:CD2	2.95	0.41
1:B:235:CYS:O	1:B:236:GLU:C	2.62	0.41
1:B:441:LEU:HD22	1:B:466:LEU:HD22	2.01	0.41
1:C:150:LEU:HD12	1:C:150:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:LEU:HD23	1:C:536:LEU:HG	2.02	0.41
1:D:37:LYS:H	1:D:37:LYS:HD3	1.85	0.41
1:D:51:CYS:O	1:D:70:TYR:CD2	2.74	0.41
1:D:172:PHE:HD2	1:D:209:PRO:HD3	1.79	0.41
1:D:557:ASP:HA	1:D:584:GLY:O	2.21	0.41
1:A:10:ARG:C	1:A:12:LEU:N	2.79	0.41
1:A:160:SER:HG	1:A:183:ASP:CG	2.17	0.41
1:A:602:ASN:OD1	1:A:605:LEU:HD23	2.20	0.41
1:B:19:VAL:HG13	1:B:20:ILE:HG23	2.03	0.41
1:B:256:ALA:CB	1:B:258:LEU:CD1	2.98	0.41
1:B:470:LEU:HA	1:B:470:LEU:HD12	1.80	0.41
1:C:10:ARG:O	1:C:12:LEU:N	2.54	0.41
1:C:470:LEU:CD1	1:C:505:LEU:HD11	2.47	0.41
1:D:68:PHE:CD2	1:D:88:THR:HG21	2.55	0.41
1:D:539:LEU:HA	1:D:539:LEU:HD12	1.81	0.41
1:A:10:ARG:O	1:A:13:MSE:N	2.38	0.41
1:A:64:LEU:C	1:A:64:LEU:CD2	2.94	0.41
1:A:217:ASN:OD1	1:A:219:TRP:N	2.46	0.41
1:A:379:LEU:HB2	1:A:404:PHE:HA	2.02	0.41
1:A:478:LEU:C	1:A:480:GLY:N	2.76	0.41
1:A:492:ASP:HA	1:A:519:ALA:HB3	2.03	0.41
1:A:597:LYS:O	1:A:598:ALA:C	2.62	0.41
1:B:43:ASN:OD1	1:B:43:ASN:N	2.54	0.41
1:B:60:ILE:HA	1:B:61:PRO:C	2.44	0.41
1:B:65:GLU:H	1:B:65:GLU:HG2	1.63	0.41
1:B:374:ASN:HD21	1:B:401:ARG:NH1	2.19	0.41
1:B:587:MSE:HG2	1:B:613:ASN:OD1	2.21	0.41
1:B:602:ASN:OD1	1:B:602:ASN:C	2.63	0.41
1:C:205:ARG:HB2	1:C:205:ARG:HH11	1.86	0.41
1:D:36:VAL:HG21	1:D:42:GLU:CD	2.45	0.41
1:D:141:LEU:HD12	1:D:141:LEU:HA	1.77	0.41
1:D:155:PRO:O	1:D:156:CYS:HB2	2.20	0.41
1:D:360:PHE:CD1	1:D:360:PHE:C	2.96	0.41
1:D:387:LEU:HD23	1:D:388:ARG:CZ	2.51	0.41
1:D:547:ASP:O	1:D:548:SER:C	2.63	0.41
1:A:193:GLU:CG	1:A:222:LYS:HD3	2.50	0.41
1:A:533:THR:N	1:A:534:PRO:CD	2.83	0.41
1:A:543:ILE:HD13	1:A:543:ILE:HG21	1.88	0.41
1:B:138:LEU:HD12	1:B:138:LEU:HA	1.80	0.41
1:B:169:TRP:CZ3	1:B:170:LEU:HD21	2.56	0.41
1:C:116:ARG:HH11	1:C:116:ARG:CG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:ASN:OD1	1:C:401:ARG:CD	2.69	0.41
1:C:524:PHE:CG	1:C:560:LEU:HD21	2.55	0.41
1:C:527:MSE:HE1	1:C:532:LEU:HG	2.01	0.41
1:C:580:VAL:CG1	1:C:605:LEU:HD11	2.51	0.41
1:D:512:ASN:ND2	1:D:514:SER:OG	2.54	0.41
1:A:32:VAL:CG2	1:A:33:LYS:N	2.84	0.40
1:B:374:ASN:HD21	1:B:401:ARG:HH11	1.69	0.40
1:C:122:SER:O	1:C:123:PRO:C	2.64	0.40
1:C:516:GLN:C	1:C:517:HIS:CG	2.99	0.40
1:D:34:LEU:HG	1:D:36:VAL:CG2	2.51	0.40
1:D:474:GLY:C	1:D:476:GLN:H	2.29	0.40
1:B:378:SER:HB2	1:B:406:HIS:CD2	2.56	0.40
1:B:441:LEU:HD11	1:B:445:LEU:CD1	2.51	0.40
1:C:97:MSE:HE3	1:C:97:MSE:HB3	2.01	0.40
1:C:441:LEU:CD1	1:C:445:LEU:CD1	3.00	0.40
1:C:615:ILE:HG23	1:C:619:GLY:HA3	2.03	0.40
1:D:270:LEU:HD21	1:D:278:LEU:CD1	2.51	0.40
1:A:263:ALA:HB1	1:A:292:GLY:CA	2.51	0.40
1:A:507:VAL:HG23	1:A:508:TRP:N	2.35	0.40
1:B:204:HIS:CD2	1:B:231:SER:HB3	2.57	0.40
1:B:533:THR:O	1:B:534:PRO:C	2.62	0.40
1:B:630:ASN:OD1	1:B:630:ASN:C	2.63	0.40
1:C:509:LEU:CD2	1:C:518:LEU:HD21	2.44	0.40
1:D:157:GLY:O	1:D:162:MSE:HE3	2.20	0.40
1:D:208:ILE:N	1:D:209:PRO:CD	2.84	0.40
1:D:359:ASN:O	1:D:363:GLN:HG3	2.21	0.40
1:D:457:VAL:HG12	1:D:458:SER:N	2.37	0.40
1:D:485:ILE:HD13	1:D:488:ILE:HD12	2.04	0.40
1:A:130:VAL:O	1:A:130:VAL:HG23	2.22	0.40
1:A:484:GLU:HA	1:A:485:ILE:HA	1.68	0.40
1:A:638:ILE:CD1	1:A:640:MSE:CE	2.88	0.40
1:B:74:HIS:HE1	1:B:89:GLU:HB2	1.71	0.40
1:B:258:LEU:CD2	1:B:262:PHE:CD2	2.99	0.40
1:B:303:LEU:HD23	1:B:304:PRO:HD2	2.03	0.40
1:B:467:GLY:O	1:B:471:ARG:HG3	2.22	0.40
1:B:509:LEU:O	1:B:512:ASN:HB3	2.21	0.40
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.80	0.40
1:C:204:HIS:CE1	1:C:234:VAL:HG21	2.57	0.40
1:D:159:PHE:O	1:D:160:SER:C	2.62	0.40
1:D:296:LEU:O	1:D:297:SER:C	2.63	0.40
1:D:397:LEU:HD11	1:D:399:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:GLN:O	1:D:545:ASP:C	2.62	0.40
1:D:627:MSE:HE1	1:D:633:LEU:HB3	2.02	0.40
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.86	0.40
1:A:246:ASN:ND2	1:A:246:ASN:C	2.80	0.40
1:A:543:ILE:HD11	1:A:553:LEU:HD22	2.03	0.40
1:B:78:CYS:HB2	1:B:132:MSE:CB	2.51	0.40
1:B:401:ARG:H	1:B:434:THR:HG22	1.87	0.40
1:B:578:THR:HG22	1:B:604:LYS:HD2	2.02	0.40
1:B:638:ILE:H	1:B:638:ILE:CD1	2.27	0.40
1:C:16:ILE:O	1:C:19:VAL:CG1	2.70	0.40
1:C:379:LEU:CD1	1:C:402:SER:HB3	2.47	0.40
1:C:477:VAL:HA	1:C:478:LEU:HA	1.73	0.40
1:D:334:LEU:O	1:D:335:THR:C	2.63	0.40
1:D:505:LEU:HA	1:D:505:LEU:HD13	1.81	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:GLN:O	1:C:649:THR:OG1[1_655]	1.32	0.88
1:C:289:GLU:OE1	1:D:513:ARG:CG[1_545]	1.55	0.65
1:C:289:GLU:OE2	1:D:513:ARG:NH2[1_545]	1.64	0.56
1:A:415:SER:OG	3:B:702:CL:CL[1_465]	1.74	0.46
1:B:35:GLU:OE2	1:D:476:GLN:NE2[1_545]	1.90	0.30

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	660/669 (99%)	628 (95%)	31 (5%)	1 (0%)	43 72
1	B	656/669 (98%)	635 (97%)	21 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	652/669 (98%)	631 (97%)	20 (3%)	1 (0%)	43	72
1	D	651/669 (97%)	628 (96%)	23 (4%)	0	100	100
All	All	2619/2676 (98%)	2522 (96%)	95 (4%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	C	11	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	585/573 (102%)	456 (78%)	129 (22%)	1	3
1	B	585/573 (102%)	454 (78%)	131 (22%)	1	3
1	C	581/573 (101%)	446 (77%)	135 (23%)	1	3
1	D	580/573 (101%)	434 (75%)	146 (25%)	0	2
All	All	2331/2292 (102%)	1790 (77%)	541 (23%)	1	3

All (541) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	17	LYS
1	A	24	ILE
1	A	25	LYS
1	A	29	LYS
1	A	30	LYS
1	A	32	VAL
1	A	37	LYS
1	A	41	VAL
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	50	SER
1	A	51	CYS
1	A	54	PHE
1	A	59	ARG
1	A	63	LYS
1	A	64	LEU
1	A	65	GLU
1	A	67	THR
1	A	72	GLU
1	A	76	VAL
1	A	77	ILE
1	A	80	LYS
1	A	90	LYS
1	A	92	ASN
1	A	93	MSE
1	A	96	LYS
1	A	97	MSE
1	A	103	VAL
1	A	105	GLU
1	A	107	LEU
1	A	115	ARG
1	A	117	ILE
1	A	121	LEU
1	A	125	ARG
1	A	127	MSE
1	A	129	LYS
1	A	131	SER
1	A	133	GLU
1	A	136	GLU
1	A	137	ARG
1	A	138	LEU
1	A	140	SER
1	A	144	LEU
1	A	147	SER
1	A	149	THR
1	A	152	GLU
1	A	168	ASP
1	A	173	SER
1	A	174	TYR
1	A	181	ASP
1	A	197	GLN

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Mol	Chain	Res	Type
1	A	202	LEU
1	A	224	SER
1	A	225	SER
1	A	226	LYS
1	A	229	LYS
1	A	232	THR
1	A	237	GLN
1	A	244	ARG
1	A	247	ARG
1	A	272	HIS
1	A	275	ASN
1	A	276	SER
1	A	290	ASP
1	A	296	LEU
1	A	299	GLN
1	A	302	LYS
1	A	303	LEU
1	A	318	SER
1	A	323	ASN
1	A	330	SER
1	A	347	ASN
1	A	350	ARG
1	A	352	ASP
1	A	379	LEU
1	A	381	MSE
1	A	393	CYS
1	A	400	SER
1	A	405	SER
1	A	412	VAL
1	A	418	GLN
1	A	426	LEU
1	A	427	ILE
1	A	434	THR
1	A	437	SER
1	A	444	LEU
1	A	458	SER
1	A	465	GLU
1	A	471	ARG
1	A	476	GLN
1	A	477	VAL
1	A	478	LEU
1	A	482	ILE

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Mol	Chain	Res	Type
1	A	484	GLU
1	A	485	ILE
1	A	490	SER
1	A	493	ILE
1	A	499	GLU
1	A	501	ASP
1	A	505	LEU
1	A	506	ILE
1	A	509	LEU
1	A	510	SER
1	A	522	LYS
1	A	526	ASN
1	A	527	MSE
1	A	528	LYS
1	A	530	LYS
1	A	532	LEU
1	A	541	GLN
1	A	550	LEU
1	A	565	THR
1	A	566	ILE
1	A	568	ILE
1	A	573	SER
1	A	580	VAL
1	A	594	MSE
1	A	603	THR
1	A	604	LYS
1	A	606	ARG
1	A	607	THR
1	A	609	ILE
1	A	634	ARG
1	A	640	MSE
1	A	650	ASN
1	A	656	GLU
1	A	660	LYS
1	A	667	ARG
1	B	7	ASP
1	B	11	GLU
1	B	22	ARG
1	B	23	LYS
1	B	24	ILE
1	B	26	ILE
1	B	29	LYS

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Mol	Chain	Res	Type
1	B	30	LYS
1	B	31	LYS
1	B	32	VAL
1	B	33	LYS
1	B	34	LEU
1	B	35	GLU
1	B	36	VAL
1	B	37	LYS
1	B	42	GLU
1	B	43	ASN
1	B	44	LYS
1	B	46	LEU
1	B	47	VAL
1	B	50	SER
1	B	63	LYS
1	B	65	GLU
1	B	66	LEU
1	B	67	THR
1	B	83	GLN
1	B	87	GLU
1	B	89	GLU
1	B	90	LYS
1	B	91	CYS
1	B	93	MSE
1	B	97	MSE
1	B	101	GLU
1	B	103	VAL
1	B	107	LEU
1	B	121	LEU
1	B	124	LEU
1	B	125	ARG
1	B	133	GLU
1	B	136	GLU
1	B	140	SER
1	B	144	LEU
1	B	160	SER
1	B	162	MSE
1	B	173	SER
1	B	174	TYR
1	B	177	GLU
1	B	183	ASP
1	B	184	THR

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Mol	Chain	Res	Type
1	B	187	LEU
1	B	197	GLN
1	B	202	LEU
1	B	224	SER
1	B	225	SER
1	B	226	LYS
1	B	229	LYS
1	B	232	THR
1	B	237	GLN
1	B	246	ASN
1	B	247	ARG
1	B	272	HIS
1	B	275	ASN
1	B	286	ASN
1	B	287	SER
1	B	288	LEU
1	B	290	ASP
1	B	291	ARG
1	B	295	SER
1	B	296	LEU
1	B	298	ILE
1	B	299	GLN
1	B	302	LYS
1	B	318	SER
1	B	323	ASN
1	B	330	SER
1	B	340	THR
1	B	350	ARG
1	B	354	LEU
1	B	355	SER
1	B	364	PRO
1	B	379	LEU
1	B	396	VAL
1	B	400	SER
1	B	403	VAL
1	B	407	ARG
1	B	408	LYS
1	B	412	VAL
1	B	415	SER
1	B	424	LEU
1	B	427	ILE
1	B	434	THR

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Mol	Chain	Res	Type
1	B	437	SER
1	B	445	LEU
1	B	455	LYS
1	B	458	SER
1	B	465	GLU
1	B	468	HIS
1	B	470	LEU
1	B	476	GLN
1	B	478	LEU
1	B	490	SER
1	B	499	GLU
1	B	503	SER
1	B	505	LEU
1	B	506	ILE
1	B	509	LEU
1	B	510	SER
1	B	513	ARG
1	B	522	LYS
1	B	528	LYS
1	B	541	GLN
1	B	550	LEU
1	B	558	SER
1	B	565	THR
1	B	566	ILE
1	B	575	THR
1	B	579	LYS
1	B	594	MSE
1	B	603	THR
1	B	604	LYS
1	B	605	LEU
1	B	607	THR
1	B	632	THR
1	B	634	ARG
1	B	635	PHE
1	B	637	PRO
1	B	638	ILE
1	B	656	GLU
1	B	660	LYS
1	B	666	LEU
1	B	667	ARG
1	C	8	VAL
1	C	12	LEU

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Mol	Chain	Res	Type
1	C	17	LYS
1	C	22	ARG
1	C	29	LYS
1	C	30	LYS
1	C	31	LYS
1	C	32	VAL
1	C	34	LEU
1	C	37	LYS
1	C	39	ASP
1	C	41	VAL
1	C	46	LEU
1	C	50	SER
1	C	51	CYS
1	C	52	ARG
1	C	55	LEU
1	C	56	LEU
1	C	61	PRO
1	C	64	LEU
1	C	67	THR
1	C	72	GLU
1	C	78	CYS
1	C	79	HIS
1	C	80	LYS
1	C	90	LYS
1	C	93	MSE
1	C	94	SER
1	C	97	MSE
1	C	115	ARG
1	C	126	ILE
1	C	129	LYS
1	C	131	SER
1	C	133	GLU
1	C	136	GLU
1	C	138	LEU
1	C	140	SER
1	C	144	LEU
1	C	147	SER
1	C	150	LEU
1	C	152	GLU
1	C	160	SER
1	C	168	ASP
1	C	173	SER

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Mol	Chain	Res	Type
1	C	174	TYR
1	C	181	ASP
1	C	184	THR
1	C	188	THR
1	C	194	LEU
1	C	197	GLN
1	C	202	LEU
1	C	205	ARG
1	C	224	SER
1	C	226	LYS
1	C	229	LYS
1	C	232	THR
1	C	237	GLN
1	C	247	ARG
1	C	272	HIS
1	C	275	ASN
1	C	276	SER
1	C	287	SER
1	C	288	LEU
1	C	294	SER
1	C	296	LEU
1	C	298	ILE
1	C	299	GLN
1	C	302	LYS
1	C	313	SER
1	C	318	SER
1	C	323	ASN
1	C	330	SER
1	C	352	ASP
1	C	354	LEU
1	C	379	LEU
1	C	381	MSE
1	C	384	SER
1	C	388	ARG
1	C	392	GLN
1	C	393	CYS
1	C	396	VAL
1	C	397	LEU
1	C	401	ARG
1	C	407	ARG
1	C	408	LYS
1	C	410	LYS

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Mol	Chain	Res	Type
1	C	411	GLU
1	C	412	VAL
1	C	418	GLN
1	C	421	SER
1	C	422	SER
1	C	426	LEU
1	C	434	THR
1	C	437	SER
1	C	451	ASN
1	C	455	LYS
1	C	458	SER
1	C	465	GLU
1	C	476	GLN
1	C	484	GLU
1	C	485	ILE
1	C	486	HIS
1	C	490	SER
1	C	499	GLU
1	C	500	SER
1	C	501	ASP
1	C	503	SER
1	C	505	LEU
1	C	511	LYS
1	C	513	ARG
1	C	525	ASN
1	C	527	MSE
1	C	531	ASN
1	C	533	THR
1	C	541	GLN
1	C	550	LEU
1	C	559	LYS
1	C	560	LEU
1	C	561	LYS
1	C	565	THR
1	C	566	ILE
1	C	568	ILE
1	C	580	VAL
1	C	594	MSE
1	C	603	THR
1	C	604	LYS
1	C	607	THR
1	C	632	THR

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Mol	Chain	Res	Type
1	C	637	PRO
1	C	639	PRO
1	C	647	LEU
1	C	649	THR
1	C	656	GLU
1	C	660	LYS
1	C	667	ARG
1	D	12	LEU
1	D	13	MSE
1	D	17	LYS
1	D	22	ARG
1	D	24	ILE
1	D	26	ILE
1	D	29	LYS
1	D	30	LYS
1	D	31	LYS
1	D	32	VAL
1	D	34	LEU
1	D	35	GLU
1	D	37	LYS
1	D	39	ASP
1	D	40	ARG
1	D	44	LYS
1	D	47	VAL
1	D	50	SER
1	D	52	ARG
1	D	62	SER
1	D	65	GLU
1	D	66	LEU
1	D	67	THR
1	D	68	PHE
1	D	71	LEU
1	D	77	ILE
1	D	80	LYS
1	D	83	GLN
1	D	86	VAL
1	D	89	GLU
1	D	90	LYS
1	D	93	MSE
1	D	95	MSE
1	D	96	LYS
1	D	99	SER

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Mol	Chain	Res	Type
1	D	101	GLU
1	D	104	SER
1	D	107	LEU
1	D	114	LEU
1	D	115	ARG
1	D	116	ARG
1	D	124	LEU
1	D	127	MSE
1	D	136	GLU
1	D	137	ARG
1	D	138	LEU
1	D	140	SER
1	D	141	LEU
1	D	146	ASP
1	D	147	SER
1	D	148	GLN
1	D	149	THR
1	D	150	LEU
1	D	152	GLU
1	D	168	ASP
1	D	173	SER
1	D	174	TYR
1	D	181	ASP
1	D	184	THR
1	D	188	THR
1	D	197	GLN
1	D	202	LEU
1	D	205	ARG
1	D	224	SER
1	D	225	SER
1	D	226	LYS
1	D	229	LYS
1	D	232	THR
1	D	237	GLN
1	D	247	ARG
1	D	272	HIS
1	D	275	ASN
1	D	286	ASN
1	D	288	LEU
1	D	291	ARG
1	D	293	VAL
1	D	296	LEU

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Mol	Chain	Res	Type
1	D	298	ILE
1	D	299	GLN
1	D	302	LYS
1	D	303	LEU
1	D	309	HIS
1	D	318	SER
1	D	323	ASN
1	D	330	SER
1	D	347	ASN
1	D	349	LEU
1	D	350	ARG
1	D	354	LEU
1	D	356	HIS
1	D	359	ASN
1	D	379	LEU
1	D	381	MSE
1	D	384	SER
1	D	388	ARG
1	D	396	VAL
1	D	397	LEU
1	D	400	SER
1	D	405	SER
1	D	407	ARG
1	D	408	LYS
1	D	410	LYS
1	D	427	ILE
1	D	428	GLN
1	D	434	THR
1	D	437	SER
1	D	455	LYS
1	D	458	SER
1	D	466	LEU
1	D	469	CYS
1	D	470	LEU
1	D	471	ARG
1	D	472	SER
1	D	476	GLN
1	D	477	VAL
1	D	478	LEU
1	D	484	GLU
1	D	490	SER
1	D	493	ILE

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Mol	Chain	Res	Type
1	D	505	LEU
1	D	509	LEU
1	D	513	ARG
1	D	517	HIS
1	D	525	ASN
1	D	532	LEU
1	D	541	GLN
1	D	550	LEU
1	D	566	ILE
1	D	568	ILE
1	D	580	VAL
1	D	594	MSE
1	D	603	THR
1	D	604	LYS
1	D	605	LEU
1	D	606	ARG
1	D	607	THR
1	D	609	ILE
1	D	632	THR
1	D	637	PRO
1	D	638	ILE
1	D	640	MSE
1	D	648	LYS
1	D	652	GLU
1	D	656	GLU
1	D	660	LYS
1	D	667	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	201	HIS
1	A	218	GLN
1	A	246	ASN
1	A	299	GLN
1	A	327	GLN
1	A	369	HIS
1	A	392	GLN
1	A	452	HIS
1	A	463	ASN
1	A	476	GLN

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Mol	Chain	Res	Type
1	A	512	ASN
1	A	525	ASN
1	A	650	ASN
1	B	79	HIS
1	B	148	GLN
1	B	201	HIS
1	B	204	HIS
1	B	309	HIS
1	B	323	ASN
1	B	486	HIS
1	B	525	ASN
1	B	600	GLN
1	B	645	GLN
1	C	92	ASN
1	C	109	HIS
1	C	189	GLN
1	C	204	HIS
1	C	237	GLN
1	C	246	ASN
1	C	323	ASN
1	C	369	HIS
1	C	406	HIS
1	C	418	GLN
1	C	468	HIS
1	C	476	GLN
1	C	602	ASN
1	C	659	GLN
1	D	79	HIS
1	D	109	HIS
1	D	189	GLN
1	D	204	HIS
1	D	237	GLN
1	D	323	ASN
1	D	356	HIS
1	D	369	HIS
1	D	406	HIS
1	D	512	ASN
1	D	517	HIS
1	D	602	ASN
1	D	614	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	OHB	B	701	-	10,10,10	1.92	1 (10%)	13,13,13	2.36	2 (15%)
4	ABU	C	701	-	6,6,6	1.30	2 (33%)	6,6,6	2.39	4 (66%)

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	OHB	B	701	-	-	1/4/4/4	0/1/1/1
4	ABU	C	701	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	OHB	C-N	5.59	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	ABU	O-C	2.20	1.29	1.22
4	C	701	ABU	CG-C	2.19	1.55	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	OHB	C6-C1-C	7.15	123.62	119.22
4	C	701	ABU	CB-CG-C	3.95	124.81	114.51
2	B	701	OHB	O-C-C1	2.73	123.46	120.24
4	C	701	ABU	CD-CB-CG	2.56	120.29	112.81
4	C	701	ABU	OXT-C-O	-2.43	117.09	123.33
4	C	701	ABU	OXT-C-CG	2.05	120.48	114.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	701	ABU	CD-CB-CG-C
2	B	701	OHB	N-C-C1-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	OHB	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	642/669 (95%)	-0.04	17 (2%)	57 48	8, 38, 107, 159	2 (0%)
1	B	642/669 (95%)	0.05	24 (3%)	45 37	8, 41, 113, 176	0
1	C	638/669 (95%)	-0.03	12 (1%)	66 58	13, 43, 89, 142	0
1	D	637/669 (95%)	0.32	28 (4%)	39 30	20, 52, 120, 175	0
All	All	2559/2676 (95%)	0.08	81 (3%)	50 41	8, 45, 109, 176	2 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	GLU	6.1
1	A	9	PRO	5.9
1	B	7	ASP	5.7
1	A	12	LEU	5.7
1	B	8	VAL	5.6
1	A	352	ASP	5.5
1	C	484	GLU	4.9
1	B	180	TRP	4.9
1	B	5	SER	4.7
1	B	484	GLU	4.7
1	C	485	ILE	4.5
1	C	476	GLN	4.4
1	D	37	LYS	4.2
1	D	36	VAL	3.8
1	D	180	TRP	3.7
1	A	483	ALA	3.5
1	A	290	ASP	3.4
1	C	508	TRP	3.2
1	D	476	GLN	3.1
1	B	76	VAL	3.0
1	B	6	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	508	TRP	2.9
1	C	509	LEU	2.9
1	A	81	PRO	2.9
1	D	353	ASP	2.9
1	C	478	LEU	2.8
1	D	98	VAL	2.8
1	D	140	SER	2.8
1	D	38	GLY	2.8
1	D	484	GLU	2.7
1	B	185	ILE	2.6
1	C	8	VAL	2.6
1	B	508	TRP	2.6
1	D	473	GLY	2.6
1	A	452	HIS	2.6
1	D	9	PRO	2.5
1	B	452	HIS	2.5
1	D	61	PRO	2.5
1	D	21	GLY	2.5
1	A	546	GLU	2.5
1	C	9	PRO	2.5
1	C	638	ILE	2.5
1	D	407	ARG	2.5
1	B	68	PHE	2.4
1	B	476	GLN	2.4
1	B	186	TYR	2.4
1	D	474	GLY	2.3
1	A	16	ILE	2.3
1	A	102	ASP	2.3
1	C	451	ASN	2.3
1	B	352	ASP	2.3
1	B	154	GLY	2.3
1	A	408	LYS	2.3
1	D	415	SER	2.3
1	A	79	HIS	2.2
1	B	37	LYS	2.2
1	B	356	HIS	2.2
1	D	66	LEU	2.2
1	D	304	PRO	2.2
1	C	272	HIS	2.2
1	C	38	GLY	2.2
1	D	137	ARG	2.1
1	A	481	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	374	ASN	2.1
1	A	21	GLY	2.1
1	A	513	ARG	2.1
1	A	106	VAL	2.1
1	A	480	GLY	2.1
1	B	261	ASP	2.1
1	B	353	ASP	2.1
1	D	352	ASP	2.1
1	B	219	TRP	2.1
1	D	45	VAL	2.1
1	D	528	LYS	2.1
1	D	78	CYS	2.0
1	D	455	LYS	2.0
1	B	14	GLU	2.0
1	B	32	VAL	2.0
1	D	60	ILE	2.0
1	D	547	ASP	2.0
1	B	511	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ABU	C	701	7/7	0.83	0.15	31,54,83,85	0
2	OHB	B	701	10/10	0.92	0.14	10,42,92,98	0
3	CL	B	702	1/1	0.99	0.05	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.