W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:44 am GMT

PDB ID	:	3CIA
Title	:	Crystal structure of cold-aminopeptidase from Colwellia psychrerythraea
Authors	:	Bauvois, C.; Jacquamet, L.; Borel, F.; Ferrer, J.-L.
Deposited on	:	2008-03-11
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.70 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.
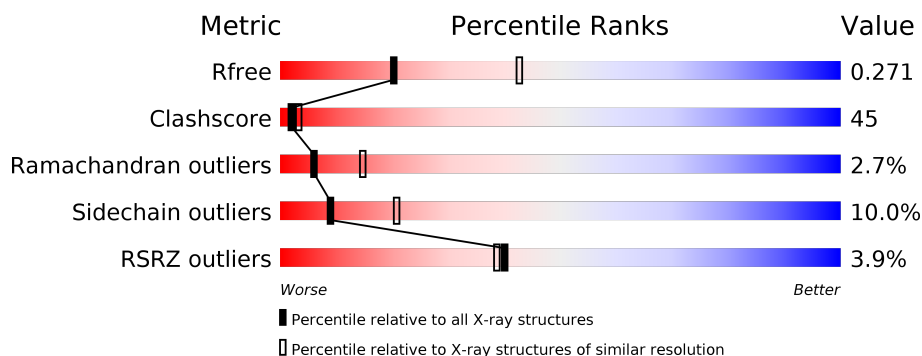
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	605	2% — 37% / 48% / 10% • •
1	B	605	5% — 36% / 47% / 12% • •
1	C	605	4% — 37% / 48% / 10% • •
1	D	605	4% — 33% / 52% / 10% • •

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	701	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 19608 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 cold-active aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4708	3023	780	892	13			
1	B	581	Total	C	N	O	S	0	0	0
			4651	2987	770	882	12			
1	C	581	Total	C	N	O	S	0	0	0
			4657	2993	770	882	12			
1	D	582	Total	C	N	O	S	0	0	0
			4669	2999	772	886	12			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	331	Total	O	0	0
			331	331		
3	B	154	Total	O	0	0
			154	154		
3	C	156	Total	O	0	0
			156	156		
3	D	278	Total	O	0	0
			278	278		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
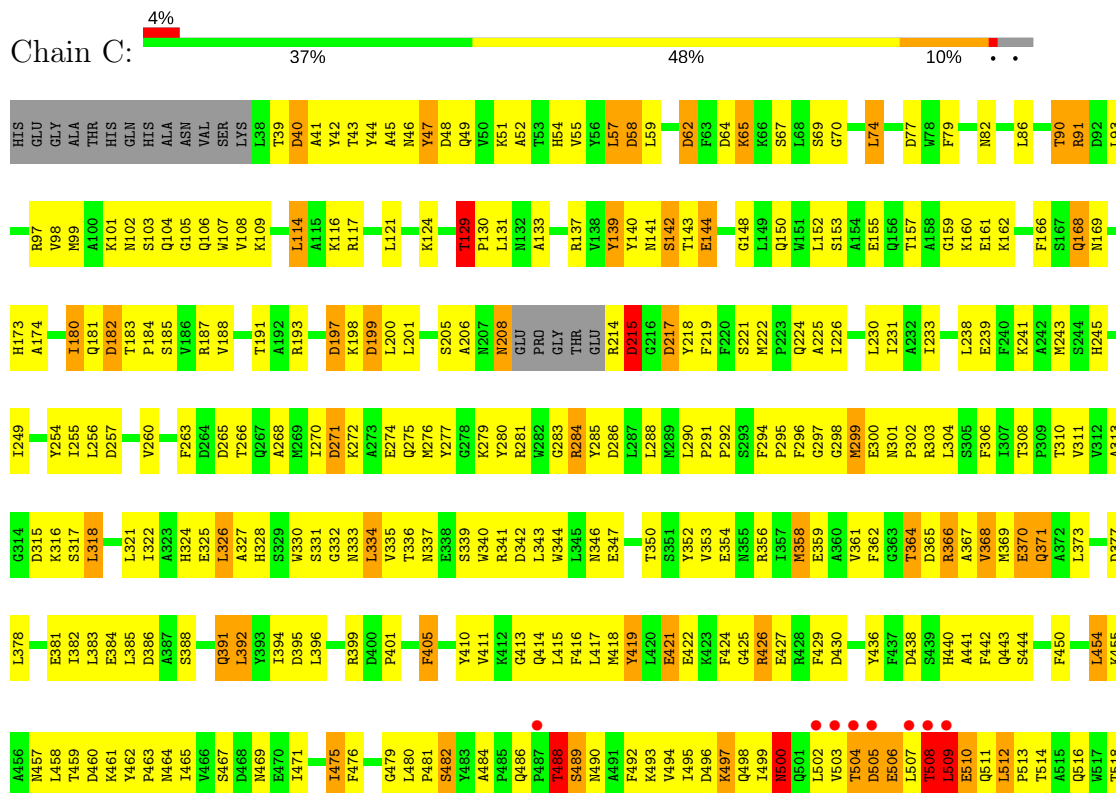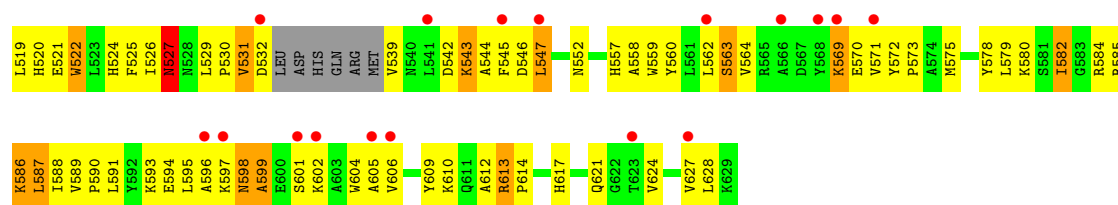
• Molecule 1: cold-active aminopeptidase
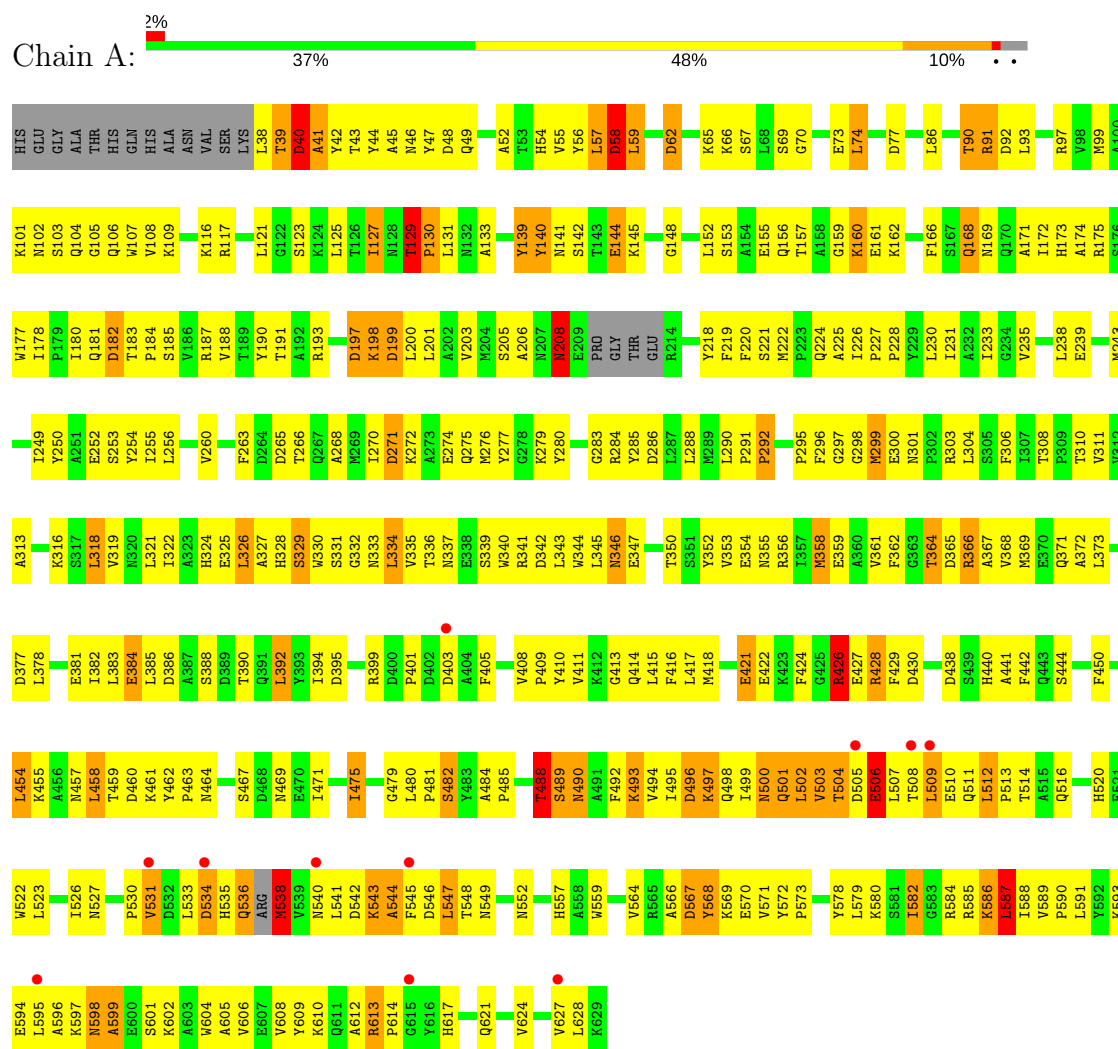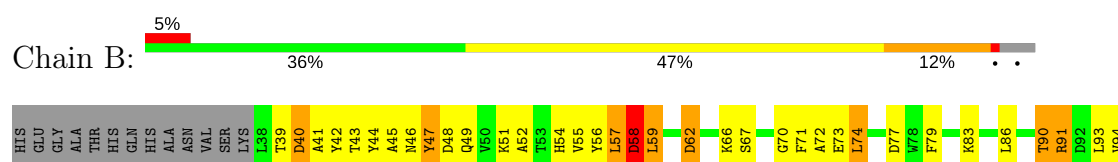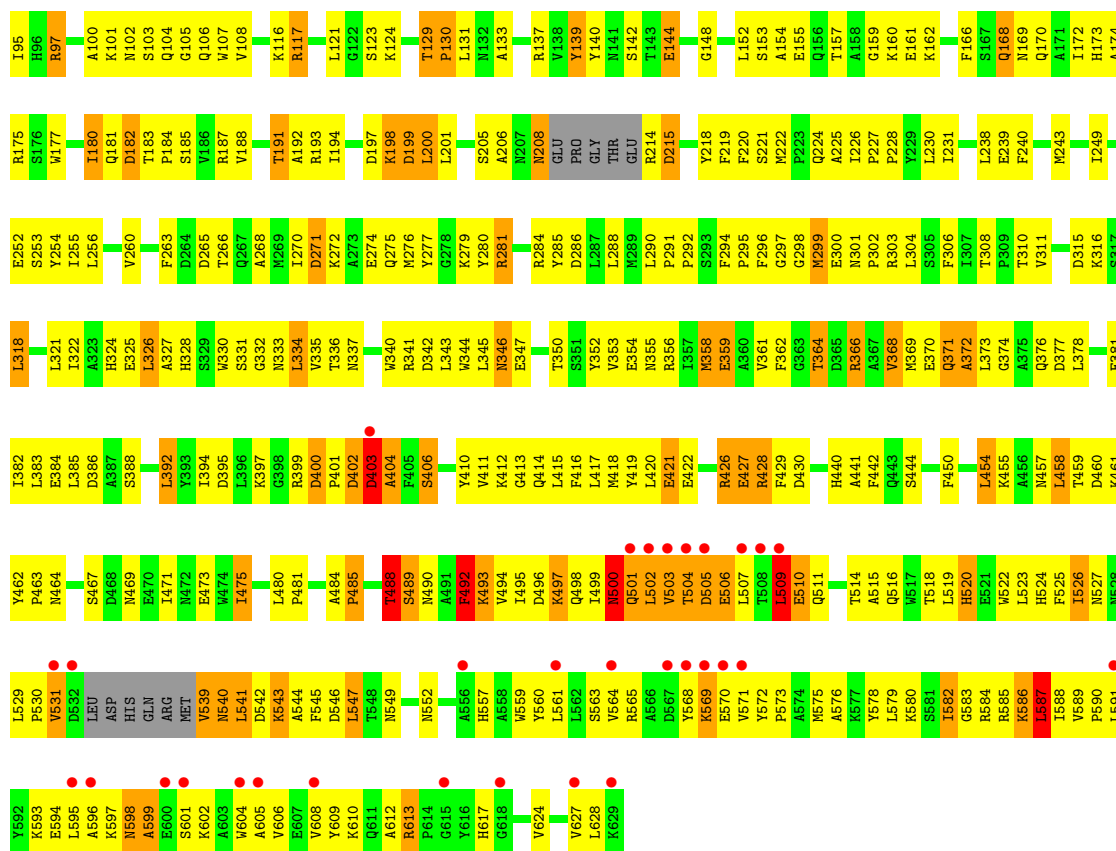
Chain A:
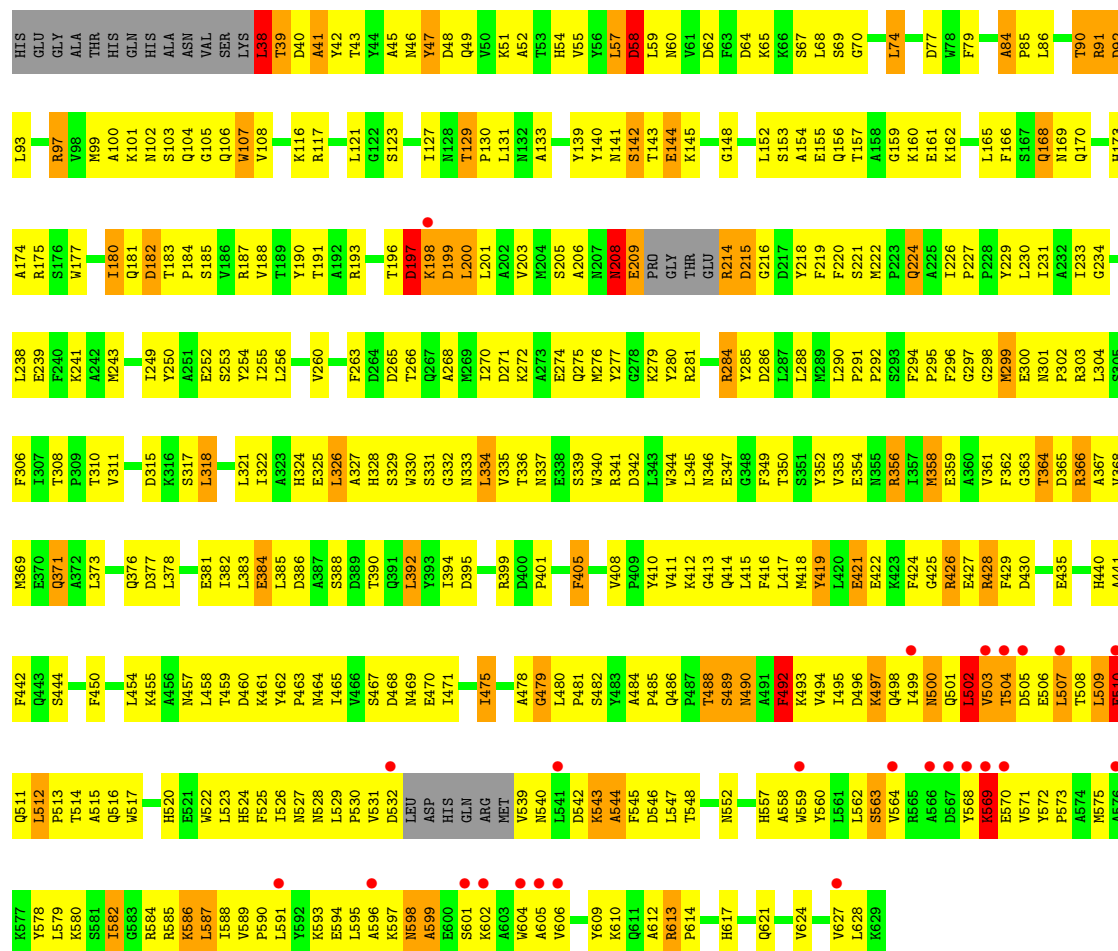
• Molecule 1: cold-active aminopeptidase

Chain B:

• Molecule 1: cold-active aminopeptidase

Chain C:

• Molecule 1: cold-active aminopeptidase

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.37Å 87.10Å 116.36Å 88.83° 70.68° 88.43°	Depositor
Resolution (Å)	46.68 – 2.70 46.69 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.68-2.70) 96.9 (46.69-2.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.249 , 0.270 0.250 , 0.271	Depositor DCC
R_{free} test set	4034 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.2	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.039 for h,-k,h-l 0.186 for -h,k,-l 0.021 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	19608	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	1.24	18/4823 (0.4%)	1.11	26/6555 (0.4%)
1	B	1.26	25/4764 (0.5%)	1.12	35/6476 (0.5%)
1	C	1.26	20/4771 (0.4%)	1.10	28/6485 (0.4%)
1	D	1.25	24/4783 (0.5%)	1.14	27/6501 (0.4%)
All	All	1.25	87/19141 (0.5%)	1.12	116/26017 (0.4%)

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	7
1	B	0	3
1	C	0	2
1	D	0	5
All	All	0	17

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	500	ASN	C-N	-18.91	0.90	1.34
1	D	140	TYR	CD2-CE2	-12.83	1.20	1.39
1	D	140	TYR	CE1-CZ	-12.36	1.22	1.38
1	C	140	TYR	CE1-CZ	-12.02	1.23	1.38
1	B	140	TYR	CE1-CZ	-9.72	1.25	1.38
1	A	47	TYR	CD2-CE2	-9.65	1.24	1.39
1	D	47	TYR	CD2-CE2	-9.47	1.25	1.39
1	A	140	TYR	CD2-CE2	-9.23	1.25	1.39
1	B	140	TYR	CD2-CE2	-9.12	1.25	1.39
1	C	139	TYR	CD2-CE2	-8.69	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	TYR	CD1-CE1	-8.59	1.26	1.39
1	B	47	TYR	CE2-CZ	-8.46	1.27	1.38
1	B	47	TYR	CD2-CE2	-8.33	1.26	1.39
1	C	47	TYR	CE2-CZ	-8.32	1.27	1.38
1	A	140	TYR	CE1-CZ	-8.32	1.27	1.38
1	C	47	TYR	CD2-CE2	-8.25	1.26	1.39
1	B	140	TYR	CG-CD1	-8.05	1.28	1.39
1	B	140	TYR	CE2-CZ	-7.91	1.28	1.38
1	C	140	TYR	CG-CD1	-7.62	1.29	1.39
1	D	47	TYR	CE2-CZ	-7.59	1.28	1.38
1	B	140	TYR	CD1-CE1	-7.55	1.28	1.39
1	A	177	TRP	CB-CG	7.48	1.63	1.50
1	C	140	TYR	CD2-CE2	-7.45	1.28	1.39
1	A	47	TYR	CD1-CE1	-7.32	1.28	1.39
1	D	139	TYR	CD2-CE2	-7.28	1.28	1.39
1	D	349	PHE	CE1-CZ	7.28	1.51	1.37
1	B	139	TYR	CD2-CE2	-7.14	1.28	1.39
1	D	208	ASN	C-N	7.04	1.50	1.34
1	B	168	GLN	C-O	-6.78	1.10	1.23
1	A	139	TYR	CD2-CE2	-6.75	1.29	1.39
1	D	177	TRP	CB-CG	6.74	1.62	1.50
1	B	488	THR	CB-CG2	-6.72	1.30	1.52
1	D	47	TYR	CE1-CZ	-6.62	1.29	1.38
1	C	47	TYR	CG-CD1	-6.57	1.30	1.39
1	D	140	TYR	CG-CD1	-6.37	1.30	1.39
1	A	47	TYR	CE1-CZ	-6.35	1.30	1.38
1	D	97	ARG	C-N	6.33	1.48	1.34
1	B	47	TYR	CG-CD2	-6.32	1.30	1.39
1	B	47	TYR	CE1-CZ	-6.28	1.30	1.38
1	B	94	VAL	CB-CG1	-6.28	1.39	1.52
1	D	140	TYR	CD1-CE1	-6.23	1.30	1.39
1	C	508	THR	C-N	-6.10	1.20	1.34
1	A	47	TYR	CE2-CZ	-6.09	1.30	1.38
1	D	492	PHE	CE1-CZ	-6.06	1.25	1.37
1	D	478	ALA	CA-CB	-6.04	1.39	1.52
1	A	168	GLN	C-O	-5.99	1.11	1.23
1	B	492	PHE	CE1-CZ	-5.97	1.26	1.37
1	D	168	GLN	C-O	-5.97	1.12	1.23
1	A	127	ILE	CA-CB	-5.95	1.41	1.54
1	C	140	TYR	CD1-CE1	-5.93	1.30	1.39
1	A	47	TYR	CG-CD1	-5.91	1.31	1.39
1	C	436	TYR	CE1-CZ	5.85	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	VAL	CB-CG1	-5.81	1.40	1.52
1	A	488	THR	CB-CG2	-5.76	1.33	1.52
1	B	177	TRP	CB-CG	5.70	1.60	1.50
1	B	359	GLU	CD-OE2	-5.67	1.19	1.25
1	D	435	GLU	CD-OE1	5.67	1.31	1.25
1	A	139	TYR	CE2-CZ	-5.67	1.31	1.38
1	B	473	GLU	CB-CG	5.62	1.62	1.52
1	B	372	ALA	CA-CB	-5.60	1.40	1.52
1	D	127	ILE	CA-CB	-5.60	1.42	1.54
1	C	419	TYR	CD1-CE1	5.60	1.47	1.39
1	D	100	ALA	C-O	-5.57	1.12	1.23
1	B	368	VAL	CB-CG2	-5.55	1.41	1.52
1	B	140	TYR	CG-CD2	-5.52	1.31	1.39
1	B	47	TYR	CD1-CE1	-5.52	1.31	1.39
1	B	139	TYR	CE2-CZ	-5.51	1.31	1.38
1	D	107	TRP	CE3-CZ3	-5.47	1.29	1.38
1	C	140	TYR	CG-CD2	-5.47	1.32	1.39
1	D	47	TYR	CD1-CE1	-5.46	1.31	1.39
1	C	370	GLU	CB-CG	5.44	1.62	1.52
1	D	419	TYR	CD1-CE1	5.44	1.47	1.39
1	C	98	VAL	CB-CG1	-5.40	1.41	1.52
1	A	140	TYR	CG-CD1	-5.37	1.32	1.39
1	C	168	GLN	C-O	-5.32	1.13	1.23
1	D	47	TYR	CG-CD1	-5.31	1.32	1.39
1	D	107	TRP	CZ3-CH2	-5.31	1.31	1.40
1	A	190	TYR	CG-CD2	5.29	1.46	1.39
1	A	47	TYR	C-O	-5.25	1.13	1.23
1	C	368	VAL	CB-CG2	-5.24	1.41	1.52
1	C	140	TYR	CE2-CZ	-5.21	1.31	1.38
1	D	139	TYR	CE2-CZ	-5.20	1.31	1.38
1	C	139	TYR	CE2-CZ	-5.17	1.31	1.38
1	C	47	TYR	CE1-CZ	-5.14	1.31	1.38
1	B	72	ALA	CA-CB	-5.09	1.41	1.52
1	B	427	GLU	CD-OE1	5.05	1.31	1.25
1	B	100	ALA	C-O	-5.04	1.13	1.23

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	ARG	O-C-N	11.59	141.24	122.70
1	D	97	ARG	CA-C-N	-9.97	95.27	117.20
1	A	599	ALA	N-CA-CB	-9.69	96.54	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	197	ASP	CB-CA-C	9.48	129.37	110.40
1	B	599	ALA	N-CA-CB	-9.22	97.19	110.10
1	D	599	ALA	N-CA-CB	-8.95	97.57	110.10
1	B	403	ASP	N-CA-CB	-8.74	94.86	110.60
1	B	402	ASP	CB-CA-C	-8.63	93.13	110.40
1	C	599	ALA	N-CA-CB	-8.60	98.07	110.10
1	B	544	ALA	N-CA-CB	-8.54	98.14	110.10
1	A	489	SER	N-CA-CB	-8.47	97.80	110.50
1	D	544	ALA	N-CA-CB	-8.47	98.24	110.10
1	A	544	ALA	N-CA-CB	-8.25	98.55	110.10
1	C	544	ALA	N-CA-CB	-8.21	98.61	110.10
1	B	403	ASP	CB-CA-C	-8.20	94.00	110.40
1	C	489	SER	N-CA-CB	-7.93	98.61	110.50
1	B	489	SER	N-CA-CB	-7.90	98.64	110.50
1	C	421	GLU	OE1-CD-OE2	-7.86	113.87	123.30
1	D	539	VAL	N-CA-CB	-7.84	94.26	111.50
1	C	539	VAL	N-CA-CB	-7.82	94.30	111.50
1	D	58	ASP	CB-CG-OD2	7.75	125.28	118.30
1	D	203	VAL	CB-CA-C	7.71	126.06	111.40
1	A	358	MET	CG-SD-CE	7.63	112.41	100.20
1	B	57	LEU	CA-CB-CG	7.58	132.73	115.30
1	D	208	ASN	C-N-CA	-7.57	102.78	121.70
1	D	489	SER	N-CA-CB	-7.55	99.18	110.50
1	B	421	GLU	OE1-CD-OE2	-7.47	114.34	123.30
1	C	598	ASN	N-CA-C	-7.42	90.96	111.00
1	A	598	ASN	N-CA-C	-7.33	91.20	111.00
1	B	117	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	D	57	LEU	CA-CB-CG	7.20	131.87	115.30
1	D	358	MET	CG-SD-CE	7.15	111.64	100.20
1	C	358	MET	CG-SD-CE	7.08	111.53	100.20
1	A	58	ASP	CB-CG-OD2	6.98	124.59	118.30
1	C	284	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	284	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	C	539	VAL	N-CA-C	-6.86	92.49	111.00
1	C	62	ASP	CB-CG-OD2	6.82	124.44	118.30
1	B	358	MET	CG-SD-CE	6.77	111.03	100.20
1	A	208	ASN	O-C-N	-6.74	111.92	122.70
1	B	208	ASN	CB-CA-C	-6.71	96.97	110.40
1	D	356	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	D	598	ASN	N-CA-C	-6.68	92.95	111.00
1	D	421	GLU	OE1-CD-OE2	-6.67	115.30	123.30
1	A	219	PHE	N-CA-C	-6.67	93.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	598	ASN	N-CA-C	-6.66	93.01	111.00
1	A	57	LEU	CA-CB-CG	6.62	130.53	115.30
1	C	57	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	421	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	D	219	PHE	N-CA-C	-6.53	93.37	111.00
1	A	208	ASN	CB-CA-C	-6.38	97.64	110.40
1	D	182	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	539	VAL	N-CA-C	-6.29	94.02	111.00
1	C	219	PHE	N-CA-C	-6.29	94.03	111.00
1	A	59	LEU	CA-CB-CG	6.26	129.71	115.30
1	B	219	PHE	N-CA-C	-6.26	94.09	111.00
1	C	182	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	400	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	402	ASP	CB-CG-OD2	6.14	123.83	118.30
1	D	92	ASP	N-CA-CB	-6.09	99.64	110.60
1	B	404	ALA	N-CA-CB	-6.08	101.58	110.10
1	A	426	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	91	ARG	CB-CA-C	5.96	122.33	110.40
1	A	91	ARG	CB-CA-C	5.90	122.20	110.40
1	D	501	GLN	N-CA-C	-5.84	95.23	111.00
1	B	200	LEU	N-CA-C	-5.82	95.30	111.00
1	D	208	ASN	CB-CA-C	-5.81	98.77	110.40
1	A	438	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	91	ARG	CB-CA-C	5.76	121.92	110.40
1	A	62	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	91	ARG	CB-CA-C	5.69	121.79	110.40
1	B	58	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	182	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	182	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	47	TYR	CB-CA-C	5.60	121.59	110.40
1	C	208	ASN	CB-CA-C	-5.59	99.22	110.40
1	A	271	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	203	VAL	CB-CA-C	5.53	121.90	111.40
1	B	488	THR	N-CA-C	-5.51	96.11	111.00
1	D	215	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	271	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	199	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	271	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	215	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	420	LEU	CB-CG-CD2	-5.34	101.91	111.00
1	B	62	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	197	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	200	LEU	O-C-N	5.32	131.21	122.70
1	B	59	LEU	CA-CB-CG	5.29	127.47	115.30
1	D	199	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	197	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	197	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	567	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	40	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	406	SER	N-CA-CB	-5.25	102.63	110.50
1	C	488	THR	N-CA-C	-5.23	96.88	111.00
1	C	217	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	198	LYS	CB-CA-C	-5.22	99.96	110.40
1	C	197	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	391	GLN	O-C-N	-5.19	114.39	122.70
1	A	587	LEU	N-CA-CB	-5.19	100.03	110.40
1	B	587	LEU	N-CA-CB	-5.17	100.05	110.40
1	B	403	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	257	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	B	281	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	D	84	ALA	N-CA-CB	-5.14	102.90	110.10
1	A	92	ASP	N-CA-C	-5.13	97.14	111.00
1	A	47	TYR	CB-CA-C	5.11	120.62	110.40
1	A	129	THR	N-CA-CB	-5.11	100.60	110.30
1	A	488	THR	N-CA-C	-5.10	97.22	111.00
1	C	199	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	342	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	40	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	191	THR	N-CA-C	-5.02	97.45	111.00
1	C	114	LEU	N-CA-C	-5.00	97.49	111.00
1	C	129	THR	N-CA-CB	-5.00	100.80	110.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ASP	Peptide
1	A	208	ASN	Mainchain
1	A	40	ASP	Peptide
1	A	506	GLU	Peptide
1	A	535	HIS	Peptide
1	A	538	MET	Peptide
1	A	568	TYR	Peptide
1	B	402	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	404	ALA	Peptide
1	B	539	VAL	Peptide
1	C	500	ASN	Mainchain
1	C	527	ASN	Peptide
1	D	197	ASP	Peptide
1	D	208	ASN	Mainchain
1	D	214	ARG	Peptide
1	D	38	LEU	Peptide
1	D	510	GLU	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	4708	0	4594	410	0
1	B	4651	0	4543	415	1
1	C	4657	0	4548	396	1
1	D	4669	0	4560	441	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	331	0	0	23	0
3	B	154	0	0	8	1
3	C	156	0	0	13	2
3	D	278	0	0	27	1
All	All	19608	0	18245	1655	3

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 45.

All (1655) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:LEU:HD12	1:D:506:GLU:O	1.34	1.27
1:A:42:TYR:OH	1:A:399:ARG:O	1.53	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:VAL:O	1:A:504:THR:HG23	1.39	1.22
1:B:42:TYR:OH	1:B:399:ARG:O	1.59	1.19
1:A:42:TYR:CE2	1:A:401:PRO:HD3	1.80	1.17
1:C:502:LEU:HB2	1:C:506:GLU:HB2	1.25	1.15
1:A:42:TYR:HE2	1:A:401:PRO:HD3	1.12	1.13
1:D:509:LEU:HG	1:D:510:GLU:N	1.59	1.12
1:D:503:VAL:HG22	1:D:506:GLU:CG	1.79	1.12
1:B:539:VAL:HG12	1:B:540:ASN:H	1.00	1.10
1:B:355:ASN:OD1	1:B:371:GLN:NE2	1.83	1.10
1:D:503:VAL:CG2	1:D:506:GLU:HG3	1.82	1.10
1:B:183:THR:HG22	1:B:185:SER:H	1.15	1.10
1:C:522:TRP:O	1:C:526:ILE:HG13	1.51	1.09
1:B:503:VAL:HG23	1:B:506:GLU:CG	1.81	1.09
1:B:144:GLU:CD	1:B:144:GLU:H	1.57	1.08
1:B:523:LEU:O	1:B:527:ASN:HB2	1.51	1.08
1:C:144:GLU:CD	1:C:144:GLU:H	1.53	1.07
1:A:504:THR:H	1:A:506:GLU:HB2	1.17	1.06
1:A:523:LEU:O	1:A:527:ASN:ND2	1.86	1.06
1:B:503:VAL:CG2	1:B:506:GLU:HG2	1.85	1.06
1:D:503:VAL:HG22	1:D:506:GLU:CD	1.75	1.06
1:D:525:PHE:O	1:D:529:LEU:HG	1.52	1.05
1:D:503:VAL:CA	1:D:506:GLU:HG3	1.84	1.05
1:D:183:THR:HG22	1:D:185:SER:H	1.21	1.05
1:C:503:VAL:O	1:C:504:THR:HG23	1.58	1.04
1:A:97:ARG:HH11	1:A:99:MET:HE3	1.20	1.04
1:B:502:LEU:HG	1:B:507:LEU:HB2	1.39	1.04
1:B:539:VAL:HG12	1:B:540:ASN:N	1.61	1.03
1:D:263:PHE:O	1:D:266:THR:HG23	1.57	1.03
1:A:183:THR:HG22	1:A:185:SER:H	1.18	1.02
1:D:503:VAL:HG22	1:D:506:GLU:HG3	1.34	1.02
1:D:503:VAL:C	1:D:506:GLU:HG3	1.77	1.02
1:C:502:LEU:HD13	1:C:506:GLU:HB3	1.41	1.02
1:D:503:VAL:O	1:D:504:THR:HG23	1.58	1.02
1:D:543:LYS:O	1:D:543:LYS:HE3	1.57	1.02
1:C:502:LEU:CD1	1:C:506:GLU:HB3	1.91	1.01
1:D:144:GLU:H	1:D:144:GLU:CD	1.57	1.01
1:C:405:PHE:HA	3:C:994:HOH:O	1.62	1.00
1:D:504:THR:N	1:D:506:GLU:HG2	1.76	1.00
1:C:368:VAL:HA	1:C:371:GLN:HG3	1.42	0.99
1:C:263:PHE:O	1:C:266:THR:HG23	1.62	0.99
1:C:509:LEU:HD23	1:C:509:LEU:N	1.78	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:VAL:C	1:D:506:GLU:CG	2.30	0.99
1:C:97:ARG:HH11	1:C:99:MET:HE3	1.28	0.99
1:D:503:VAL:C	1:D:504:THR:HG23	1.80	0.99
1:B:504:THR:HG23	1:B:504:THR:O	1.63	0.98
1:D:503:VAL:O	1:D:503:VAL:HG23	1.58	0.98
1:D:67:SER:HB2	1:D:142:SER:O	1.64	0.98
1:C:183:THR:HG22	1:C:185:SER:H	1.21	0.98
1:D:506:GLU:O	1:D:507:LEU:HB2	1.60	0.98
1:A:368:VAL:HA	1:A:371:GLN:HG3	1.43	0.98
1:C:157:THR:O	1:C:160:LYS:HE3	1.61	0.97
1:C:543:LYS:HE3	1:C:543:LYS:O	1.64	0.97
1:D:586:LYS:HG2	1:D:586:LYS:O	1.63	0.97
1:B:502:LEU:CG	1:B:507:LEU:HB2	1.94	0.97
1:A:263:PHE:O	1:A:266:THR:HG23	1.64	0.97
1:B:503:VAL:HG23	1:B:506:GLU:HG2	1.36	0.97
1:B:263:PHE:O	1:B:266:THR:HG23	1.65	0.96
1:B:502:LEU:CD1	1:B:507:LEU:HB2	1.95	0.96
1:B:157:THR:O	1:B:160:LYS:HE3	1.65	0.95
1:D:509:LEU:HG	1:D:510:GLU:H	1.30	0.94
1:A:586:LYS:HG2	1:A:586:LYS:O	1.65	0.94
1:A:157:THR:O	1:A:160:LYS:HE3	1.67	0.93
1:B:373:LEU:HD13	1:B:492:PHE:CZ	2.05	0.92
1:D:42:TYR:OH	1:D:399:ARG:O	1.86	0.92
1:B:400:ASP:HB3	1:B:403:ASP:HB2	1.52	0.92
1:A:543:LYS:HE3	1:A:543:LYS:O	1.69	0.92
1:B:67:SER:HB2	1:B:142:SER:O	1.71	0.90
1:D:157:THR:O	1:D:160:LYS:HE3	1.70	0.90
1:C:503:VAL:C	1:C:504:THR:HG23	1.92	0.90
1:C:40:ASP:OD2	1:C:183:THR:HG23	1.72	0.90
1:B:543:LYS:O	1:B:543:LYS:HE3	1.72	0.90
1:C:507:LEU:HD11	3:C:971:HOH:O	1.70	0.90
1:A:361:VAL:HG23	1:A:362:PHE:CD1	2.06	0.90
1:B:341:ARG:HD2	1:B:394:ILE:O	1.72	0.89
1:B:522:TRP:O	1:B:526:ILE:HD13	1.72	0.89
1:B:586:LYS:HG2	1:B:586:LYS:O	1.71	0.89
1:D:522:TRP:O	1:D:526:ILE:HG13	1.73	0.89
1:C:67:SER:HB2	1:C:142:SER:O	1.71	0.89
1:B:522:TRP:O	1:B:526:ILE:HG23	1.71	0.89
1:A:144:GLU:CD	1:A:144:GLU:H	1.76	0.88
1:C:502:LEU:HB2	1:C:506:GLU:CB	2.03	0.88
1:C:361:VAL:HG23	1:C:362:PHE:CD1	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ILE:CD1	1:A:587:LEU:HD23	2.04	0.88
1:B:529:LEU:HD23	1:B:530:PRO:N	1.87	0.88
1:A:567:ASP:O	1:A:569:LYS:HD2	1.74	0.87
1:B:355:ASN:CG	1:B:371:GLN:HE21	1.78	0.87
1:D:40:ASP:OD2	1:D:183:THR:HG23	1.75	0.86
1:A:530:PRO:O	1:A:533:LEU:HD13	1.75	0.86
1:D:153:SER:OG	1:D:155:GLU:HG2	1.75	0.86
1:A:523:LEU:O	1:A:527:ASN:HB2	1.75	0.86
1:A:500:ASN:N	1:A:500:ASN:HD22	1.70	0.86
1:C:97:ARG:HH11	1:C:99:MET:CE	1.89	0.86
1:A:67:SER:HB2	1:A:142:SER:O	1.76	0.85
1:B:510:GLU:H	1:B:510:GLU:CD	1.77	0.85
1:D:500:ASN:HD22	1:D:500:ASN:H	1.23	0.85
1:D:361:VAL:HG23	1:D:362:PHE:CD1	2.12	0.85
1:B:502:LEU:HG	1:B:507:LEU:CB	2.05	0.84
1:C:144:GLU:CD	1:C:144:GLU:N	2.30	0.84
1:A:102:ASN:HB2	3:A:960:HOH:O	1.77	0.84
1:A:168:GLN:O	1:A:168:GLN:HG3	1.78	0.84
1:A:567:ASP:HB3	1:A:569:LYS:CE	2.08	0.84
1:B:373:LEU:HD13	1:B:492:PHE:CE2	2.12	0.84
1:C:464:ASN:HD22	1:D:241:LYS:HB3	1.42	0.83
1:D:296:PHE:HD2	3:D:970:HOH:O	1.60	0.83
1:D:503:VAL:CB	1:D:506:GLU:HG3	2.08	0.83
1:A:97:ARG:HH11	1:A:99:MET:CE	1.92	0.83
1:B:361:VAL:HG23	1:B:362:PHE:CD1	2.13	0.83
1:B:334:LEU:CD2	1:B:441:ALA:HA	2.08	0.83
1:C:586:LYS:HG2	1:C:586:LYS:O	1.76	0.83
1:A:198:LYS:O	1:A:199:ASP:HB2	1.77	0.83
1:C:582:ILE:CD1	1:C:587:LEU:HD23	2.08	0.83
1:B:503:VAL:O	1:B:504:THR:HB	1.76	0.83
1:C:271:ASP:OD1	3:C:924:HOH:O	1.97	0.82
1:D:168:GLN:HE22	1:D:299:MET:HG2	1.44	0.82
1:D:405:PHE:O	3:D:761:HOH:O	1.96	0.82
1:D:584:ARG:O	1:D:588:ILE:HG12	1.78	0.82
1:A:40:ASP:OD2	1:A:183:THR:HG23	1.79	0.82
1:C:153:SER:OG	1:C:155:GLU:HG2	1.80	0.82
1:D:502:LEU:HD11	1:D:507:LEU:HD12	1.59	0.82
1:B:539:VAL:CG1	1:B:540:ASN:H	1.84	0.81
1:A:42:TYR:CE2	1:A:401:PRO:CD	2.61	0.81
1:B:198:LYS:O	1:B:199:ASP:HB2	1.79	0.81
1:D:341:ARG:HD2	1:D:394:ILE:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:LYS:HD2	1:B:570:GLU:N	1.94	0.81
1:D:455:LYS:O	1:D:460:ASP:HB2	1.80	0.81
1:C:512:LEU:HB3	1:C:513:PRO:CD	2.11	0.80
1:A:567:ASP:HB3	1:A:569:LYS:HE3	1.63	0.80
1:B:102:ASN:HB2	3:B:795:HOH:O	1.81	0.80
1:B:208:ASN:OD1	1:B:208:ASN:O	2.00	0.80
1:B:153:SER:OG	1:B:155:GLU:HG2	1.81	0.80
1:A:169:ASN:O	3:A:715:HOH:O	1.98	0.80
1:D:334:LEU:CD2	1:D:441:ALA:HA	2.12	0.80
1:A:199:ASP:OD2	3:A:825:HOH:O	2.00	0.79
1:B:504:THR:CG2	1:B:504:THR:O	2.30	0.79
1:C:502:LEU:CB	1:C:506:GLU:HB2	2.10	0.79
1:D:489:SER:HB3	1:D:492:PHE:HB2	1.64	0.79
1:D:168:GLN:HG3	1:D:168:GLN:O	1.81	0.79
1:D:503:VAL:O	1:D:504:THR:CG2	2.30	0.79
1:A:153:SER:OG	1:A:155:GLU:HG2	1.83	0.79
1:A:503:VAL:H	1:A:506:GLU:HB3	1.48	0.79
1:B:547:LEU:H	1:B:547:LEU:HD12	1.47	0.79
1:A:341:ARG:HD2	1:A:394:ILE:O	1.81	0.79
1:D:168:GLN:HB3	3:D:737:HOH:O	1.82	0.79
1:B:368:VAL:CG1	1:B:368:VAL:O	2.30	0.78
1:B:509:LEU:HB2	1:B:510:GLU:OE2	1.83	0.78
1:C:208:ASN:OD1	1:C:208:ASN:O	2.01	0.78
1:D:296:PHE:CD2	3:D:970:HOH:O	2.35	0.78
1:C:508:THR:O	1:C:509:LEU:O	2.02	0.78
1:D:428:ARG:CD	3:D:956:HOH:O	2.32	0.78
1:C:418:MET:O	1:C:422:GLU:HG3	1.83	0.78
1:A:199:ASP:O	1:A:200:LEU:HD12	1.84	0.78
1:A:99:MET:HE1	1:A:109:LYS:HB2	1.64	0.78
1:D:500:ASN:N	1:D:500:ASN:HD22	1.81	0.78
1:C:503:VAL:O	1:C:504:THR:CG2	2.30	0.78
1:D:295:PRO:HG2	1:D:296:PHE:HD1	1.49	0.78
1:D:424:PHE:O	3:D:873:HOH:O	2.02	0.78
1:C:168:GLN:HE22	1:C:299:MET:HG2	1.49	0.77
1:A:334:LEU:CD2	1:A:441:ALA:HA	2.14	0.77
1:B:144:GLU:CD	1:B:144:GLU:N	2.35	0.77
1:A:101:LYS:O	3:A:981:HOH:O	2.03	0.77
1:C:341:ARG:HD2	1:C:394:ILE:O	1.84	0.77
1:C:419:TYR:CE1	3:C:976:HOH:O	2.37	0.77
1:B:547:LEU:HD12	1:B:547:LEU:N	2.00	0.77
1:A:424:PHE:O	3:A:866:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:LYS:HD2	1:D:570:GLU:N	2.00	0.76
1:D:57:LEU:HB3	1:D:59:LEU:CD2	2.15	0.76
1:A:208:ASN:OD1	1:A:208:ASN:O	2.04	0.76
1:B:580:LYS:HA	1:B:612:ALA:HB2	1.67	0.76
1:D:503:VAL:O	1:D:503:VAL:CG2	2.29	0.76
1:B:539:VAL:C	1:B:541:LEU:H	1.88	0.76
1:A:405:PHE:O	3:A:732:HOH:O	2.04	0.76
1:A:502:LEU:HB2	1:A:506:GLU:O	1.85	0.76
1:B:271:ASP:OD1	3:B:763:HOH:O	2.02	0.76
1:B:381:GLU:O	1:B:385:LEU:HB2	1.84	0.76
1:A:168:GLN:HB3	3:A:703:HOH:O	1.84	0.76
1:B:509:LEU:HD21	1:B:511:GLN:HB2	1.69	0.75
1:B:569:LYS:HD2	1:B:570:GLU:H	1.50	0.75
1:C:334:LEU:CD2	1:C:441:ALA:HA	2.17	0.75
1:B:582:ILE:CD1	1:B:587:LEU:HD23	2.17	0.75
1:C:509:LEU:CD2	1:C:509:LEU:N	2.49	0.75
1:C:492:PHE:O	1:C:495:ILE:HB	1.87	0.75
1:D:606:VAL:O	1:D:610:LYS:HD3	1.86	0.75
1:B:168:GLN:HE22	1:B:299:MET:HG2	1.51	0.75
1:B:418:MET:O	1:B:422:GLU:HG3	1.87	0.75
1:B:503:VAL:O	1:B:504:THR:CB	2.34	0.75
1:B:539:VAL:CG1	1:B:540:ASN:N	2.37	0.74
1:C:547:LEU:H	1:C:547:LEU:HD12	1.52	0.74
1:D:582:ILE:CD1	1:D:587:LEU:HD23	2.17	0.74
1:B:584:ARG:O	1:B:588:ILE:HG12	1.87	0.74
1:B:503:VAL:HB	1:B:506:GLU:OE1	1.87	0.74
1:C:543:LYS:CE	1:C:543:LYS:O	2.35	0.74
1:C:606:VAL:O	1:C:610:LYS:HD3	1.88	0.74
1:D:144:GLU:N	1:D:144:GLU:CD	2.39	0.74
1:D:58:ASP:O	1:D:70:GLY:HA3	1.88	0.74
1:B:609:TYR:O	1:B:613:ARG:HB2	1.88	0.74
1:C:579:LEU:HD21	1:C:591:LEU:HD23	1.67	0.74
1:B:334:LEU:HD22	1:B:441:ALA:HA	1.70	0.74
1:B:606:VAL:O	1:B:610:LYS:HD3	1.87	0.74
1:A:503:VAL:O	1:A:504:THR:CG2	2.29	0.74
1:D:503:VAL:C	1:D:506:GLU:HG2	2.01	0.74
1:C:381:GLU:O	1:C:385:LEU:HB2	1.88	0.73
1:C:290:LEU:HD21	1:C:306:PHE:HD2	1.53	0.73
1:C:569:LYS:HD2	1:C:570:GLU:N	2.02	0.73
1:D:543:LYS:CE	1:D:543:LYS:O	2.33	0.73
1:A:418:MET:O	1:A:422:GLU:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ARG:O	1:A:588:ILE:HG12	1.87	0.73
1:D:503:VAL:CG2	1:D:506:GLU:CG	2.52	0.73
1:A:543:LYS:O	1:A:543:LYS:CE	2.36	0.73
1:C:424:PHE:O	3:C:929:HOH:O	2.06	0.73
1:C:41:ALA:O	1:C:42:TYR:HB2	1.86	0.73
1:A:533:LEU:O	1:A:536:GLN:N	2.18	0.72
1:A:606:VAL:O	1:A:610:LYS:HD3	1.89	0.72
1:C:295:PRO:HG2	1:C:296:PHE:HD1	1.52	0.72
1:D:169:ASN:O	3:D:746:HOH:O	2.06	0.72
1:B:102:ASN:HD21	1:B:106:GLN:HB2	1.54	0.72
1:A:501:GLN:HG2	1:A:508:THR:HG23	1.69	0.72
1:A:523:LEU:O	1:A:527:ASN:CB	2.37	0.72
1:B:290:LEU:HD21	1:B:306:PHE:HD2	1.55	0.72
1:A:580:LYS:HA	1:A:612:ALA:HB2	1.72	0.72
1:A:290:LEU:HD21	1:A:306:PHE:HD2	1.54	0.72
1:B:510:GLU:N	1:B:510:GLU:CD	2.42	0.71
1:C:580:LYS:HA	1:C:612:ALA:HB2	1.70	0.71
1:B:359:GLU:HG2	1:B:364:THR:HG22	1.72	0.71
1:C:582:ILE:HD11	1:C:584:ARG:HB3	1.71	0.71
1:D:418:MET:O	1:D:422:GLU:HG3	1.89	0.71
1:D:378:LEU:O	1:D:382:ILE:HG12	1.90	0.71
1:D:586:LYS:CG	1:D:586:LYS:O	2.35	0.71
1:A:295:PRO:HG2	1:A:296:PHE:HD1	1.55	0.71
1:C:527:ASN:OD1	1:C:558:ALA:HB1	1.90	0.71
1:D:503:VAL:CG2	1:D:506:GLU:CD	2.56	0.71
1:C:168:GLN:HE22	1:C:299:MET:CG	2.03	0.71
1:D:580:LYS:HA	1:D:612:ALA:HB2	1.71	0.71
1:C:46:ASN:C	1:C:48:ASP:H	1.94	0.71
1:A:144:GLU:N	1:A:144:GLU:CD	2.43	0.71
1:A:222:MET:SD	1:A:224:GLN:HB2	2.31	0.70
1:D:168:GLN:HE22	1:D:299:MET:CG	2.03	0.70
1:A:58:ASP:O	1:A:70:GLY:HA3	1.92	0.70
1:B:168:GLN:HG3	1:B:168:GLN:O	1.87	0.70
1:B:411:VAL:O	1:B:415:LEU:HG	1.90	0.70
1:B:539:VAL:C	1:B:541:LEU:N	2.40	0.70
1:C:503:VAL:HG23	1:C:506:GLU:HG2	1.73	0.70
1:D:42:TYR:CE2	1:D:401:PRO:HD3	2.26	0.70
1:D:500:ASN:N	1:D:500:ASN:ND2	2.39	0.70
1:B:503:VAL:HG23	1:B:506:GLU:OE1	1.91	0.70
1:B:543:LYS:O	1:B:543:LYS:CE	2.40	0.70
1:C:584:ARG:O	1:C:588:ILE:HG12	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:609:TYR:O	1:C:613:ARG:HB2	1.91	0.70
1:B:183:THR:HG22	1:B:185:SER:N	2.00	0.70
1:C:58:ASP:O	1:C:70:GLY:HA3	1.92	0.70
1:C:596:ALA:HA	1:C:602:LYS:HB2	1.73	0.70
1:D:290:LEU:HD21	1:D:306:PHE:HD2	1.56	0.70
1:C:57:LEU:HB3	1:C:59:LEU:CD2	2.22	0.69
1:A:378:LEU:O	1:A:382:ILE:HG12	1.92	0.69
1:A:411:VAL:O	1:A:415:LEU:HG	1.92	0.69
1:B:58:ASP:O	1:B:70:GLY:HA3	1.92	0.69
1:A:384:GLU:OE1	3:A:832:HOH:O	2.10	0.69
1:B:57:LEU:HB3	1:B:59:LEU:CD2	2.21	0.69
1:A:536:GLN:HA	1:A:536:GLN:OE1	1.90	0.69
1:A:547:LEU:HD12	1:A:547:LEU:H	1.57	0.69
1:C:598:ASN:HB3	1:C:601:SER:HB3	1.74	0.69
1:A:183:THR:HG22	1:A:185:SER:N	2.01	0.69
1:B:503:VAL:HG23	1:B:506:GLU:CD	2.13	0.69
1:B:503:VAL:CB	1:B:506:GLU:OE1	2.40	0.69
1:B:509:LEU:CD2	1:B:509:LEU:H	2.06	0.69
1:C:455:LYS:O	1:C:460:ASP:HB2	1.93	0.69
1:B:503:VAL:HG21	1:B:506:GLU:HG2	1.72	0.69
1:A:523:LEU:C	1:A:527:ASN:HD22	1.93	0.69
1:D:503:VAL:CA	1:D:506:GLU:CG	2.68	0.69
1:A:455:LYS:O	1:A:460:ASP:HB2	1.93	0.68
1:C:494:VAL:HG12	1:C:494:VAL:O	1.93	0.68
1:A:103:SER:N	3:A:960:HOH:O	2.16	0.68
1:A:504:THR:N	1:A:506:GLU:HB2	1.99	0.68
1:C:168:GLN:O	1:C:168:GLN:HG3	1.89	0.68
1:C:180:ILE:HG12	1:C:181:GLN:H	1.58	0.68
1:B:503:VAL:CG2	1:B:506:GLU:OE1	2.42	0.68
1:C:547:LEU:N	1:C:547:LEU:HD12	2.09	0.68
1:A:168:GLN:HE22	1:A:299:MET:HG2	1.57	0.68
1:A:582:ILE:HD11	1:A:587:LEU:HD23	1.74	0.68
1:A:500:ASN:N	1:A:500:ASN:ND2	2.38	0.68
1:A:543:LYS:CD	1:A:543:LYS:O	2.40	0.68
1:D:197:ASP:HB3	1:D:198:LYS:O	1.93	0.68
1:C:358:MET:CE	1:C:366:ARG:HH12	2.06	0.68
1:D:502:LEU:HD12	1:D:507:LEU:HB2	1.74	0.68
1:A:392:LEU:HD23	1:A:475:ILE:HG22	1.74	0.68
1:D:369:MET:SD	1:D:520:HIS:HB2	2.33	0.68
1:A:547:LEU:N	1:A:547:LEU:HD12	2.09	0.68
1:B:509:LEU:HD22	1:B:509:LEU:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:MET:HG2	1:A:568:TYR:CG	2.29	0.67
1:D:97:ARG:HD3	1:D:99:MET:CE	2.24	0.67
1:A:492:PHE:O	1:A:495:ILE:HB	1.93	0.67
1:A:499:ILE:HG13	1:A:500:ASN:ND2	2.10	0.67
1:A:174:ALA:HB3	1:A:182:ASP:OD1	1.95	0.67
1:C:569:LYS:HD2	1:C:570:GLU:H	1.59	0.67
1:C:464:ASN:ND2	1:D:241:LYS:HD3	2.09	0.67
1:D:547:LEU:HD12	1:D:547:LEU:N	2.08	0.67
1:D:208:ASN:OD1	1:D:208:ASN:O	2.12	0.67
1:B:295:PRO:HG2	1:B:296:PHE:HD1	1.59	0.67
1:B:525:PHE:CD1	1:B:526:ILE:HG22	2.30	0.67
1:C:502:LEU:CB	1:C:506:GLU:CB	2.71	0.67
1:D:547:LEU:H	1:D:547:LEU:HD12	1.59	0.67
1:B:358:MET:CE	1:B:366:ARG:HH12	2.08	0.67
1:B:529:LEU:C	1:B:529:LEU:HD23	2.13	0.67
1:C:596:ALA:HA	1:C:602:LYS:CB	2.23	0.67
1:D:609:TYR:O	1:D:613:ARG:HB2	1.95	0.67
1:A:494:VAL:HG12	1:A:494:VAL:O	1.95	0.67
1:D:582:ILE:HD11	1:D:584:ARG:HB3	1.75	0.66
1:B:400:ASP:HB3	1:B:403:ASP:CB	2.24	0.66
1:B:514:THR:HG21	1:B:545:PHE:CZ	2.29	0.66
1:B:46:ASN:C	1:B:48:ASP:H	1.98	0.66
1:D:359:GLU:HG2	1:D:364:THR:HG22	1.75	0.66
1:B:582:ILE:HD11	1:B:584:ARG:HB3	1.78	0.66
1:B:579:LEU:HD21	1:B:591:LEU:HD23	1.77	0.66
1:A:507:LEU:HD11	3:A:970:HOH:O	1.95	0.66
1:A:533:LEU:HD23	1:A:538:MET:HE3	1.78	0.66
1:D:334:LEU:HD21	1:D:441:ALA:HA	1.76	0.66
1:B:509:LEU:CD2	1:B:509:LEU:N	2.59	0.66
1:D:224:GLN:OE1	3:D:792:HOH:O	2.14	0.66
1:D:509:LEU:CG	1:D:510:GLU:N	2.43	0.66
1:A:46:ASN:C	1:A:48:ASP:H	1.96	0.66
1:C:334:LEU:HD22	1:C:441:ALA:HA	1.77	0.66
1:D:143:THR:HB	1:D:144:GLU:OE2	1.96	0.66
1:D:200:LEU:O	1:D:218:TYR:OH	2.13	0.66
1:D:46:ASN:C	1:D:48:ASP:H	1.98	0.66
1:D:368:VAL:HA	1:D:371:GLN:HG3	1.77	0.66
1:B:540:ASN:OD1	1:B:541:LEU:N	2.29	0.65
1:C:586:LYS:CG	1:C:586:LYS:O	2.44	0.65
1:D:503:VAL:H	1:D:506:GLU:CB	2.09	0.65
1:C:503:VAL:C	1:C:504:THR:CG2	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:VAL:O	1:D:415:LEU:HG	1.96	0.65
1:A:301:ASN:HB2	1:A:304:LEU:O	1.96	0.65
1:A:586:LYS:O	1:A:586:LYS:CG	2.39	0.65
1:B:272:LYS:HG3	1:B:361:VAL:HG12	1.78	0.65
1:B:455:LYS:O	1:B:460:ASP:HB2	1.95	0.65
1:B:529:LEU:HD23	1:B:530:PRO:CD	2.27	0.65
1:D:381:GLU:O	1:D:385:LEU:HB2	1.95	0.65
1:B:358:MET:HE3	1:B:366:ARG:HH12	1.61	0.65
1:C:359:GLU:HG2	1:C:364:THR:HG22	1.78	0.65
1:B:539:VAL:O	1:B:541:LEU:N	2.30	0.65
1:C:272:LYS:HG3	1:C:361:VAL:HG12	1.79	0.65
1:A:500:ASN:HD22	1:A:500:ASN:H	1.45	0.65
1:B:489:SER:HB3	1:B:492:PHE:HB2	1.78	0.65
1:D:504:THR:N	1:D:506:GLU:CG	2.49	0.65
1:D:595:LEU:HD21	1:D:604:TRP:CE3	2.31	0.65
1:A:66:LYS:HB2	1:A:144:GLU:HB3	1.79	0.65
1:B:502:LEU:HD11	1:B:507:LEU:HB2	1.78	0.65
1:B:543:LYS:O	1:B:543:LYS:CD	2.44	0.65
1:C:514:THR:HG21	1:C:545:PHE:CZ	2.32	0.65
1:D:358:MET:CE	1:D:366:ARG:HH12	2.10	0.65
1:C:311:VAL:HG11	1:C:321:LEU:CD2	2.27	0.65
1:D:169:ASN:ND2	1:D:231:ILE:O	2.30	0.65
1:D:506:GLU:O	1:D:507:LEU:CB	2.35	0.65
1:B:507:LEU:C	1:B:507:LEU:HD23	2.18	0.64
1:A:144:GLU:N	1:A:144:GLU:OE2	2.30	0.64
1:A:198:LYS:O	1:A:199:ASP:CB	2.46	0.64
1:C:226:ILE:HD12	1:C:230:LEU:HB2	1.78	0.64
1:C:97:ARG:HD3	1:C:99:MET:HE3	1.80	0.64
1:A:568:TYR:C	1:A:570:GLU:H	2.00	0.64
1:A:52:ALA:O	1:A:188:VAL:HG12	1.97	0.64
1:D:209:GLU:HB3	3:D:768:HOH:O	1.96	0.64
1:D:579:LEU:HD21	1:D:591:LEU:HD23	1.79	0.64
1:A:57:LEU:HB3	1:A:59:LEU:CD2	2.28	0.64
1:A:534:ASP:OD1	3:A:1001:HOH:O	2.15	0.64
1:B:308:THR:O	1:B:311:VAL:HG22	1.98	0.64
1:D:457:ASN:O	1:D:461:LYS:HE2	1.98	0.64
1:A:359:GLU:HG2	1:A:364:THR:HG22	1.80	0.64
1:B:359:GLU:CG	1:B:364:THR:HG22	2.28	0.64
1:B:525:PHE:HD1	1:B:526:ILE:HG22	1.61	0.64
1:D:334:LEU:HD22	1:D:441:ALA:HA	1.78	0.64
1:A:514:THR:HG21	1:A:545:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:HD21	1:B:441:ALA:HA	1.78	0.63
1:A:102:ASN:HD21	1:A:106:GLN:HB2	1.62	0.63
1:A:598:ASN:HB3	1:A:601:SER:HB3	1.80	0.63
1:B:369:MET:SD	1:B:520:HIS:HB2	2.38	0.63
1:A:381:GLU:O	1:A:385:LEU:HB2	1.97	0.63
1:A:206:ALA:HA	1:A:222:MET:HE3	1.80	0.63
1:A:334:LEU:HD22	1:A:441:ALA:HA	1.78	0.63
1:B:494:VAL:HG12	1:B:494:VAL:O	1.96	0.63
1:A:369:MET:SD	1:A:520:HIS:HB2	2.39	0.63
1:B:129:THR:HG23	1:B:133:ALA:CB	2.29	0.63
1:B:159:GLY:O	1:B:160:LYS:HB2	1.99	0.63
1:B:311:VAL:HG11	1:B:321:LEU:CD2	2.29	0.63
1:B:378:LEU:O	1:B:382:ILE:HG12	1.99	0.63
1:D:144:GLU:N	1:D:144:GLU:OE2	2.30	0.63
1:B:392:LEU:HD23	1:B:475:ILE:HG22	1.81	0.62
1:B:492:PHE:CE1	1:B:520:HIS:O	2.51	0.62
1:C:183:THR:HG22	1:C:185:SER:N	2.05	0.62
1:C:40:ASP:O	1:C:43:THR:HG22	2.00	0.62
1:A:334:LEU:HD23	1:A:442:PHE:H	1.63	0.62
1:A:342:ASP:OD2	3:A:977:HOH:O	2.15	0.62
1:D:359:GLU:CG	1:D:364:THR:HG22	2.29	0.62
1:D:57:LEU:HB3	1:D:59:LEU:HD22	1.81	0.62
1:A:538:MET:HG2	1:A:568:TYR:CD2	2.33	0.62
1:B:52:ALA:O	1:B:188:VAL:HG12	1.99	0.62
1:C:369:MET:SD	1:C:520:HIS:HB2	2.39	0.62
1:D:183:THR:HG22	1:D:185:SER:N	2.04	0.62
1:D:43:THR:OG1	1:D:45:ALA:HB3	1.99	0.62
1:B:586:LYS:O	1:B:586:LYS:CG	2.43	0.62
1:C:40:ASP:OD1	1:C:41:ALA:O	2.17	0.62
1:C:503:VAL:HB	1:C:506:GLU:OE1	1.99	0.62
1:A:90:THR:OG1	1:A:93:LEU:HD22	1.99	0.62
1:B:206:ALA:HB1	1:B:221:SER:C	2.20	0.62
1:B:168:GLN:HE22	1:B:299:MET:CG	2.12	0.62
1:C:543:LYS:O	1:C:543:LYS:CD	2.48	0.62
1:C:57:LEU:HD12	1:C:59:LEU:HD21	1.81	0.62
1:D:503:VAL:N	1:D:506:GLU:HB2	2.14	0.62
1:C:102:ASN:HD21	1:C:106:GLN:HB2	1.65	0.62
1:C:311:VAL:HG11	1:C:321:LEU:HD23	1.81	0.62
1:C:419:TYR:CD1	3:C:976:HOH:O	2.53	0.62
1:D:503:VAL:C	1:D:504:THR:CG2	2.54	0.62
1:A:276:MET:CE	1:A:356:ARG:HB3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LEU:HD21	1:A:591:LEU:HD23	1.82	0.62
1:B:368:VAL:HG12	1:B:368:VAL:O	1.99	0.62
1:C:277:TYR:OH	1:C:356:ARG:HG3	2.00	0.62
1:C:502:LEU:HD12	1:C:506:GLU:HB3	1.81	0.62
1:A:361:VAL:CG2	1:A:362:PHE:CD1	2.83	0.62
1:D:514:THR:HG21	1:D:545:PHE:CZ	2.35	0.62
1:A:334:LEU:CD2	1:A:442:PHE:H	2.13	0.61
1:B:518:THR:O	1:B:522:TRP:HD1	1.83	0.61
1:D:494:VAL:O	1:D:494:VAL:CG1	2.48	0.61
1:A:609:TYR:O	1:A:613:ARG:HB2	2.00	0.61
1:C:359:GLU:CG	1:C:364:THR:HG22	2.30	0.61
1:D:308:THR:O	1:D:311:VAL:HG22	2.00	0.61
1:C:55:VAL:HG12	1:C:57:LEU:HD22	1.81	0.61
1:C:200:LEU:O	1:C:218:TYR:OH	2.16	0.61
1:A:297:GLY:O	1:A:308:THR:HG22	2.00	0.61
1:A:494:VAL:O	1:A:498:GLN:HG3	2.01	0.61
1:D:596:ALA:HB1	1:D:602:LYS:HG3	1.81	0.61
1:B:184:PRO:HB2	1:B:337:ASN:O	2.01	0.61
1:C:596:ALA:HB1	1:C:602:LYS:HG3	1.82	0.61
1:D:327:ALA:HB3	1:D:350:THR:HG23	1.83	0.61
1:C:174:ALA:HB3	1:C:182:ASP:OD1	2.01	0.61
1:B:499:ILE:O	1:B:501:GLN:N	2.34	0.61
1:D:596:ALA:HA	1:D:602:LYS:CB	2.31	0.61
1:A:352:TYR:CZ	1:A:429:PHE:HE2	2.19	0.61
1:C:42:TYR:HA	1:C:121:LEU:CD2	2.30	0.61
1:C:411:VAL:O	1:C:415:LEU:HG	2.00	0.61
1:D:334:LEU:CD2	1:D:442:PHE:H	2.14	0.61
1:D:503:VAL:O	1:D:504:THR:CB	2.46	0.61
1:A:334:LEU:HD21	1:A:441:ALA:HA	1.83	0.60
1:D:301:ASN:HB2	1:D:304:LEU:O	2.01	0.60
1:A:426:ARG:O	1:A:430:ASP:HB2	2.00	0.60
1:C:243:MET:HG2	1:C:260:VAL:HG13	1.83	0.60
1:C:308:THR:O	1:C:311:VAL:HG22	2.01	0.60
1:C:324:HIS:CE1	1:C:350:THR:HG22	2.36	0.60
1:C:503:VAL:O	1:C:504:THR:CB	2.49	0.60
1:C:464:ASN:ND2	1:D:241:LYS:HB3	2.15	0.60
1:A:595:LEU:HD21	1:A:604:TRP:CE3	2.36	0.60
1:A:567:ASP:HB3	1:A:569:LYS:NZ	2.15	0.60
1:D:271:ASP:O	1:D:275:GLN:HG3	2.01	0.60
1:C:358:MET:HE3	1:C:366:ARG:HH12	1.65	0.60
1:C:373:LEU:HD13	1:C:492:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:VAL:N	1:D:506:GLU:HG3	2.16	0.60
1:A:180:ILE:HG12	1:A:181:GLN:H	1.66	0.60
1:A:457:ASN:O	1:A:461:LYS:HE2	2.02	0.60
1:C:464:ASN:HD21	1:D:241:LYS:HD3	1.67	0.60
1:A:168:GLN:O	1:A:168:GLN:CG	2.34	0.60
1:A:536:GLN:CA	1:A:536:GLN:OE1	2.49	0.60
1:B:284:ARG:HD3	1:B:286:ASP:OD2	2.00	0.60
1:D:303:ARG:NH1	3:D:974:HOH:O	2.33	0.60
1:D:40:ASP:OD1	1:D:41:ALA:O	2.20	0.60
1:D:582:ILE:HG13	1:D:584:ARG:H	1.67	0.60
1:D:569:LYS:HD2	1:D:570:GLU:H	1.67	0.60
1:D:97:ARG:HD3	1:D:99:MET:HE2	1.83	0.60
1:A:290:LEU:HD21	1:A:306:PHE:CD2	2.37	0.59
1:A:489:SER:HB3	1:A:492:PHE:HB2	1.83	0.59
1:B:492:PHE:O	1:B:495:ILE:HB	2.02	0.59
1:C:522:TRP:O	1:C:526:ILE:CG1	2.39	0.59
1:C:283:GLY:HA2	3:C:988:HOH:O	2.02	0.59
1:D:129:THR:HG23	1:D:133:ALA:CB	2.32	0.59
1:D:159:GLY:O	1:D:160:LYS:HB2	2.02	0.59
1:A:368:VAL:HA	1:A:371:GLN:CG	2.26	0.59
1:C:169:ASN:ND2	1:C:231:ILE:O	2.36	0.59
1:C:43:THR:OG1	1:C:45:ALA:HB3	2.01	0.59
1:C:391:GLN:OE1	1:C:476:PHE:O	2.19	0.59
1:C:578:TYR:OH	1:C:587:LEU:HG	2.03	0.59
1:A:54:HIS:CE1	1:A:191:THR:HG23	2.38	0.59
1:C:276:MET:CE	1:C:356:ARG:HB3	2.32	0.59
1:D:42:TYR:HA	1:D:121:LEU:CD2	2.33	0.59
1:A:42:TYR:HA	1:A:121:LEU:CD2	2.32	0.59
1:B:494:VAL:CG1	1:B:494:VAL:O	2.49	0.59
1:C:421:GLU:OE1	1:C:426:ARG:HD3	2.03	0.59
1:D:199:ASP:O	1:D:200:LEU:HD12	2.03	0.59
1:A:543:LYS:HD2	1:A:543:LYS:O	2.03	0.59
1:D:598:ASN:HB3	1:D:601:SER:HB3	1.83	0.59
1:D:90:THR:OG1	1:D:93:LEU:HD22	2.02	0.59
1:D:55:VAL:HG22	1:D:74:LEU:HD13	1.84	0.59
1:A:501:GLN:HG2	1:A:508:THR:CG2	2.33	0.59
1:B:42:TYR:HA	1:B:121:LEU:CD2	2.33	0.59
1:B:605:ALA:CB	1:B:628:LEU:HD11	2.33	0.59
1:C:205:SER:O	1:C:222:MET:HE3	2.03	0.59
1:C:288:LEU:HB2	1:C:304:LEU:HD11	1.85	0.59
1:A:288:LEU:HB2	1:A:304:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:CD2	1:B:442:PHE:H	2.16	0.59
1:B:54:HIS:CE1	1:B:191:THR:HG23	2.37	0.59
1:A:169:ASN:ND2	1:A:231:ILE:O	2.36	0.58
1:A:582:ILE:HD11	1:A:584:ARG:HB3	1.85	0.58
1:C:457:ASN:O	1:C:461:LYS:HE2	2.03	0.58
1:C:494:VAL:CG1	1:C:494:VAL:O	2.50	0.58
1:C:582:ILE:HG13	1:C:584:ARG:H	1.68	0.58
1:B:492:PHE:HE1	1:B:520:HIS:O	1.86	0.58
1:D:364:THR:O	1:D:368:VAL:HG13	2.03	0.58
1:B:503:VAL:HG23	1:B:506:GLU:CB	2.33	0.58
1:C:168:GLN:O	1:C:168:GLN:CG	2.44	0.58
1:C:276:MET:HE3	1:C:356:ARG:HB3	1.86	0.58
1:D:249:ILE:HD12	1:D:260:VAL:HG22	1.85	0.58
1:B:500:ASN:C	1:B:502:LEU:H	2.06	0.58
1:D:38:LEU:HB2	1:D:39:THR:HG22	1.84	0.58
1:C:368:VAL:HA	1:C:371:GLN:CG	2.27	0.58
1:D:494:VAL:O	1:D:494:VAL:HG12	1.98	0.58
1:B:57:LEU:HD12	1:B:59:LEU:HD21	1.85	0.58
1:D:503:VAL:H	1:D:506:GLU:HB2	1.67	0.58
1:A:536:GLN:O	1:A:536:GLN:OE1	2.22	0.58
1:B:461:LYS:HE3	1:B:462:TYR:CE2	2.39	0.58
1:C:370:GLU:HG2	1:C:520:HIS:CD2	2.39	0.58
1:D:361:VAL:CG2	1:D:362:PHE:CD1	2.84	0.58
1:A:359:GLU:CG	1:A:364:THR:HG22	2.34	0.58
1:A:364:THR:O	1:A:368:VAL:HG13	2.04	0.58
1:B:335:VAL:HG13	1:B:440:HIS:HB3	1.84	0.58
1:B:42:TYR:CZ	1:B:399:ARG:O	2.55	0.58
1:B:43:THR:OG1	1:B:45:ALA:HB3	2.04	0.58
1:C:274:GLU:HG2	1:C:279:LYS:HA	1.86	0.58
1:C:373:LEU:HD13	1:C:492:PHE:CE2	2.39	0.58
1:D:180:ILE:HG12	1:D:181:GLN:H	1.67	0.58
1:C:254:TYR:CE2	1:C:255:ILE:HB	2.39	0.58
1:C:481:PRO:HD2	1:C:484:ALA:HB2	1.86	0.58
1:D:276:MET:CE	1:D:356:ARG:HB3	2.33	0.58
1:D:488:THR:O	1:D:488:THR:HG22	2.04	0.58
1:B:276:MET:CE	1:B:356:ARG:HB3	2.34	0.57
1:C:368:VAL:HG12	1:C:371:GLN:NE2	2.18	0.57
1:C:97:ARG:NH1	1:C:99:MET:CE	2.66	0.57
1:D:174:ALA:HB3	1:D:182:ASP:OD1	2.04	0.57
1:D:584:ARG:HD3	1:D:587:LEU:HD22	1.86	0.57
1:B:174:ALA:HB3	1:B:182:ASP:OD1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:VAL:HG13	1:B:368:VAL:O	2.01	0.57
1:C:334:LEU:HD21	1:C:441:ALA:HA	1.85	0.57
1:C:507:LEU:CD2	1:C:508:THR:HG22	2.34	0.57
1:B:168:GLN:O	1:B:168:GLN:CG	2.44	0.57
1:C:284:ARG:HD3	1:C:286:ASP:OD2	2.03	0.57
1:C:378:LEU:O	1:C:382:ILE:HG12	2.05	0.57
1:D:596:ALA:HA	1:D:602:LYS:HB2	1.86	0.57
1:B:514:THR:C	1:B:516:GLN:H	2.08	0.57
1:A:277:TYR:OH	1:A:356:ARG:HG3	2.05	0.57
1:A:582:ILE:HG13	1:A:584:ARG:H	1.68	0.57
1:C:492:PHE:CD2	1:C:524:HIS:CD2	2.93	0.57
1:D:335:VAL:HG13	1:D:440:HIS:HB3	1.85	0.57
1:B:90:THR:OG1	1:B:93:LEU:HD22	2.05	0.57
1:C:594:GLU:HA	1:C:597:LYS:HD3	1.87	0.57
1:A:341:ARG:HH11	1:A:395:ASP:HA	1.70	0.57
1:A:55:VAL:HG22	1:A:74:LEU:HD13	1.87	0.57
1:B:332:GLY:HA2	1:B:346:ASN:OD1	2.05	0.57
1:D:222:MET:HA	1:D:222:MET:HE2	1.87	0.57
1:D:334:LEU:HD23	1:D:442:PHE:H	1.70	0.57
1:A:337:ASN:H	1:A:337:ASN:ND2	2.02	0.57
1:A:421:GLU:OE1	1:A:426:ARG:HD3	2.05	0.57
1:C:392:LEU:HD23	1:C:475:ILE:HG22	1.86	0.57
1:D:152:LEU:HD13	1:D:291:PRO:HG3	1.86	0.57
1:D:392:LEU:HD23	1:D:475:ILE:HG22	1.86	0.57
1:D:512:LEU:HB3	1:D:513:PRO:CD	2.35	0.57
1:D:55:VAL:HG12	1:D:57:LEU:HD22	1.85	0.57
1:A:568:TYR:O	1:A:570:GLU:N	2.38	0.57
1:C:504:THR:O	1:C:505:ASP:HB2	2.05	0.57
1:D:107:TRP:NE1	3:D:706:HOH:O	2.27	0.57
1:D:324:HIS:CE1	1:D:350:THR:HG22	2.39	0.57
1:A:131:LEU:HD12	3:A:1016:HOH:O	2.05	0.56
1:D:97:ARG:HB2	3:D:709:HOH:O	2.04	0.56
1:A:522:TRP:O	1:A:526:ILE:HG13	2.05	0.56
1:B:301:ASN:HB2	1:B:304:LEU:O	2.05	0.56
1:B:499:ILE:C	1:B:501:GLN:H	2.08	0.56
1:C:361:VAL:CG2	1:C:362:PHE:CD1	2.86	0.56
1:D:373:LEU:HD13	1:D:492:PHE:CZ	2.40	0.56
1:A:336:THR:O	1:A:444:SER:HA	2.05	0.56
1:B:290:LEU:HD21	1:B:306:PHE:CD2	2.38	0.56
1:C:199:ASP:O	1:C:200:LEU:HD12	2.05	0.56
1:C:283:GLY:N	3:C:988:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:VAL:HG11	1:D:321:LEU:CD2	2.35	0.56
1:D:503:VAL:N	1:D:506:GLU:CB	2.67	0.56
1:D:57:LEU:HD12	1:D:59:LEU:HD21	1.86	0.56
1:A:159:GLY:O	1:A:160:LYS:HB2	2.04	0.56
1:B:284:ARG:HG3	1:B:285:TYR:N	2.21	0.56
1:C:243:MET:CE	1:C:249:ILE:HG13	2.36	0.56
1:C:373:LEU:O	1:C:377:ASP:OD1	2.24	0.56
1:D:142:SER:OG	3:D:763:HOH:O	2.09	0.56
1:A:206:ALA:HB1	1:A:221:SER:C	2.25	0.56
1:A:499:ILE:CG1	1:A:500:ASN:ND2	2.69	0.56
1:C:512:LEU:HB3	1:C:513:PRO:HD3	1.87	0.56
1:A:201:LEU:HD23	1:A:238:LEU:HB2	1.87	0.56
1:C:54:HIS:CE1	1:C:191:THR:HG23	2.40	0.56
1:C:271:ASP:O	1:C:275:GLN:HG3	2.06	0.56
1:A:40:ASP:OD1	1:A:41:ALA:O	2.23	0.56
1:C:206:ALA:O	1:C:303:ARG:NH1	2.38	0.56
1:C:358:MET:CE	1:C:366:ARG:NH1	2.69	0.56
1:A:97:ARG:HD3	1:A:99:MET:HE3	1.88	0.56
1:B:297:GLY:O	1:B:308:THR:HG22	2.06	0.56
1:C:294:PHE:CD1	1:C:295:PRO:HD2	2.41	0.56
1:B:129:THR:HG23	1:B:133:ALA:HB2	1.88	0.56
1:C:102:ASN:C	1:C:104:GLN:H	2.09	0.56
1:C:55:VAL:HG22	1:C:74:LEU:HD13	1.88	0.56
1:A:594:GLU:HA	1:A:597:LYS:HD3	1.88	0.56
1:C:593:LYS:HE2	1:C:627:VAL:HG11	1.88	0.56
1:D:153:SER:OG	1:D:156:GLN:HG3	2.06	0.56
1:D:332:GLY:HA2	1:D:346:ASN:OD1	2.06	0.56
1:C:245:HIS:HD2	3:C:987:HOH:O	1.89	0.55
1:C:502:LEU:CD1	1:C:506:GLU:CB	2.77	0.55
1:C:90:THR:OG1	1:C:93:LEU:HD22	2.06	0.55
1:D:205:SER:O	1:D:222:MET:HE3	2.05	0.55
1:D:243:MET:HG2	1:D:260:VAL:HG13	1.88	0.55
1:D:274:GLU:HG2	1:D:279:LYS:HA	1.87	0.55
1:D:496:ASP:O	1:D:499:ILE:HG12	2.06	0.55
1:D:502:LEU:CD1	1:D:507:LEU:HB2	2.36	0.55
1:C:358:MET:HE3	1:C:366:ARG:NH1	2.19	0.55
1:D:337:ASN:H	1:D:337:ASN:ND2	2.03	0.55
1:B:206:ALA:HA	1:B:222:MET:HE3	1.86	0.55
1:A:97:ARG:NH1	1:A:99:MET:HE3	2.05	0.55
1:C:512:LEU:HB3	1:C:513:PRO:HD2	1.89	0.55
1:B:169:ASN:ND2	1:B:231:ILE:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:HG12	1:B:181:GLN:H	1.70	0.55
1:B:288:LEU:CB	1:B:304:LEU:HD11	2.37	0.55
1:B:547:LEU:H	1:B:547:LEU:CD1	2.17	0.55
1:C:529:LEU:HD23	1:C:562:LEU:HD21	1.88	0.55
1:D:405:PHE:HA	3:D:750:HOH:O	2.07	0.55
1:A:494:VAL:O	1:A:494:VAL:CG1	2.48	0.55
1:B:311:VAL:HG11	1:B:321:LEU:HD23	1.89	0.55
1:B:542:ASP:O	1:B:546:ASP:HA	2.07	0.55
1:C:129:THR:HG23	1:C:133:ALA:CB	2.36	0.55
1:C:65:LYS:O	1:C:144:GLU:OE1	2.25	0.55
1:D:52:ALA:O	1:D:188:VAL:HG12	2.07	0.55
1:D:199:ASP:C	1:D:200:LEU:HD12	2.27	0.55
1:D:557:HIS:HE1	1:D:590:PRO:HG2	1.71	0.55
1:B:324:HIS:CE1	1:B:350:THR:HG22	2.42	0.55
1:B:494:VAL:O	1:B:498:GLN:HG3	2.07	0.55
1:B:543:LYS:O	1:B:543:LYS:HD2	2.06	0.55
1:C:334:LEU:CD2	1:C:442:PHE:H	2.20	0.55
1:D:503:VAL:N	1:D:506:GLU:CG	2.70	0.55
1:D:284:ARG:HG3	1:D:285:TYR:N	2.21	0.55
1:D:492:PHE:O	1:D:495:ILE:HB	2.06	0.55
1:A:288:LEU:CB	1:A:304:LEU:HD11	2.36	0.55
1:B:503:VAL:CG2	1:B:506:GLU:CG	2.59	0.55
1:B:507:LEU:CD2	1:B:507:LEU:C	2.75	0.55
1:C:162:LYS:HE3	1:C:199:ASP:HB3	1.88	0.55
1:C:572:TYR:N	1:C:573:PRO:HD2	2.22	0.55
1:A:347:GLU:OE1	1:A:347:GLU:CA	2.55	0.54
1:A:373:LEU:HD13	1:A:492:PHE:CZ	2.42	0.54
1:A:55:VAL:HG12	1:A:57:LEU:HD22	1.89	0.54
1:D:578:TYR:OH	1:D:587:LEU:HG	2.08	0.54
1:D:596:ALA:CB	1:D:602:LYS:HG3	2.38	0.54
1:B:288:LEU:HB2	1:B:304:LEU:HD11	1.89	0.54
1:B:509:LEU:CD2	1:B:511:GLN:HB2	2.36	0.54
1:C:461:LYS:HE3	1:C:462:TYR:CE2	2.42	0.54
1:D:254:TYR:CE2	1:D:255:ILE:HB	2.42	0.54
1:D:560:TYR:HB3	1:D:575:MET:CE	2.37	0.54
1:A:276:MET:HE3	1:A:356:ARG:HB3	1.88	0.54
1:A:605:ALA:O	1:A:608:VAL:HG22	2.06	0.54
1:B:226:ILE:HD12	1:B:230:LEU:HB2	1.89	0.54
1:D:543:LYS:CD	1:D:543:LYS:O	2.56	0.54
1:A:46:ASN:C	1:A:48:ASP:N	2.60	0.54
1:C:496:ASP:O	1:C:499:ILE:HG12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLN:O	1:D:108:VAL:HG13	2.07	0.54
1:D:328:HIS:HE1	1:D:347:GLU:OE1	1.91	0.54
1:D:542:ASP:O	1:D:546:ASP:HA	2.08	0.54
1:A:358:MET:CE	1:A:366:ARG:HH12	2.20	0.54
1:D:290:LEU:HD21	1:D:306:PHE:CD2	2.40	0.54
1:B:347:GLU:HB3	1:B:410:TYR:CD2	2.41	0.54
1:C:42:TYR:OH	1:C:399:ARG:O	2.17	0.54
1:D:494:VAL:O	1:D:498:GLN:HG3	2.06	0.54
1:A:523:LEU:O	1:A:527:ASN:CG	2.44	0.54
1:A:540:ASN:O	1:A:544:ALA:CB	2.56	0.54
1:A:578:TYR:OH	1:A:587:LEU:HG	2.07	0.54
1:B:501:GLN:O	1:B:502:LEU:HB2	2.08	0.54
1:B:509:LEU:N	1:B:509:LEU:HD23	2.22	0.54
1:B:584:ARG:HD3	1:B:587:LEU:HD22	1.90	0.54
1:C:243:MET:HE2	1:C:249:ILE:HG13	1.90	0.54
1:D:358:MET:HE3	1:D:366:ARG:HH12	1.73	0.54
1:B:344:TRP:HH2	1:B:450:PHE:CE2	2.25	0.54
1:C:265:ASP:O	1:C:268:ALA:HB3	2.08	0.54
1:C:488:THR:O	1:C:488:THR:HG22	2.07	0.54
1:C:542:ASP:O	1:C:546:ASP:HA	2.08	0.54
1:C:494:VAL:O	1:C:498:GLN:HG3	2.06	0.54
1:C:585:ARG:O	1:C:587:LEU:N	2.38	0.54
1:D:524:HIS:O	1:D:528:ASN:HB2	2.07	0.54
1:A:531:VAL:O	1:A:531:VAL:HG12	2.08	0.53
1:A:57:LEU:HD12	1:A:59:LEU:HD21	1.90	0.53
1:B:582:ILE:HD11	1:B:587:LEU:HD23	1.90	0.53
1:C:341:ARG:HH11	1:C:395:ASP:HA	1.73	0.53
1:C:99:MET:HE1	1:C:109:LYS:HB2	1.89	0.53
1:A:533:LEU:O	1:A:536:GLN:HB2	2.08	0.53
1:B:421:GLU:OE1	1:B:426:ARG:HD3	2.08	0.53
1:B:334:LEU:HD23	1:B:442:PHE:H	1.73	0.53
1:C:206:ALA:HB1	1:C:221:SER:C	2.29	0.53
1:C:46:ASN:C	1:C:48:ASP:N	2.60	0.53
1:B:131:LEU:HD12	3:B:805:HOH:O	2.08	0.53
1:B:243:MET:HG2	1:B:260:VAL:HG13	1.90	0.53
1:C:595:LEU:HD21	1:C:604:TRP:CE3	2.42	0.53
1:D:596:ALA:HA	1:D:602:LYS:HA	1.91	0.53
1:A:308:THR:O	1:A:311:VAL:HG22	2.09	0.53
1:A:481:PRO:HD2	1:A:484:ALA:HB2	1.90	0.53
1:A:503:VAL:N	1:A:506:GLU:HB3	2.21	0.53
1:B:91:ARG:NH2	1:B:175:ARG:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:VAL:HG12	1:C:371:GLN:HE21	1.73	0.53
1:C:512:LEU:CB	1:C:513:PRO:CD	2.78	0.53
1:D:284:ARG:HD3	1:D:286:ASP:OD2	2.09	0.53
1:D:284:ARG:NH1	1:D:286:ASP:OD1	2.35	0.53
1:C:152:LEU:HD13	1:C:291:PRO:HG3	1.90	0.53
1:C:300:GLU:O	1:C:300:GLU:HG2	2.08	0.53
1:C:498:GLN:HB3	1:C:512:LEU:CD2	2.39	0.53
1:A:368:VAL:CA	1:A:371:GLN:HG3	2.30	0.53
1:B:201:LEU:HD23	1:B:238:LEU:HB2	1.90	0.53
1:B:378:LEU:HD21	1:B:480:LEU:HD21	1.91	0.53
1:D:288:LEU:HB2	1:D:304:LEU:HD11	1.90	0.53
1:D:421:GLU:OE1	1:D:426:ARG:HD3	2.08	0.53
1:A:347:GLU:HA	1:A:347:GLU:OE1	2.08	0.53
1:A:405:PHE:HA	3:A:719:HOH:O	2.08	0.53
1:B:373:LEU:O	1:B:377:ASP:OD1	2.27	0.53
1:C:284:ARG:HG3	1:C:285:TYR:N	2.23	0.53
1:C:344:TRP:HH2	1:C:450:PHE:CE2	2.27	0.53
1:D:226:ILE:HD12	1:D:230:LEU:HB2	1.91	0.53
1:A:263:PHE:CD1	1:A:322:ILE:HG13	2.43	0.53
1:A:596:ALA:HA	1:A:602:LYS:CB	2.38	0.53
1:B:311:VAL:HG11	1:B:321:LEU:HD22	1.91	0.53
1:B:361:VAL:CG2	1:B:362:PHE:CD1	2.90	0.53
1:B:42:TYR:CD2	1:B:121:LEU:HD21	2.43	0.53
1:B:46:ASN:C	1:B:48:ASP:N	2.61	0.53
1:B:573:PRO:O	1:B:576:ALA:HB3	2.09	0.53
1:C:222:MET:HA	1:C:222:MET:HE2	1.91	0.53
1:C:369:MET:HG3	1:C:492:PHE:CE1	2.44	0.53
1:D:184:PRO:HG3	1:D:340:TRP:CZ2	2.43	0.53
1:D:358:MET:CE	1:D:366:ARG:NH1	2.72	0.53
1:D:560:TYR:HB3	1:D:575:MET:HE2	1.91	0.53
1:A:533:LEU:O	1:A:536:GLN:CB	2.57	0.53
1:B:298:GLY:C	1:B:325:GLU:OE2	2.47	0.53
1:A:485:PRO:HA	3:A:951:HOH:O	2.09	0.53
1:A:542:ASP:O	1:A:546:ASP:N	2.42	0.53
1:B:224:GLN:NE2	1:B:281:ARG:O	2.42	0.53
1:B:318:LEU:HD21	1:B:552:ASN:ND2	2.23	0.53
1:C:180:ILE:HG12	1:C:181:GLN:N	2.23	0.53
1:C:335:VAL:HG13	1:C:440:HIS:HB3	1.90	0.53
1:D:224:GLN:NE2	1:D:281:ARG:O	2.41	0.53
1:B:103:SER:N	3:B:795:HOH:O	2.22	0.52
1:A:324:HIS:CE1	1:A:350:THR:HG22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HE3	1:A:462:TYR:CE2	2.44	0.52
1:B:277:TYR:OH	1:B:356:ARG:HG3	2.09	0.52
1:B:524:HIS:O	1:B:525:PHE:C	2.45	0.52
1:C:239:GLU:HB2	1:C:256:LEU:HD22	1.91	0.52
1:A:284:ARG:HG3	1:A:285:TYR:N	2.24	0.52
1:B:542:ASP:HB2	1:B:559:TRP:HZ2	1.74	0.52
1:C:557:HIS:HE1	1:C:590:PRO:HG2	1.74	0.52
1:A:327:ALA:HB3	1:A:350:THR:HG23	1.91	0.52
1:B:249:ILE:HD12	1:B:260:VAL:HG22	1.90	0.52
1:B:254:TYR:CG	1:B:255:ILE:N	2.77	0.52
1:B:591:LEU:O	1:B:595:LEU:HB2	2.09	0.52
1:C:159:GLY:O	1:C:160:LYS:HB2	2.08	0.52
1:D:277:TYR:CE1	1:D:353:VAL:HG22	2.45	0.52
1:A:332:GLY:C	1:A:336:THR:HG22	2.30	0.52
1:A:43:THR:OG1	1:A:45:ALA:HB3	2.10	0.52
1:B:274:GLU:HG2	1:B:279:LYS:HA	1.92	0.52
1:B:457:ASN:O	1:B:461:LYS:HE2	2.09	0.52
1:C:310:THR:HG21	1:C:582:ILE:HD12	1.91	0.52
1:D:129:THR:HG23	1:D:133:ALA:HB3	1.90	0.52
1:D:582:ILE:HD11	1:D:587:LEU:HD23	1.90	0.52
1:A:512:LEU:HB3	1:A:513:PRO:CD	2.40	0.52
1:B:295:PRO:HD3	1:B:617:HIS:HB2	1.91	0.52
1:B:332:GLY:C	1:B:336:THR:HG22	2.29	0.52
1:C:386:ASP:O	1:C:388:SER:N	2.38	0.52
1:C:378:LEU:HD21	1:C:480:LEU:HD21	1.90	0.52
1:C:557:HIS:CE1	1:C:590:PRO:HG2	2.45	0.52
1:C:582:ILE:HD11	1:C:587:LEU:HD23	1.90	0.52
1:D:168:GLN:CG	1:D:168:GLN:O	2.38	0.52
1:D:214:ARG:NH1	3:D:705:HOH:O	2.41	0.52
1:D:280:TYR:HH	1:D:285:TYR:HD1	1.56	0.52
1:A:337:ASN:HD22	1:A:337:ASN:H	1.58	0.52
1:B:373:LEU:HD13	1:B:492:PHE:HZ	1.69	0.52
1:B:336:THR:O	1:B:444:SER:HA	2.10	0.52
1:C:101:LYS:HD2	1:C:107:TRP:CZ2	2.45	0.52
1:C:463:PRO:O	1:C:464:ASN:HB2	2.08	0.52
1:D:341:ARG:HH11	1:D:395:ASP:HA	1.75	0.52
1:D:97:ARG:HH11	1:D:99:MET:CE	2.23	0.52
1:A:596:ALA:HB1	1:A:602:LYS:HG3	1.92	0.52
1:B:598:ASN:HB3	1:B:601:SER:HB3	1.91	0.52
1:A:206:ALA:HA	1:A:222:MET:CE	2.40	0.52
1:A:205:SER:OG	1:A:301:ASN:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ARG:O	1:B:430:ASP:HB2	2.09	0.52
1:B:459:THR:HG21	1:B:471:ILE:HD11	1.92	0.52
1:D:294:PHE:HE2	1:D:298:GLY:HA2	1.75	0.52
1:D:300:GLU:HG2	1:D:300:GLU:O	2.10	0.52
1:D:326:LEU:HD22	1:D:330:TRP:HZ3	1.74	0.52
1:D:467:SER:O	1:D:469:ASN:N	2.43	0.52
1:D:527:ASN:OD1	1:D:558:ALA:HB1	2.09	0.52
1:A:271:ASP:O	1:A:275:GLN:HG3	2.09	0.51
1:A:326:LEU:HD22	1:A:330:TRP:HZ3	1.75	0.51
1:B:596:ALA:HA	1:B:602:LYS:CB	2.40	0.51
1:C:90:THR:HG23	1:C:91:ARG:N	2.24	0.51
1:A:226:ILE:HD12	1:A:230:LEU:HB2	1.91	0.51
1:A:168:GLN:HE22	1:A:299:MET:CG	2.22	0.51
1:A:496:ASP:O	1:A:499:ILE:HG12	2.09	0.51
1:A:540:ASN:O	1:A:544:ALA:HB3	2.10	0.51
1:B:557:HIS:HE1	1:B:590:PRO:HG2	1.76	0.51
1:C:180:ILE:CG1	1:C:181:GLN:H	2.22	0.51
1:D:378:LEU:HD13	1:D:411:VAL:HB	1.92	0.51
1:D:514:THR:C	1:D:516:GLN:H	2.13	0.51
1:C:168:GLN:NE2	1:C:299:MET:CG	2.73	0.51
1:C:519:LEU:HD13	1:C:519:LEU:C	2.29	0.51
1:D:46:ASN:C	1:D:48:ASP:N	2.59	0.51
1:D:504:THR:C	1:D:506:GLU:HG2	2.30	0.51
1:A:277:TYR:CE1	1:A:353:VAL:HG22	2.46	0.51
1:B:55:VAL:HG22	1:B:74:LEU:HD13	1.92	0.51
1:C:327:ALA:HB3	1:C:350:THR:HG23	1.92	0.51
1:D:295:PRO:HG2	1:D:296:PHE:CD1	2.36	0.51
1:A:311:VAL:HG11	1:A:321:LEU:CD2	2.41	0.51
1:C:560:TYR:HB3	1:C:575:MET:CE	2.41	0.51
1:D:344:TRP:HH2	1:D:450:PHE:CE2	2.29	0.51
1:C:106:GLN:O	1:C:108:VAL:HG13	2.11	0.51
1:C:263:PHE:CD1	1:C:322:ILE:HG13	2.46	0.51
1:C:52:ALA:O	1:C:188:VAL:HG12	2.10	0.51
1:C:596:ALA:HA	1:C:602:LYS:HA	1.93	0.51
1:D:297:GLY:O	1:D:308:THR:HG22	2.11	0.51
1:D:263:PHE:CD1	1:D:322:ILE:HG13	2.46	0.51
1:D:272:LYS:HG3	1:D:361:VAL:HG12	1.91	0.51
1:D:428:ARG:HD3	3:D:956:HOH:O	2.02	0.51
1:D:336:THR:O	1:D:444:SER:HA	2.10	0.51
1:D:40:ASP:HB3	1:D:47:TYR:OH	2.10	0.51
1:D:254:TYR:CG	1:D:255:ILE:N	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ILE:HD12	3:A:724:HOH:O	2.11	0.51
1:B:557:HIS:CE1	1:B:590:PRO:HG2	2.46	0.51
1:C:295:PRO:HG2	1:C:296:PHE:CD1	2.39	0.51
1:D:548:THR:OG1	1:D:571:VAL:HG12	2.11	0.51
1:A:249:ILE:HD12	1:A:260:VAL:HG22	1.93	0.51
1:A:284:ARG:NH1	1:A:286:ASP:OD1	2.40	0.51
1:B:529:LEU:C	1:B:529:LEU:CD2	2.79	0.51
1:C:454:LEU:HD23	1:C:454:LEU:O	2.10	0.51
1:A:392:LEU:HD23	1:A:475:ILE:CG2	2.40	0.51
1:B:529:LEU:HD23	1:B:530:PRO:HD2	1.93	0.51
1:D:373:LEU:O	1:D:377:ASP:OD1	2.28	0.51
1:D:38:LEU:CB	1:D:39:THR:HG22	2.41	0.51
1:D:591:LEU:O	1:D:595:LEU:HB2	2.11	0.51
1:A:159:GLY:C	1:A:161:GLU:H	2.15	0.50
1:C:280:TYR:HH	1:C:285:TYR:HD1	1.58	0.50
1:C:328:HIS:HE1	1:C:347:GLU:OE1	1.94	0.50
1:C:57:LEU:HB3	1:C:59:LEU:HD22	1.94	0.50
1:A:162:LYS:HD3	1:A:200:LEU:CD1	2.41	0.50
1:C:101:LYS:HB3	1:C:101:LYS:HZ3	1.77	0.50
1:C:144:GLU:N	1:C:144:GLU:OE2	2.30	0.50
1:C:336:THR:O	1:C:444:SER:HA	2.10	0.50
1:D:271:ASP:HA	3:D:951:HOH:O	2.10	0.50
1:A:373:LEU:O	1:A:377:ASP:OD1	2.30	0.50
1:A:548:THR:OG1	1:A:571:VAL:HG12	2.11	0.50
1:C:317:SER:OG	1:C:318:LEU:HD22	2.11	0.50
1:C:563:SER:CB	1:C:571:VAL:HG21	2.41	0.50
1:D:277:TYR:CD1	1:D:353:VAL:HG13	2.46	0.50
1:D:428:ARG:HG2	3:D:956:HOH:O	2.11	0.50
1:A:42:TYR:CE2	1:A:401:PRO:CG	2.94	0.50
1:B:205:SER:HB2	1:B:302:PRO:HG2	1.93	0.50
1:C:455:LYS:HA	1:C:459:THR:HB	1.94	0.50
1:D:502:LEU:CD1	1:D:506:GLU:O	2.30	0.50
1:D:605:ALA:CB	1:D:628:LEU:HD11	2.42	0.50
1:A:129:THR:HG23	1:A:133:ALA:CB	2.41	0.50
1:A:148:GLY:CA	1:A:173:HIS:HB3	2.41	0.50
1:A:298:GLY:C	1:A:325:GLU:OE2	2.49	0.50
1:B:153:SER:O	1:B:157:THR:HG23	2.12	0.50
1:B:180:ILE:CG1	1:B:181:GLN:H	2.25	0.50
1:B:378:LEU:HD13	1:B:411:VAL:HB	1.92	0.50
1:B:392:LEU:HD23	1:B:475:ILE:CG2	2.42	0.50
1:C:596:ALA:CB	1:C:602:LYS:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:THR:HA	1:D:367:ALA:HB3	1.94	0.50
1:D:504:THR:O	1:D:506:GLU:OE2	2.30	0.50
1:A:503:VAL:HG23	1:A:506:GLU:HG2	1.93	0.50
1:A:584:ARG:HD3	1:A:587:LEU:HD22	1.93	0.50
1:A:97:ARG:NH1	1:A:99:MET:CE	2.68	0.50
1:B:162:LYS:HD3	1:B:200:LEU:CD1	2.41	0.50
1:C:332:GLY:HA2	1:C:346:ASN:OD1	2.12	0.50
1:A:605:ALA:CB	1:A:628:LEU:HD11	2.42	0.50
1:B:206:ALA:O	1:B:303:ARG:NH1	2.45	0.50
1:B:208:ASN:OD1	1:B:208:ASN:C	2.50	0.50
1:B:397:LYS:HA	3:B:798:HOH:O	2.12	0.50
1:A:129:THR:HG23	1:A:133:ALA:HB3	1.94	0.50
1:A:274:GLU:HG2	1:A:279:LYS:HA	1.94	0.50
1:B:129:THR:HG23	1:B:133:ALA:HB3	1.93	0.50
1:C:129:THR:HG23	1:C:133:ALA:HB2	1.93	0.50
1:C:130:PRO:O	1:C:131:LEU:C	2.48	0.50
1:C:162:LYS:HD3	1:C:200:LEU:CD1	2.41	0.50
1:C:46:ASN:O	1:C:48:ASP:N	2.45	0.50
1:D:102:ASN:C	1:D:104:GLN:H	2.15	0.50
1:D:594:GLU:HA	1:D:597:LYS:HD3	1.94	0.50
1:B:488:THR:HG22	1:B:488:THR:O	2.11	0.50
1:B:57:LEU:HB3	1:B:59:LEU:HD22	1.93	0.50
1:C:143:THR:HB	1:C:144:GLU:OE2	2.11	0.50
1:C:596:ALA:HA	1:C:602:LYS:CA	2.41	0.50
1:D:481:PRO:HD2	1:D:484:ALA:HB2	1.94	0.50
1:B:184:PRO:HG3	1:B:340:TRP:CZ2	2.47	0.49
1:B:294:PHE:CD1	1:B:295:PRO:HD2	2.47	0.49
1:B:500:ASN:HD22	1:B:500:ASN:N	2.10	0.49
1:D:416:PHE:CD1	1:D:416:PHE:O	2.65	0.49
1:D:54:HIS:CE1	1:D:191:THR:HG23	2.47	0.49
1:A:54:HIS:HE1	1:A:191:THR:HG23	1.75	0.49
1:A:514:THR:C	1:A:516:GLN:H	2.15	0.49
1:B:206:ALA:HA	1:B:222:MET:CE	2.42	0.49
1:B:270:ILE:O	1:B:270:ILE:HG22	2.12	0.49
1:C:290:LEU:HD21	1:C:306:PHE:CD2	2.40	0.49
1:D:414:GLN:O	1:D:418:MET:HG3	2.11	0.49
1:D:510:GLU:O	1:D:512:LEU:N	2.37	0.49
1:D:310:THR:HG21	1:D:582:ILE:HD12	1.94	0.49
1:A:498:GLN:C	1:A:500:ASN:N	2.65	0.49
1:B:582:ILE:HG13	1:B:584:ARG:H	1.78	0.49
1:D:326:LEU:O	1:D:326:LEU:CD2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:GLY:C	1:D:336:THR:HG22	2.32	0.49
1:A:239:GLU:HB2	1:A:256:LEU:HD22	1.94	0.49
1:B:503:VAL:O	1:B:504:THR:CG2	2.61	0.49
1:B:578:TYR:OH	1:B:587:LEU:HG	2.11	0.49
1:C:301:ASN:HB2	1:C:304:LEU:O	2.12	0.49
1:C:396:LEU:O	1:C:399:ARG:NE	2.37	0.49
1:C:298:GLY:C	1:C:325:GLU:OE2	2.51	0.49
1:C:584:ARG:HD3	1:C:587:LEU:HD22	1.93	0.49
1:D:180:ILE:CG1	1:D:181:GLN:H	2.25	0.49
1:D:206:ALA:HB1	1:D:221:SER:C	2.32	0.49
1:D:337:ASN:H	1:D:337:ASN:HD22	1.61	0.49
1:D:613:ARG:HB3	1:D:614:PRO:HD3	1.94	0.49
1:C:288:LEU:CB	1:C:304:LEU:HD11	2.43	0.49
1:D:277:TYR:OH	1:D:356:ARG:HG3	2.13	0.49
1:D:428:ARG:CG	3:D:956:HOH:O	2.60	0.49
1:A:538:MET:HG3	1:A:538:MET:O	2.13	0.49
1:A:596:ALA:HA	1:A:602:LYS:HB2	1.94	0.49
1:B:44:TYR:CD2	1:B:124:LYS:HB2	2.48	0.49
1:B:326:LEU:HD22	1:B:330:TRP:HZ3	1.78	0.49
1:B:580:LYS:HA	1:B:612:ALA:CB	2.39	0.49
1:C:153:SER:O	1:C:157:THR:HG23	2.13	0.49
1:A:101:LYS:HZ3	1:A:101:LYS:HB3	1.76	0.49
1:A:284:ARG:HD3	1:A:286:ASP:OD2	2.13	0.49
1:A:57:LEU:HB3	1:A:59:LEU:HD22	1.93	0.49
1:B:276:MET:HE1	1:B:356:ARG:HB3	1.94	0.49
1:C:504:THR:O	1:C:504:THR:OG1	2.30	0.49
1:C:507:LEU:HD23	1:C:508:THR:HG22	1.94	0.49
1:D:321:LEU:O	1:D:324:HIS:HB3	2.13	0.49
1:A:321:LEU:O	1:A:324:HIS:HB3	2.13	0.49
1:C:364:THR:O	1:C:368:VAL:HG13	2.13	0.49
1:D:168:GLN:NE2	1:D:299:MET:CG	2.73	0.49
1:D:463:PRO:O	1:D:464:ASN:HB2	2.13	0.49
1:A:180:ILE:HG12	1:A:181:GLN:N	2.28	0.49
1:A:359:GLU:HG3	1:A:364:THR:HA	1.94	0.49
1:C:152:LEU:HD13	1:C:291:PRO:CG	2.42	0.49
1:C:324:HIS:CE1	1:C:350:THR:CG2	2.95	0.49
1:C:392:LEU:HD23	1:C:475:ILE:CG2	2.42	0.49
1:D:116:LYS:HD3	1:D:117:ARG:N	2.27	0.49
1:D:311:VAL:HG11	1:D:321:LEU:HD22	1.95	0.49
1:D:184:PRO:HB2	1:D:337:ASN:O	2.13	0.49
1:D:426:ARG:O	1:D:430:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:LYS:HE3	1:D:462:TYR:CE2	2.48	0.49
1:D:503:VAL:O	1:D:504:THR:OG1	2.29	0.49
1:A:106:GLN:O	1:A:108:VAL:HG13	2.13	0.48
1:B:605:ALA:HB1	1:B:628:LEU:HD11	1.94	0.48
1:C:54:HIS:HE1	1:C:191:THR:HG23	1.78	0.48
1:D:215:ASP:OD1	1:D:216:GLY:N	2.46	0.48
1:D:609:TYR:O	1:D:609:TYR:CG	2.65	0.48
1:A:254:TYR:CE2	1:A:255:ILE:HB	2.48	0.48
1:A:542:ASP:O	1:A:546:ASP:HA	2.14	0.48
1:C:503:VAL:O	1:C:504:THR:OG1	2.30	0.48
1:D:277:TYR:CE1	1:D:353:VAL:HG13	2.48	0.48
1:D:373:LEU:HD13	1:D:492:PHE:CE2	2.47	0.48
1:D:504:THR:O	1:D:504:THR:OG1	2.30	0.48
1:B:102:ASN:ND2	1:B:106:GLN:HB2	2.25	0.48
1:D:557:HIS:CE1	1:D:590:PRO:HG2	2.47	0.48
1:A:184:PRO:HB2	1:A:337:ASN:O	2.13	0.48
1:A:272:LYS:HG3	1:A:361:VAL:HG12	1.96	0.48
1:B:428:ARG:HG3	1:B:462:TYR:CZ	2.48	0.48
1:B:455:LYS:HA	1:B:459:THR:HB	1.95	0.48
1:B:55:VAL:HG12	1:B:57:LEU:HD22	1.96	0.48
1:C:41:ALA:O	1:C:42:TYR:CB	2.57	0.48
1:C:542:ASP:HB2	1:C:559:TRP:HZ2	1.78	0.48
1:D:159:GLY:C	1:D:161:GLU:H	2.16	0.48
1:A:493:LYS:O	1:A:497:LYS:HD2	2.14	0.48
1:B:315:ASP:O	1:B:316:LYS:HB2	2.12	0.48
1:B:595:LEU:HD21	1:B:604:TRP:CE3	2.49	0.48
1:C:184:PRO:HB2	1:C:337:ASN:O	2.14	0.48
1:C:543:LYS:HA	1:C:543:LYS:HD2	1.45	0.48
1:D:347:GLU:OE1	1:D:347:GLU:CA	2.60	0.48
1:A:335:VAL:HG13	1:A:440:HIS:HB3	1.94	0.48
1:A:332:GLY:HA2	1:A:346:ASN:OD1	2.13	0.48
1:A:580:LYS:HA	1:A:612:ALA:CB	2.42	0.48
1:B:504:THR:O	1:B:505:ASP:CB	2.60	0.48
1:C:294:PHE:HE2	1:C:298:GLY:HA2	1.79	0.48
1:D:69:SER:HB3	1:D:141:ASN:HB2	1.95	0.48
1:D:347:GLU:HA	1:D:347:GLU:OE1	2.12	0.48
1:D:359:GLU:HG3	1:D:364:THR:HA	1.95	0.48
1:D:74:LEU:HD22	1:D:74:LEU:N	2.28	0.48
1:A:102:ASN:C	1:A:104:GLN:H	2.17	0.48
1:A:507:LEU:HD23	1:A:507:LEU:C	2.34	0.48
1:A:596:ALA:HA	1:A:602:LYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:HIS:O	1:B:333:ASN:HB2	2.14	0.48
1:C:162:LYS:HD3	1:C:200:LEU:HD12	1.96	0.48
1:C:613:ARG:N	1:C:614:PRO:HD2	2.28	0.48
1:D:102:ASN:HD21	1:D:106:GLN:HB2	1.79	0.48
1:D:294:PHE:CD1	1:D:295:PRO:HD2	2.49	0.48
1:D:358:MET:HE3	1:D:366:ARG:NH1	2.29	0.48
1:D:392:LEU:HD23	1:D:475:ILE:CG2	2.43	0.48
1:D:596:ALA:HA	1:D:602:LYS:CA	2.44	0.48
1:A:153:SER:HG	1:A:155:GLU:HG2	1.78	0.48
1:B:284:ARG:NH2	3:B:702:HOH:O	2.17	0.48
1:B:514:THR:C	1:B:516:GLN:N	2.66	0.48
1:B:585:ARG:O	1:B:587:LEU:N	2.44	0.48
1:C:321:LEU:O	1:C:324:HIS:HB3	2.14	0.48
1:D:152:LEU:HD13	1:D:291:PRO:CG	2.44	0.48
1:D:376:GLN:HE22	1:D:524:HIS:CE1	2.30	0.48
1:B:159:GLY:C	1:B:161:GLU:H	2.17	0.48
1:C:283:GLY:CA	3:C:988:HOH:O	2.60	0.48
1:C:343:LEU:HD13	1:C:343:LEU:O	2.13	0.48
1:D:384:GLU:OE1	3:D:843:HOH:O	2.20	0.48
1:A:42:TYR:HD2	1:A:172:ILE:HD13	1.79	0.48
1:A:585:ARG:O	1:A:587:LEU:N	2.41	0.48
1:A:585:ARG:C	1:A:587:LEU:H	2.18	0.48
1:B:352:TYR:CZ	1:B:429:PHE:HE2	2.32	0.48
1:B:46:ASN:O	1:B:48:ASP:N	2.47	0.48
1:B:579:LEU:HD23	1:B:588:ILE:HG22	1.96	0.48
1:C:241:LYS:HE3	3:C:985:HOH:O	2.14	0.48
1:C:359:GLU:HG3	1:C:364:THR:HA	1.96	0.48
1:C:525:PHE:O	1:C:529:LEU:HB2	2.14	0.48
1:A:243:MET:HG2	1:A:260:VAL:HG13	1.96	0.47
1:A:184:PRO:HG3	1:A:340:TRP:CZ2	2.48	0.47
1:B:40:ASP:OD1	1:B:41:ALA:O	2.32	0.47
1:C:459:THR:HG21	1:C:471:ILE:HD11	1.96	0.47
1:D:101:LYS:HZ3	1:D:105:GLY:HA2	1.79	0.47
1:D:206:ALA:HA	1:D:222:MET:CE	2.44	0.47
1:D:522:TRP:O	1:D:526:ILE:CG1	2.54	0.47
1:D:595:LEU:HD21	1:D:604:TRP:CZ3	2.49	0.47
1:A:91:ARG:NH2	1:A:175:ARG:HD2	2.29	0.47
1:A:263:PHE:C	1:A:265:ASP:H	2.17	0.47
1:A:328:HIS:HE1	1:A:347:GLU:OE1	1.98	0.47
1:A:378:LEU:HD21	1:A:480:LEU:HD21	1.95	0.47
1:B:300:GLU:HG2	1:B:300:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:THR:O	1:B:516:GLN:N	2.47	0.47
1:B:605:ALA:HB3	1:B:628:LEU:HD11	1.96	0.47
1:C:378:LEU:HD13	1:C:411:VAL:HB	1.95	0.47
1:D:288:LEU:CB	1:D:304:LEU:HD11	2.44	0.47
1:D:39:THR:O	1:D:39:THR:OG1	2.30	0.47
1:D:46:ASN:O	1:D:48:ASP:N	2.47	0.47
1:A:116:LYS:HD3	1:A:117:ARG:N	2.29	0.47
1:B:106:GLN:O	1:B:108:VAL:HG13	2.14	0.47
1:B:493:LYS:O	1:B:497:LYS:HD2	2.14	0.47
1:B:504:THR:OG1	1:B:540:ASN:ND2	2.47	0.47
1:B:585:ARG:C	1:B:587:LEU:H	2.18	0.47
1:C:40:ASP:OD1	1:C:40:ASP:C	2.53	0.47
1:C:514:THR:C	1:C:516:GLN:H	2.16	0.47
1:A:280:TYR:HH	1:A:285:TYR:HD1	1.60	0.47
1:A:39:THR:O	1:A:339:SER:HB3	2.14	0.47
1:B:596:ALA:HA	1:B:602:LYS:HA	1.95	0.47
1:C:297:GLY:O	1:C:308:THR:HG22	2.14	0.47
1:D:160:LYS:HA	1:D:160:LYS:HD3	1.70	0.47
1:A:326:LEU:O	1:A:326:LEU:CD2	2.61	0.47
1:A:344:TRP:HH2	1:A:450:PHE:CE2	2.30	0.47
1:B:42:TYR:HA	1:B:121:LEU:HD21	1.97	0.47
1:B:572:TYR:N	1:B:573:PRO:HD2	2.29	0.47
1:C:507:LEU:CD1	3:C:971:HOH:O	2.43	0.47
1:D:378:LEU:HD21	1:D:480:LEU:HD21	1.96	0.47
1:D:579:LEU:HD23	1:D:588:ILE:HG22	1.97	0.47
1:A:298:GLY:HA2	1:A:306:PHE:O	2.15	0.47
1:C:585:ARG:C	1:C:587:LEU:H	2.18	0.47
1:D:129:THR:HG23	1:D:133:ALA:HB2	1.96	0.47
1:D:517:TRP:CH2	1:D:525:PHE:CD2	3.02	0.47
1:A:613:ARG:HB3	1:A:614:PRO:HD3	1.96	0.47
1:B:327:ALA:HB3	1:B:350:THR:HG23	1.96	0.47
1:B:543:LYS:HA	1:B:543:LYS:HD2	1.52	0.47
1:D:298:GLY:HA2	1:D:306:PHE:O	2.14	0.47
1:D:311:VAL:HG11	1:D:321:LEU:HD23	1.96	0.47
1:A:263:PHE:HB3	1:A:266:THR:CG2	2.44	0.47
1:B:454:LEU:O	1:B:454:LEU:HD23	2.14	0.47
1:B:518:THR:O	1:B:522:TRP:CD1	2.66	0.47
1:C:208:ASN:OD1	1:C:208:ASN:C	2.52	0.47
1:C:263:PHE:C	1:C:265:ASP:H	2.17	0.47
1:D:459:THR:HG21	1:D:471:ILE:HD11	1.97	0.47
1:A:361:VAL:HG23	1:A:362:PHE:HD1	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:GLY:C	1:C:161:GLU:H	2.18	0.47
1:D:352:TYR:CZ	1:D:429:PHE:HE2	2.32	0.47
1:D:428:ARG:HG3	1:D:462:TYR:CZ	2.49	0.47
1:A:162:LYS:HD3	1:A:200:LEU:HD12	1.96	0.47
1:A:358:MET:CE	1:A:366:ARG:NH1	2.78	0.47
1:A:39:THR:O	1:A:40:ASP:HB2	2.14	0.47
1:A:310:THR:HG21	1:A:582:ILE:HD12	1.96	0.47
1:B:130:PRO:O	1:B:131:LEU:C	2.52	0.47
1:B:542:ASP:O	1:B:546:ASP:N	2.48	0.47
1:C:184:PRO:HG3	1:C:340:TRP:CZ2	2.50	0.47
1:C:489:SER:HB3	1:C:492:PHE:HB2	1.97	0.47
1:D:166:PHE:HB2	1:D:306:PHE:HE2	1.80	0.47
1:D:252:GLU:O	1:D:253:SER:HB2	2.15	0.47
1:A:488:THR:HG22	1:A:488:THR:O	2.14	0.47
1:D:365:ASP:O	1:D:369:MET:HB2	2.15	0.47
1:D:509:LEU:CG	1:D:510:GLU:H	2.11	0.47
1:D:585:ARG:C	1:D:587:LEU:H	2.17	0.47
1:A:228:PRO:C	1:A:230:LEU:H	2.18	0.46
1:A:328:HIS:HA	1:A:331:SER:O	2.15	0.46
1:B:560:TYR:HB3	1:B:575:MET:CE	2.45	0.46
1:C:311:VAL:HG11	1:C:321:LEU:HD22	1.96	0.46
1:C:347:GLU:HB3	1:C:410:TYR:CD2	2.50	0.46
1:C:42:TYR:CD2	1:C:121:LEU:HD21	2.49	0.46
1:D:413:GLY:O	1:D:417:LEU:HG	2.15	0.46
1:D:563:SER:CB	1:D:571:VAL:HG21	2.45	0.46
1:A:455:LYS:HA	1:A:459:THR:HB	1.96	0.46
1:A:543:LYS:HA	1:A:543:LYS:HD2	1.49	0.46
1:C:547:LEU:H	1:C:547:LEU:CD1	2.25	0.46
1:C:605:ALA:CB	1:C:628:LEU:HD11	2.46	0.46
1:A:208:ASN:OD1	1:A:208:ASN:C	2.53	0.46
1:A:325:GLU:OE1	1:A:325:GLU:HA	2.16	0.46
1:A:328:HIS:O	1:A:330:TRP:N	2.48	0.46
1:A:347:GLU:HB3	1:A:410:TYR:CD2	2.51	0.46
1:A:46:ASN:O	1:A:48:ASP:N	2.48	0.46
1:B:116:LYS:HD3	1:B:117:ARG:N	2.31	0.46
1:C:166:PHE:HB2	1:C:306:PHE:HE2	1.80	0.46
1:D:512:LEU:CB	1:D:513:PRO:CD	2.92	0.46
1:A:489:SER:O	1:A:490:ASN:C	2.52	0.46
1:B:416:PHE:CD1	1:B:416:PHE:O	2.69	0.46
1:C:265:ASP:OD2	1:C:316:LYS:HD3	2.15	0.46
1:C:530:PRO:C	1:C:532:ASP:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:SER:HB2	1:D:302:PRO:HG2	1.97	0.46
1:A:295:PRO:HD3	1:A:617:HIS:HB2	1.97	0.46
1:A:459:THR:HG21	1:A:471:ILE:HD11	1.98	0.46
1:C:467:SER:O	1:C:469:ASN:N	2.49	0.46
1:C:510:GLU:O	1:C:512:LEU:N	2.47	0.46
1:D:328:HIS:O	1:D:330:TRP:N	2.49	0.46
1:A:572:TYR:N	1:A:573:PRO:HD2	2.30	0.46
1:C:337:ASN:H	1:C:337:ASN:ND2	2.12	0.46
1:A:596:ALA:CB	1:A:602:LYS:HG3	2.46	0.46
1:B:400:ASP:CB	1:B:403:ASP:HB2	2.34	0.46
1:B:596:ALA:HA	1:B:602:LYS:HB2	1.98	0.46
1:C:352:TYR:CZ	1:C:429:PHE:HE2	2.34	0.46
1:C:613:ARG:HB3	1:C:614:PRO:HD3	1.98	0.46
1:A:265:ASP:OD2	1:A:316:LYS:HD3	2.16	0.46
1:A:507:LEU:CD1	3:A:970:HOH:O	2.60	0.46
1:A:56:TYR:HB3	1:A:73:GLU:HB3	1.98	0.46
1:B:243:MET:CE	1:B:249:ILE:HG13	2.45	0.46
1:B:288:LEU:CD2	1:B:304:LEU:HD11	2.45	0.46
1:B:454:LEU:O	1:B:454:LEU:CD2	2.64	0.46
1:B:606:VAL:HG13	1:B:610:LYS:NZ	2.30	0.46
1:C:197:ASP:C	1:C:198:LYS:O	2.51	0.46
1:C:281:ARG:NH2	1:C:438:ASP:OD1	2.45	0.46
1:C:504:THR:O	1:C:505:ASP:CB	2.64	0.46
1:D:276:MET:HE3	1:D:356:ARG:HB3	1.98	0.46
1:A:200:LEU:O	1:A:218:TYR:OH	2.28	0.46
1:A:254:TYR:CG	1:A:255:ILE:N	2.84	0.46
1:B:303:ARG:NH1	3:B:737:HOH:O	2.48	0.46
1:B:400:ASP:HA	1:B:401:PRO:HD3	1.74	0.46
1:C:201:LEU:HD23	1:C:238:LEU:HB2	1.97	0.46
1:C:426:ARG:O	1:C:430:ASP:HB2	2.16	0.46
1:D:180:ILE:HG12	1:D:181:GLN:N	2.30	0.46
1:D:224:GLN:HG3	3:D:976:HOH:O	2.16	0.46
1:D:166:PHE:HA	1:D:233:ILE:O	2.16	0.46
1:A:153:SER:OG	1:A:156:GLN:HG3	2.16	0.46
1:A:326:LEU:O	1:A:326:LEU:HD23	2.15	0.46
1:B:271:ASP:O	1:B:275:GLN:HG3	2.15	0.46
1:B:280:TYR:HH	1:B:285:TYR:HD1	1.64	0.46
1:D:347:GLU:HB3	1:D:410:TYR:CD2	2.51	0.46
1:D:589:VAL:CG1	1:D:593:LYS:HE3	2.46	0.46
1:A:300:GLU:HG2	1:A:300:GLU:O	2.16	0.45
1:A:510:GLU:O	1:A:512:LEU:N	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:VAL:HG13	1:A:610:LYS:NZ	2.31	0.45
1:C:270:ILE:O	1:C:270:ILE:HG22	2.16	0.45
1:C:168:GLN:NE2	1:C:299:MET:HG3	2.32	0.45
1:C:514:THR:C	1:C:516:GLN:N	2.69	0.45
1:C:526:ILE:O	1:C:529:LEU:HB3	2.16	0.45
1:D:547:LEU:CD1	1:D:547:LEU:N	2.79	0.45
1:D:542:ASP:HB2	1:D:559:TRP:HZ2	1.81	0.45
1:D:613:ARG:HB3	1:D:614:PRO:CD	2.46	0.45
1:A:283:GLY:N	3:A:989:HOH:O	2.49	0.45
1:A:354:GLU:O	1:A:358:MET:HG2	2.15	0.45
1:A:481:PRO:O	1:A:482:SER:CB	2.62	0.45
1:B:503:VAL:O	1:B:504:THR:HG22	2.16	0.45
1:C:277:TYR:CD1	1:C:353:VAL:HG13	2.51	0.45
1:C:42:TYR:CE2	1:C:401:PRO:HD3	2.51	0.45
1:C:507:LEU:HD22	1:C:508:THR:HG22	1.98	0.45
1:C:518:THR:O	1:C:521:GLU:N	2.49	0.45
1:D:467:SER:C	1:D:469:ASN:H	2.19	0.45
1:D:559:TRP:NE1	1:D:571:VAL:HG11	2.32	0.45
1:A:361:VAL:CG2	1:A:362:PHE:HD1	2.29	0.45
1:A:416:PHE:CD1	1:A:416:PHE:O	2.69	0.45
1:B:254:TYR:CE2	1:B:255:ILE:HB	2.51	0.45
1:B:295:PRO:HB3	1:B:617:HIS:HB3	1.98	0.45
1:B:326:LEU:O	1:B:326:LEU:HD23	2.16	0.45
1:B:56:TYR:HB3	1:B:73:GLU:HB3	1.98	0.45
1:B:569:LYS:HA	1:B:572:TYR:CD1	2.51	0.45
1:C:160:LYS:HD3	1:C:160:LYS:HA	1.64	0.45
1:C:187:ARG:NH1	1:C:225:ALA:O	2.48	0.45
1:C:249:ILE:HD12	1:C:260:VAL:HA	1.99	0.45
1:C:324:HIS:ND1	1:C:350:THR:HG22	2.31	0.45
1:D:489:SER:O	1:D:490:ASN:C	2.53	0.45
1:D:507:LEU:HB3	1:D:508:THR:H	1.63	0.45
1:D:582:ILE:CG1	1:D:584:ARG:H	2.29	0.45
1:A:467:SER:C	1:A:469:ASN:H	2.19	0.45
1:B:500:ASN:O	1:B:502:LEU:N	2.49	0.45
1:B:520:HIS:ND1	1:B:520:HIS:N	2.65	0.45
1:C:44:TYR:CD2	1:C:124:LYS:HB2	2.51	0.45
1:C:263:PHE:HB3	1:C:266:THR:CG2	2.47	0.45
1:C:42:TYR:HA	1:C:121:LEU:CD1	2.46	0.45
1:D:270:ILE:O	1:D:270:ILE:HG22	2.15	0.45
1:D:568:TYR:CE2	1:D:571:VAL:HG13	2.51	0.45
1:A:166:PHE:HA	1:A:233:ILE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:O	1:A:253:SER:HB2	2.17	0.45
1:A:313:ALA:HB2	1:A:318:LEU:HD23	1.98	0.45
1:A:42:TYR:HA	1:A:121:LEU:HD21	1.97	0.45
1:A:559:TRP:CZ2	1:A:568:TYR:CE1	3.05	0.45
1:A:69:SER:HB3	1:A:141:ASN:CB	2.45	0.45
1:B:263:PHE:CD1	1:B:322:ILE:HG13	2.51	0.45
1:B:500:ASN:C	1:B:502:LEU:N	2.68	0.45
1:B:542:ASP:O	1:B:546:ASP:CA	2.64	0.45
1:C:101:LYS:HZ3	1:C:105:GLY:HA2	1.82	0.45
1:D:295:PRO:HD3	1:D:617:HIS:HB2	1.98	0.45
1:B:358:MET:HE3	1:B:366:ARG:NH1	2.27	0.45
1:B:539:VAL:O	1:B:543:LYS:N	2.43	0.45
1:C:334:LEU:HD23	1:C:442:PHE:H	1.82	0.45
1:C:454:LEU:CD2	1:C:454:LEU:O	2.65	0.45
1:C:74:LEU:HD22	1:C:74:LEU:N	2.32	0.45
1:A:311:VAL:HG11	1:A:321:LEU:HD22	1.99	0.45
1:A:394:ILE:O	1:A:394:ILE:HG23	2.16	0.45
1:B:137:ARG:HG2	1:B:139:TYR:CE2	2.51	0.45
1:B:239:GLU:HB2	1:B:256:LEU:HD22	1.99	0.45
1:B:561:LEU:O	1:B:565:ARG:HG3	2.17	0.45
1:C:116:LYS:HD3	1:C:117:ARG:N	2.31	0.45
1:C:339:SER:OG	1:C:342:ASP:OD2	2.29	0.45
1:D:239:GLU:HB2	1:D:256:LEU:HD22	1.98	0.45
1:A:175:ARG:HA	1:A:178:ILE:O	2.17	0.45
1:A:152:LEU:HD13	1:A:291:PRO:HG3	1.98	0.45
1:A:386:ASP:O	1:A:388:SER:N	2.47	0.45
1:A:533:LEU:CD2	1:A:538:MET:HE3	2.45	0.45
1:A:591:LEU:O	1:A:595:LEU:HB2	2.16	0.45
1:A:595:LEU:HD21	1:A:604:TRP:CZ3	2.52	0.45
1:B:263:PHE:C	1:B:265:ASP:H	2.19	0.45
1:B:498:GLN:C	1:B:500:ASN:N	2.70	0.45
1:D:318:LEU:HD21	1:D:552:ASN:ND2	2.31	0.45
1:D:298:GLY:C	1:D:325:GLU:OE2	2.55	0.45
1:D:572:TYR:N	1:D:573:PRO:HD2	2.31	0.45
1:A:206:ALA:O	1:A:303:ARG:NH1	2.50	0.45
1:B:359:GLU:HG3	1:B:364:THR:HA	1.98	0.45
1:C:148:GLY:CA	1:C:173:HIS:HB3	2.47	0.45
1:C:205:SER:HB2	1:C:302:PRO:HG2	1.99	0.45
1:D:198:LYS:O	1:D:199:ASP:HB2	2.16	0.45
1:D:201:LEU:HD23	1:D:238:LEU:HB2	1.98	0.45
1:D:495:ILE:O	1:D:499:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LYS:HB2	1:D:79:PHE:CE1	2.51	0.45
1:A:270:ILE:HG22	1:A:270:ILE:O	2.17	0.45
1:A:97:ARG:HG3	1:A:139:TYR:CD2	2.52	0.45
1:B:414:GLN:O	1:B:418:MET:HG3	2.17	0.45
1:D:526:ILE:O	1:D:562:LEU:HD22	2.17	0.45
1:A:265:ASP:O	1:A:268:ALA:HB3	2.16	0.44
1:B:180:ILE:HG12	1:B:181:GLN:N	2.32	0.44
1:C:206:ALA:HA	1:C:222:MET:HE3	2.00	0.44
1:C:365:ASP:O	1:C:369:MET:HB2	2.17	0.44
1:D:187:ARG:HG2	1:D:227:PRO:HD3	1.99	0.44
1:D:249:ILE:CD1	1:D:260:VAL:HA	2.47	0.44
1:D:290:LEU:HD11	1:D:306:PHE:HB3	2.00	0.44
1:D:455:LYS:HA	1:D:459:THR:HB	1.99	0.44
1:D:373:LEU:HD21	1:D:523:LEU:HD12	1.98	0.44
1:B:328:HIS:HE1	1:B:347:GLU:OE1	2.01	0.44
1:C:464:ASN:HD22	1:D:241:LYS:CB	2.19	0.44
1:C:467:SER:C	1:C:469:ASN:H	2.20	0.44
1:D:543:LYS:HD2	1:D:543:LYS:HA	1.49	0.44
1:A:365:ASP:O	1:A:369:MET:HB2	2.16	0.44
1:A:495:ILE:HA	1:A:498:GLN:HE21	1.82	0.44
1:A:605:ALA:HB1	1:A:628:LEU:HD11	1.98	0.44
1:A:593:LYS:HE2	1:A:627:VAL:HG11	2.00	0.44
1:B:200:LEU:O	1:B:218:TYR:OH	2.28	0.44
1:B:263:PHE:HB3	1:B:266:THR:CG2	2.47	0.44
1:B:62:ASP:C	1:B:62:ASP:OD1	2.56	0.44
1:C:311:VAL:HG21	1:C:321:LEU:HD23	2.00	0.44
1:C:395:ASP:O	1:C:399:ARG:NH2	2.51	0.44
1:D:97:ARG:HD3	1:D:99:MET:HE3	1.98	0.44
1:A:613:ARG:HD2	1:A:621:GLN:NE2	2.32	0.44
1:A:613:ARG:HB3	1:A:614:PRO:CD	2.48	0.44
1:B:101:LYS:HZ3	1:B:105:GLY:HA2	1.83	0.44
1:B:463:PRO:O	1:B:464:ASN:HB2	2.17	0.44
1:C:413:GLY:O	1:C:417:LEU:HG	2.17	0.44
1:C:580:LYS:HA	1:C:612:ALA:CB	2.42	0.44
1:D:229:TYR:HA	3:D:746:HOH:O	2.18	0.44
1:D:300:GLU:HG3	1:D:333:ASN:OD1	2.18	0.44
1:D:426:ARG:O	1:D:427:GLU:C	2.55	0.44
1:D:60:ASN:O	1:D:68:LEU:HA	2.17	0.44
1:D:613:ARG:N	1:D:614:PRO:HD2	2.33	0.44
1:A:130:PRO:O	1:A:131:LEU:C	2.53	0.44
1:A:295:PRO:HG2	1:A:296:PHE:CD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:HD3	1:A:617:HIS:CB	2.48	0.44
1:B:321:LEU:O	1:B:324:HIS:HB3	2.17	0.44
1:B:54:HIS:HE1	1:B:191:THR:HG23	1.81	0.44
1:C:206:ALA:HA	1:C:222:MET:CE	2.48	0.44
1:C:332:GLY:C	1:C:336:THR:HG22	2.37	0.44
1:C:277:TYR:CE1	1:C:353:VAL:HG22	2.52	0.44
1:D:130:PRO:O	1:D:131:LEU:C	2.53	0.44
1:D:497:LYS:O	1:D:500:ASN:ND2	2.50	0.44
1:D:498:GLN:C	1:D:500:ASN:N	2.69	0.44
1:A:427:GLU:HG3	1:A:428:ARG:CZ	2.48	0.44
1:B:347:GLU:CA	1:B:347:GLU:OE1	2.66	0.44
1:D:354:GLU:O	1:D:358:MET:HG2	2.17	0.44
1:D:514:THR:C	1:D:516:GLN:N	2.70	0.44
1:A:101:LYS:HD2	1:A:107:TRP:CZ2	2.53	0.44
1:A:69:SER:HB3	1:A:141:ASN:HB2	1.98	0.44
1:A:547:LEU:CD1	1:A:547:LEU:H	2.26	0.44
1:B:298:GLY:HA2	1:B:306:PHE:O	2.17	0.44
1:D:416:PHE:CD1	1:D:416:PHE:C	2.89	0.44
1:A:62:ASP:OD1	1:A:62:ASP:C	2.56	0.44
1:B:354:GLU:O	1:B:358:MET:HG2	2.18	0.44
1:B:341:ARG:HH11	1:B:395:ASP:HA	1.83	0.44
1:C:137:ARG:HG2	1:C:139:TYR:CE2	2.53	0.44
1:C:464:ASN:HB3	1:D:241:LYS:HA	2.00	0.44
1:A:239:GLU:O	1:A:250:TYR:HA	2.17	0.44
1:B:471:ILE:O	1:B:475:ILE:HG12	2.18	0.44
1:B:502:LEU:HG	1:B:507:LEU:HB3	1.96	0.44
1:C:313:ALA:HB2	1:C:318:LEU:HD23	1.99	0.44
1:C:414:GLN:O	1:C:418:MET:HG3	2.18	0.44
1:A:102:ASN:ND2	1:A:106:GLN:HB2	2.32	0.43
1:B:187:ARG:NH1	1:B:225:ALA:O	2.50	0.43
1:C:325:GLU:OE1	1:C:325:GLU:HA	2.17	0.43
1:C:564:VAL:HG23	1:C:572:TYR:OH	2.17	0.43
1:D:564:VAL:HG23	1:D:572:TYR:OH	2.18	0.43
1:A:102:ASN:CA	3:A:960:HOH:O	2.65	0.43
1:A:324:HIS:ND1	1:A:350:THR:HG22	2.32	0.43
1:A:463:PRO:O	1:A:464:ASN:HB2	2.18	0.43
1:B:265:ASP:O	1:B:268:ALA:HB3	2.17	0.43
1:B:295:PRO:HD3	1:B:617:HIS:CB	2.47	0.43
1:C:298:GLY:HA2	1:C:306:PHE:O	2.17	0.43
1:C:318:LEU:HD21	1:C:552:ASN:ND2	2.32	0.43
1:C:354:GLU:O	1:C:358:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:O	1:A:235:VAL:HA	2.18	0.43
1:A:328:HIS:C	1:A:330:TRP:N	2.71	0.43
1:B:102:ASN:CB	3:B:795:HOH:O	2.55	0.43
1:B:252:GLU:O	1:B:253:SER:HB2	2.18	0.43
1:B:427:GLU:HG3	1:B:428:ARG:CZ	2.49	0.43
1:B:569:LYS:HA	1:B:572:TYR:CE1	2.53	0.43
1:C:526:ILE:O	1:C:529:LEU:CB	2.67	0.43
1:D:471:ILE:O	1:D:475:ILE:HG12	2.18	0.43
1:D:530:PRO:C	1:D:532:ASP:H	2.21	0.43
1:A:249:ILE:HD12	1:A:260:VAL:HA	1.99	0.43
1:A:303:ARG:NH1	3:A:782:HOH:O	2.45	0.43
1:A:42:TYR:HE2	1:A:401:PRO:CD	2.02	0.43
1:A:564:VAL:HG23	1:A:572:TYR:OH	2.18	0.43
1:B:162:LYS:HD3	1:B:200:LEU:HD12	2.01	0.43
1:B:318:LEU:HD21	1:B:552:ASN:HD21	1.83	0.43
1:B:370:GLU:HG2	1:B:520:HIS:CD2	2.52	0.43
1:B:83:LYS:HD2	1:D:363:GLY:HA2	2.00	0.43
1:C:500:ASN:C	1:C:502:LEU:H	2.21	0.43
1:C:531:VAL:HG12	1:C:531:VAL:O	2.19	0.43
1:A:300:GLU:HG3	1:A:333:ASN:OD1	2.19	0.43
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.87	0.43
1:A:546:ASP:OD1	1:A:549:ASN:HB2	2.17	0.43
1:A:598:ASN:O	1:A:601:SER:N	2.51	0.43
1:B:214:ARG:HB3	1:B:215:ASP:H	1.45	0.43
1:B:227:PRO:HD2	1:B:230:LEU:HD12	2.01	0.43
1:B:343:LEU:HD13	1:B:343:LEU:O	2.18	0.43
1:C:102:ASN:ND2	1:C:106:GLN:HB2	2.31	0.43
1:C:51:LYS:HB2	1:C:79:PHE:CZ	2.53	0.43
1:D:197:ASP:O	1:D:216:GLY:HA3	2.18	0.43
1:D:486:GLN:NE2	1:D:486:GLN:HA	2.33	0.43
1:A:103:SER:C	1:A:104:GLN:CG	2.87	0.43
1:A:277:TYR:CE1	1:A:353:VAL:HG13	2.53	0.43
1:A:390:THR:HA	1:A:408:VAL:HG21	2.00	0.43
1:B:228:PRO:C	1:B:230:LEU:H	2.21	0.43
1:B:277:TYR:CE1	1:B:353:VAL:HG22	2.54	0.43
1:B:467:SER:O	1:B:469:ASN:N	2.51	0.43
1:C:328:HIS:HA	1:C:331:SER:O	2.18	0.43
1:C:42:TYR:HA	1:C:121:LEU:HD21	1.99	0.43
1:C:503:VAL:C	1:C:506:GLU:OE1	2.57	0.43
1:D:326:LEU:HD23	1:D:326:LEU:O	2.19	0.43
1:D:588:ILE:HG13	1:D:589:VAL:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HD2	3:A:987:HOH:O	2.17	0.43
1:A:277:TYR:CD1	1:A:353:VAL:HG13	2.53	0.43
1:A:414:GLN:O	1:A:418:MET:HG3	2.18	0.43
1:A:467:SER:O	1:A:469:ASN:N	2.52	0.43
1:A:624:VAL:HA	1:A:627:VAL:HG22	2.00	0.43
1:B:101:LYS:HB3	1:B:101:LYS:HZ3	1.84	0.43
1:B:467:SER:C	1:B:469:ASN:H	2.22	0.43
1:B:609:TYR:O	1:B:609:TYR:CG	2.71	0.43
1:C:364:THR:HA	1:C:367:ALA:HB3	2.00	0.43
1:C:591:LEU:O	1:C:595:LEU:HB2	2.18	0.43
1:D:220:PHE:CD1	1:D:220:PHE:N	2.86	0.43
1:D:367:ALA:O	1:D:371:GLN:HG3	2.19	0.43
1:D:416:PHE:O	1:D:419:TYR:HB3	2.19	0.43
1:A:596:ALA:HA	1:A:602:LYS:CA	2.48	0.43
1:B:166:PHE:HB2	1:B:306:PHE:HE2	1.82	0.43
1:B:152:LEU:HD13	1:B:291:PRO:CG	2.48	0.43
1:B:519:LEU:C	1:B:519:LEU:HD13	2.39	0.43
1:D:92:ASP:OD1	1:D:145:LYS:HE2	2.19	0.43
1:A:153:SER:O	1:A:157:THR:HG23	2.18	0.43
1:A:160:LYS:HD3	1:A:160:LYS:HA	1.58	0.43
1:A:416:PHE:CD1	1:A:416:PHE:C	2.86	0.43
1:A:534:ASP:H	1:A:566:ALA:HB1	1.83	0.43
1:B:563:SER:CB	1:B:571:VAL:HG21	2.48	0.43
1:B:310:THR:HG21	1:B:582:ILE:HD12	2.00	0.43
1:C:465:ILE:HD12	1:C:465:ILE:N	2.34	0.43
1:C:543:LYS:O	1:C:543:LYS:HD2	2.19	0.43
1:D:148:GLY:CA	1:D:173:HIS:HB3	2.48	0.43
1:D:290:LEU:CD1	1:D:306:PHE:HB3	2.48	0.43
1:D:390:THR:HA	1:D:408:VAL:HG21	2.00	0.43
1:D:42:TYR:HA	1:D:121:LEU:HD21	2.00	0.43
1:D:51:LYS:HB2	1:D:79:PHE:CZ	2.53	0.43
1:D:613:ARG:HE	1:D:621:GLN:HB3	1.84	0.43
1:A:283:GLY:HA2	3:A:989:HOH:O	2.19	0.43
1:B:102:ASN:C	1:B:104:GLN:H	2.21	0.43
1:B:542:ASP:HB2	1:B:559:TRP:CZ2	2.53	0.43
1:B:588:ILE:HG13	1:B:589:VAL:N	2.32	0.43
1:C:547:LEU:N	1:C:547:LEU:CD1	2.81	0.43
1:C:589:VAL:CG1	1:C:593:LYS:HE3	2.49	0.43
1:A:542:ASP:O	1:A:546:ASP:CA	2.67	0.42
1:A:557:HIS:CE1	1:A:590:PRO:HG2	2.54	0.42
1:B:294:PHE:HE2	1:B:298:GLY:HA2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ASP:O	1:B:403:ASP:HB2	2.20	0.42
1:C:254:TYR:CG	1:C:255:ILE:N	2.86	0.42
1:A:220:PHE:N	1:A:220:PHE:CD1	2.87	0.42
1:A:596:ALA:O	1:A:597:LYS:HG3	2.20	0.42
1:B:426:ARG:O	1:B:427:GLU:C	2.57	0.42
1:C:249:ILE:CD1	1:C:260:VAL:HA	2.48	0.42
1:C:315:ASP:O	1:C:316:LYS:HB2	2.19	0.42
1:C:42:TYR:HA	1:C:121:LEU:HD22	1.99	0.42
1:D:290:LEU:HD22	1:D:294:PHE:CD1	2.54	0.42
1:A:180:ILE:CG1	1:A:181:GLN:H	2.32	0.42
1:A:613:ARG:N	1:A:614:PRO:HD2	2.35	0.42
1:B:160:LYS:HA	1:B:160:LYS:HD3	1.70	0.42
1:B:40:ASP:OD2	1:B:183:THR:HG23	2.20	0.42
1:B:568:TYR:CE2	1:B:571:VAL:HG13	2.54	0.42
1:C:542:ASP:O	1:C:546:ASP:CA	2.67	0.42
1:D:42:TYR:CD2	1:D:121:LEU:HD21	2.55	0.42
1:D:345:LEU:HD21	1:D:450:PHE:CG	2.54	0.42
1:D:504:THR:CA	1:D:506:GLU:HG2	2.46	0.42
1:A:358:MET:HE3	1:A:366:ARG:HH12	1.84	0.42
1:A:498:GLN:C	1:A:500:ASN:H	2.22	0.42
1:A:534:ASP:OD1	1:A:566:ALA:O	2.37	0.42
1:B:277:TYR:CD1	1:B:353:VAL:HG13	2.54	0.42
1:B:311:VAL:HG21	1:B:321:LEU:HD23	2.00	0.42
1:B:326:LEU:O	1:B:326:LEU:CD2	2.68	0.42
1:B:372:ALA:C	1:B:374:GLY:N	2.73	0.42
1:B:541:LEU:HD23	1:B:541:LEU:HA	1.89	0.42
1:D:165:LEU:O	1:D:234:GLY:HA2	2.20	0.42
1:D:263:PHE:HB3	1:D:266:THR:CG2	2.50	0.42
1:D:427:GLU:HG3	1:D:428:ARG:CZ	2.49	0.42
1:D:580:LYS:HA	1:D:612:ALA:CB	2.43	0.42
1:A:187:ARG:NH1	1:A:225:ALA:O	2.53	0.42
1:B:220:PHE:N	1:B:220:PHE:CD1	2.87	0.42
1:B:222:MET:SD	1:B:224:GLN:HB2	2.59	0.42
1:B:361:VAL:HG23	1:B:362:PHE:HD1	1.79	0.42
1:C:272:LYS:CG	1:C:361:VAL:HG12	2.49	0.42
1:C:497:LYS:O	1:C:500:ASN:HB2	2.19	0.42
1:C:498:GLN:C	1:C:500:ASN:N	2.72	0.42
1:C:370:GLU:CG	1:C:520:HIS:CD2	3.02	0.42
1:D:101:LYS:HD2	1:D:107:TRP:CZ2	2.55	0.42
1:D:317:SER:OG	1:D:318:LEU:HD22	2.19	0.42
1:A:358:MET:HE3	1:A:366:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:THR:H	1:A:506:GLU:CB	2.08	0.42
1:A:557:HIS:HE1	1:A:590:PRO:HG2	1.83	0.42
1:C:69:SER:HB3	1:C:141:ASN:HB2	2.02	0.42
1:C:328:HIS:O	1:C:333:ASN:HB2	2.19	0.42
1:C:277:TYR:CE1	1:C:353:VAL:HG13	2.55	0.42
1:C:416:PHE:O	1:C:419:TYR:HB3	2.19	0.42
1:D:239:GLU:O	1:D:250:TYR:HA	2.20	0.42
1:D:324:HIS:CE1	1:D:350:THR:CG2	3.02	0.42
1:D:498:GLN:C	1:D:500:ASN:H	2.22	0.42
1:D:624:VAL:HA	1:D:627:VAL:HG22	2.01	0.42
1:B:416:PHE:O	1:B:419:TYR:HB3	2.19	0.42
1:B:413:GLY:O	1:B:417:LEU:HG	2.19	0.42
1:C:166:PHE:HA	1:C:233:ILE:O	2.20	0.42
1:C:315:ASP:OD1	1:C:317:SER:CB	2.68	0.42
1:D:168:GLN:HE21	1:D:170:GLN:HB3	1.84	0.42
1:D:295:PRO:HB3	1:D:617:HIS:HB3	2.01	0.42
1:D:502:LEU:H	1:D:502:LEU:HG	1.46	0.42
1:A:148:GLY:HA3	1:A:173:HIS:HB3	2.02	0.42
1:B:148:GLY:CA	1:B:173:HIS:HB3	2.49	0.42
1:B:180:ILE:CG1	1:B:181:GLN:N	2.82	0.42
1:C:624:VAL:HA	1:C:627:VAL:HG22	2.01	0.42
1:D:276:MET:HE1	1:D:356:ARG:HB3	1.99	0.42
1:D:394:ILE:HD12	3:D:754:HOH:O	2.19	0.42
1:D:467:SER:OG	1:D:470:GLU:OE2	2.29	0.42
1:A:228:PRO:C	1:A:230:LEU:N	2.71	0.42
1:A:291:PRO:HA	1:A:292:PRO:HD3	1.87	0.42
1:A:542:ASP:HB2	1:A:559:TRP:HZ2	1.85	0.42
1:B:369:MET:HG2	1:B:492:PHE:CE1	2.55	0.42
1:C:129:THR:HG23	1:C:133:ALA:HB3	2.01	0.42
1:C:150:GLN:HG3	1:C:152:LEU:HG	2.02	0.42
1:C:361:VAL:CG2	1:C:362:PHE:HD1	2.30	0.42
1:C:426:ARG:O	1:C:427:GLU:C	2.58	0.42
1:C:467:SER:C	1:C:469:ASN:N	2.73	0.42
1:C:520:HIS:N	1:C:520:HIS:ND1	2.67	0.42
1:C:582:ILE:CG1	1:C:584:ARG:H	2.32	0.42
1:D:304:LEU:HD12	1:D:306:PHE:CE1	2.55	0.42
1:D:392:LEU:HB2	1:D:475:ILE:HA	2.01	0.42
1:A:101:LYS:HG3	1:A:107:TRP:CE2	2.55	0.42
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.88	0.42
1:A:566:ALA:O	1:A:567:ASP:HB2	2.20	0.42
1:B:101:LYS:HD2	1:B:107:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:HA	1:B:162:LYS:O	2.20	0.42
1:B:192:ALA:HB1	1:B:194:ILE:HD11	2.02	0.42
1:B:496:ASP:O	1:B:499:ILE:HG12	2.20	0.42
1:B:546:ASP:OD1	1:B:549:ASN:HB2	2.20	0.42
1:B:560:TYR:HB3	1:B:575:MET:HE2	2.01	0.42
1:C:542:ASP:O	1:C:546:ASP:N	2.52	0.42
1:D:465:ILE:N	1:D:465:ILE:HD12	2.35	0.42
1:D:90:THR:HG23	1:D:91:ARG:N	2.34	0.42
1:A:125:LEU:HD21	1:A:127:ILE:HD11	2.02	0.41
1:A:171:ALA:HB3	1:A:401:PRO:HB2	2.01	0.41
1:A:318:LEU:HD21	1:A:552:ASN:ND2	2.35	0.41
1:A:276:MET:HE1	1:A:356:ARG:HB3	2.00	0.41
1:B:416:PHE:CD1	1:B:416:PHE:C	2.91	0.41
1:B:481:PRO:HD2	1:B:484:ALA:HB2	2.01	0.41
1:B:526:ILE:HG12	1:B:527:ASN:N	2.34	0.41
1:B:57:LEU:HB3	1:B:59:LEU:HD23	2.01	0.41
1:B:594:GLU:HA	1:B:597:LYS:HD3	2.01	0.41
1:C:481:PRO:O	1:C:482:SER:CB	2.68	0.41
1:D:196:THR:OG1	1:D:218:TYR:HE1	2.03	0.41
1:D:412:LYS:NZ	1:D:479:GLY:O	2.43	0.41
1:D:54:HIS:HE1	1:D:191:THR:HG23	1.84	0.41
1:A:227:PRO:HA	1:A:228:PRO:HD3	1.92	0.41
1:A:313:ALA:HB2	1:A:318:LEU:CD2	2.50	0.41
1:A:343:LEU:HD13	1:A:343:LEU:O	2.20	0.41
1:A:372:ALA:O	1:A:373:LEU:C	2.57	0.41
1:A:454:LEU:O	1:A:454:LEU:CD2	2.69	0.41
1:C:217:ASP:C	1:C:217:ASP:OD1	2.59	0.41
1:C:304:LEU:HD12	1:C:306:PHE:CE1	2.55	0.41
1:C:356:ARG:HD2	1:C:356:ARG:HA	1.92	0.41
1:D:328:HIS:C	1:D:330:TRP:N	2.71	0.41
1:D:295:PRO:HD3	1:D:617:HIS:CB	2.50	0.41
1:A:101:LYS:HZ3	1:A:105:GLY:HA2	1.83	0.41
1:A:74:LEU:N	1:A:74:LEU:HD22	2.35	0.41
1:B:240:PHE:C	1:B:240:PHE:CD2	2.93	0.41
1:B:345:LEU:HD21	1:B:450:PHE:CG	2.55	0.41
1:D:90:THR:HG22	1:D:123:SER:O	2.20	0.41
1:D:154:ALA:HA	1:D:162:LYS:O	2.20	0.41
1:D:180:ILE:CG1	1:D:181:GLN:N	2.83	0.41
1:D:208:ASN:OD1	1:D:208:ASN:C	2.58	0.41
1:D:302:PRO:O	1:D:303:ARG:HB2	2.20	0.41
1:D:617:HIS:NE2	3:D:737:HOH:O	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:VAL:O	1:A:319:VAL:CG1	2.67	0.41
1:A:509:LEU:HB3	1:A:510:GLU:H	1.67	0.41
1:A:514:THR:C	1:A:516:GLN:N	2.73	0.41
1:B:295:PRO:HG2	1:B:296:PHE:CD1	2.46	0.41
1:B:345:LEU:HA	1:B:345:LEU:HD23	1.88	0.41
1:B:596:ALA:HA	1:B:602:LYS:CA	2.50	0.41
1:B:95:ILE:N	1:B:95:ILE:HD13	2.35	0.41
1:C:104:GLN:HB2	1:C:106:GLN:HG3	2.02	0.41
1:C:180:ILE:CG1	1:C:181:GLN:N	2.80	0.41
1:C:198:LYS:O	1:C:199:ASP:HB2	2.20	0.41
1:D:249:ILE:HD12	1:D:260:VAL:HA	2.02	0.41
1:D:512:LEU:HB3	1:D:513:PRO:HD3	2.02	0.41
1:D:568:TYR:CD2	1:D:571:VAL:HG13	2.55	0.41
1:D:605:ALA:HB3	1:D:628:LEU:HD11	2.01	0.41
1:A:399:ARG:HD2	1:A:403:ASP:OD2	2.20	0.41
1:B:593:LYS:HE2	1:B:627:VAL:HG11	2.02	0.41
1:C:290:LEU:HD11	1:C:306:PHE:CD2	2.55	0.41
1:D:156:GLN:NE2	3:D:800:HOH:O	2.54	0.41
1:D:265:ASP:O	1:D:268:ALA:HB3	2.20	0.41
1:D:42:TYR:HA	1:D:121:LEU:HD22	2.01	0.41
1:A:44:TYR:CD2	3:A:713:HOH:O	2.57	0.41
1:A:428:ARG:HG3	1:A:462:TYR:CZ	2.54	0.41
1:A:512:LEU:CB	1:A:513:PRO:CD	2.98	0.41
1:B:66:LYS:HB2	1:B:144:GLU:HB3	2.03	0.41
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.86	0.41
1:C:114:LEU:HD12	1:C:114:LEU:HA	1.94	0.41
1:C:222:MET:HE3	1:C:222:MET:HB2	1.77	0.41
1:C:295:PRO:HD3	1:C:617:HIS:HB2	2.02	0.41
1:C:326:LEU:HD22	1:C:330:TRP:HZ3	1.85	0.41
1:C:613:ARG:HD2	1:C:621:GLN:NE2	2.35	0.41
1:D:101:LYS:HB3	1:D:101:LYS:HZ3	1.85	0.41
1:D:290:LEU:HD11	1:D:306:PHE:CB	2.51	0.41
1:D:425:GLY:HA3	3:D:873:HOH:O	2.20	0.41
1:D:613:ARG:HD2	1:D:621:GLN:NE2	2.35	0.41
1:A:140:TYR:N	1:A:140:TYR:CD1	2.89	0.41
1:A:152:LEU:HD13	1:A:291:PRO:CG	2.51	0.41
1:A:413:GLY:O	1:A:417:LEU:HG	2.21	0.41
1:B:168:GLN:HE21	1:B:170:GLN:HB3	1.86	0.41
1:B:228:PRO:C	1:B:230:LEU:N	2.74	0.41
1:B:568:TYR:CD2	1:B:571:VAL:HG13	2.56	0.41
1:C:214:ARG:HB3	1:C:215:ASP:H	1.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:CD1	1:C:306:PHE:HB3	2.51	0.41
1:C:495:ILE:HA	1:C:498:GLN:HE21	1.85	0.41
1:D:386:ASP:O	1:D:388:SER:N	2.45	0.41
1:B:328:HIS:C	1:B:330:TRP:N	2.73	0.41
1:C:347:GLU:OE1	1:C:347:GLU:CA	2.69	0.41
1:C:40:ASP:HB3	1:C:47:TYR:OH	2.21	0.41
1:D:43:THR:HG21	1:D:47:TYR:HE1	1.86	0.41
1:D:542:ASP:O	1:D:546:ASP:CA	2.68	0.41
1:A:329:SER:O	1:A:334:LEU:HB2	2.21	0.41
1:A:364:THR:HA	1:A:367:ALA:HB3	2.03	0.41
1:B:392:LEU:HD13	1:B:412:LYS:HD3	2.03	0.41
1:C:328:HIS:C	1:C:330:TRP:N	2.74	0.41
1:D:91:ARG:NH2	1:D:175:ARG:HD2	2.36	0.41
1:D:294:PHE:HA	1:D:295:PRO:HD2	1.88	0.41
1:D:467:SER:C	1:D:469:ASN:N	2.74	0.41
1:D:517:TRP:HH2	1:D:525:PHE:CD2	2.39	0.41
1:D:74:LEU:CD2	1:D:74:LEU:N	2.84	0.41
1:A:243:MET:CE	1:A:249:ILE:HG13	2.51	0.41
1:B:228:PRO:HA	1:B:231:ILE:HG13	2.03	0.41
1:B:324:HIS:ND1	1:B:350:THR:HG22	2.36	0.41
1:B:400:ASP:HB3	1:B:403:ASP:CG	2.41	0.41
1:B:43:THR:HG21	1:B:47:TYR:HE1	1.86	0.41
1:B:499:ILE:C	1:B:501:GLN:N	2.72	0.41
1:B:376:GLN:OE1	1:B:524:HIS:CD2	2.74	0.41
1:B:564:VAL:HG23	1:B:572:TYR:OH	2.20	0.41
1:B:531:VAL:CG1	1:B:565:ARG:HB3	2.51	0.41
1:B:595:LEU:HD21	1:B:604:TRP:CZ3	2.56	0.41
1:B:624:VAL:HA	1:B:627:VAL:HG22	2.03	0.41
1:C:369:MET:CG	1:C:492:PHE:CE1	3.04	0.41
1:C:97:ARG:NH1	1:C:99:MET:HE3	2.13	0.41
1:D:190:TYR:CD1	1:D:222:MET:HB3	2.56	0.41
1:D:540:ASN:O	1:D:544:ALA:CB	2.68	0.41
1:D:62:ASP:OD1	1:D:64:ASP:N	2.53	0.41
1:D:84:ALA:HA	1:D:85:PRO:HD3	1.95	0.41
1:A:249:ILE:CD1	1:A:260:VAL:HA	2.50	0.41
1:A:344:TRP:HA	1:A:409:PRO:HB2	2.03	0.41
1:A:454:LEU:O	1:A:454:LEU:HD23	2.21	0.41
1:A:90:THR:HG23	1:A:91:ARG:N	2.35	0.41
1:B:172:ILE:HA	1:B:182:ASP:OD2	2.21	0.41
1:B:332:GLY:C	1:B:336:THR:CG2	2.89	0.41
1:B:51:LYS:HB2	1:B:79:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:N	1:B:74:LEU:HD22	2.35	0.41
1:C:313:ALA:HB2	1:C:318:LEU:CD2	2.51	0.41
1:C:440:HIS:O	1:C:443:GLN:HB2	2.21	0.41
1:C:579:LEU:HD23	1:C:588:ILE:HG22	2.03	0.41
1:C:609:TYR:O	1:C:609:TYR:CG	2.74	0.41
1:C:62:ASP:OD1	1:C:64:ASP:N	2.54	0.41
1:D:148:GLY:HA3	1:D:173:HIS:HB3	2.03	0.41
1:D:175:ARG:HH21	1:D:182:ASP:HB3	1.86	0.41
1:D:324:HIS:ND1	1:D:350:THR:HG22	2.35	0.41
1:D:547:LEU:H	1:D:547:LEU:CD1	2.29	0.41
1:A:144:GLU:OE2	1:A:145:LYS:N	2.53	0.40
1:A:162:LYS:HE3	1:A:199:ASP:HB3	2.03	0.40
1:A:297:GLY:HA2	1:A:308:THR:HG21	2.02	0.40
1:A:355:ASN:O	1:A:358:MET:HB2	2.22	0.40
1:A:471:ILE:O	1:A:475:ILE:HG12	2.21	0.40
1:B:222:MET:HE3	1:B:222:MET:HB2	1.64	0.40
1:B:297:GLY:HA2	1:B:308:THR:HG21	2.03	0.40
1:B:372:ALA:O	1:B:373:LEU:C	2.57	0.40
1:B:372:ALA:O	1:B:374:GLY:N	2.54	0.40
1:B:539:VAL:O	1:B:540:ASN:C	2.59	0.40
1:C:514:THR:O	1:C:516:GLN:N	2.53	0.40
1:C:527:ASN:OD1	1:C:558:ALA:CB	2.66	0.40
1:D:523:LEU:O	1:D:527:ASN:HB2	2.22	0.40
1:A:373:LEU:HA	1:A:373:LEU:HD12	1.85	0.40
1:B:356:ARG:HA	1:B:356:ARG:HD2	1.90	0.40
1:B:386:ASP:O	1:B:388:SER:N	2.45	0.40
1:B:458:LEU:HA	1:B:458:LEU:HD23	1.91	0.40
1:B:484:ALA:O	1:B:485:PRO:C	2.59	0.40
1:B:582:ILE:CG1	1:B:583:GLY:N	2.82	0.40
1:B:70:GLY:O	1:B:71:PHE:HB3	2.21	0.40
1:B:90:THR:HG23	1:B:91:ARG:N	2.36	0.40
1:D:296:PHE:N	1:D:296:PHE:CD1	2.88	0.40
1:D:41:ALA:C	1:D:43:THR:H	2.25	0.40
1:A:534:ASP:HA	1:A:566:ALA:O	2.20	0.40
1:B:137:ARG:HH11	1:B:137:ARG:HD3	1.66	0.40
1:B:276:MET:HE3	1:B:356:ARG:HB3	2.03	0.40
1:D:339:SER:OG	1:D:342:ASP:OD2	2.37	0.40
1:D:502:LEU:HD11	1:D:507:LEU:CD1	2.40	0.40
1:A:567:ASP:CB	1:A:569:LYS:HE3	2.43	0.40
1:A:588:ILE:HG13	1:A:589:VAL:N	2.36	0.40
1:B:205:SER:O	1:B:222:MET:HE3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:HD22	1:B:304:LEU:HD11	2.03	0.40
1:B:358:MET:CE	1:B:366:ARG:NH1	2.79	0.40
1:B:569:LYS:CD	1:B:570:GLU:N	2.76	0.40
1:D:168:GLN:NE2	1:D:299:MET:HG3	2.35	0.40
1:D:263:PHE:C	1:D:265:ASP:H	2.25	0.40
1:A:290:LEU:N	1:A:290:LEU:HD12	2.37	0.40
1:B:605:ALA:O	1:B:608:VAL:HG22	2.21	0.40
1:C:337:ASN:HD22	1:C:337:ASN:H	1.70	0.40
1:C:425:GLY:HA3	3:C:929:HOH:O	2.21	0.40
1:D:315:ASP:OD1	1:D:317:SER:CB	2.70	0.40
1:D:328:HIS:HA	1:D:331:SER:O	2.21	0.40
1:D:373:LEU:HA	1:D:373:LEU:HD12	1.88	0.40
1:D:486:GLN:HG3	3:D:820:HOH:O	2.21	0.40

All (3) 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:B:97:ARG:NH1	1:C:217:ASP:OD1[1_545]	1.80	0.40
3:C:946:HOH:O	3:D:797:HOH:O[1_565]	2.03	0.17
3:B:712:HOH:O	3:C:856:HOH:O[1_545]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/605 (96%)	484 (83%)	81 (14%)	16 (3%)	6	14
1	B	575/605 (95%)	481 (84%)	81 (14%)	13 (2%)	7	19
1	C	575/605 (95%)	478 (83%)	84 (15%)	13 (2%)	7	19
1	D	576/605 (95%)	482 (84%)	74 (13%)	20 (4%)	4	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2307/2420 (95%)	1925 (83%)	320 (14%)	62 (3%)	6　15

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	41	ALA
1	A	509	LEU
1	A	511	GLN
1	B	504	THR
1	B	509	LEU
1	B	540	ASN
1	C	509	LEU
1	D	507	LEU
1	D	509	LEU
1	D	511	GLN
1	D	586	LYS
1	A	198	LYS
1	A	329	SER
1	A	504	THR
1	A	586	LYS
1	A	599	ALA
1	B	500	ASN
1	B	501	GLN
1	B	586	LYS
1	C	504	THR
1	C	511	GLN
1	C	586	LYS
1	D	329	SER
1	D	502	LEU
1	D	504	THR
1	A	479	GLY
1	B	515	ALA
1	B	599	ALA
1	C	103	SER
1	D	41	ALA
1	D	468	ASP
1	A	496	ASP
1	A	587	LEU
1	C	479	GLY
1	C	563	SER
1	C	587	LEU

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Mol	Chain	Res	Type
1	D	197	ASP
1	D	563	SER
1	D	569	LYS
1	D	587	LEU
1	A	292	PRO
1	B	292	PRO
1	B	502	LEU
1	B	587	LEU
1	C	500	ASN
1	C	599	ALA
1	D	292	PRO
1	D	479	GLY
1	A	199	ASP
1	A	502	LEU
1	A	534	ASP
1	C	292	PRO
1	C	531	VAL
1	D	103	SER
1	D	515	ALA
1	D	599	ALA
1	B	180	ILE
1	B	531	VAL
1	C	180	ILE
1	D	531	VAL
1	D	180	ILE

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	502/517 (97%)	454 (90%)	48 (10%)	10	22
1	B	495/517 (96%)	441 (89%)	54 (11%)	7	17
1	C	496/517 (96%)	447 (90%)	49 (10%)	9	21
1	D	498/517 (96%)	449 (90%)	49 (10%)	9	21
All	All	1991/2068 (96%)	1791 (90%)	200 (10%)	9	21

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	39	THR
1	A	49	GLN
1	A	58	ASP
1	A	65	LYS
1	A	74	LEU
1	A	77	ASP
1	A	86	LEU
1	A	90	THR
1	A	123	SER
1	A	129	THR
1	A	130	PRO
1	A	144	GLU
1	A	160	LYS
1	A	193	ARG
1	A	299	MET
1	A	318	LEU
1	A	326	LEU
1	A	334	LEU
1	A	346	ASN
1	A	364	THR
1	A	366	ARG
1	A	383	LEU
1	A	384	GLU
1	A	392	LEU
1	A	426	ARG
1	A	428	ARG
1	A	454	LEU
1	A	458	LEU
1	A	475	ILE
1	A	482	SER
1	A	488	THR
1	A	490	ASN
1	A	493	LYS
1	A	497	LYS
1	A	500	ASN
1	A	501	GLN
1	A	503	VAL
1	A	505	ASP
1	A	506	GLU
1	A	512	LEU
1	A	536	GLN

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Mol	Chain	Res	Type
1	A	538	MET
1	A	541	LEU
1	A	543	LYS
1	A	547	LEU
1	A	582	ILE
1	A	613	ARG
1	B	39	THR
1	B	49	GLN
1	B	58	ASP
1	B	74	LEU
1	B	77	ASP
1	B	86	LEU
1	B	90	THR
1	B	97	ARG
1	B	123	SER
1	B	129	THR
1	B	130	PRO
1	B	144	GLU
1	B	193	ARG
1	B	198	LYS
1	B	215	ASP
1	B	299	MET
1	B	318	LEU
1	B	326	LEU
1	B	331	SER
1	B	334	LEU
1	B	346	ASN
1	B	364	THR
1	B	366	ARG
1	B	371	GLN
1	B	383	LEU
1	B	384	GLU
1	B	392	LEU
1	B	403	ASP
1	B	406	SER
1	B	426	ARG
1	B	428	ARG
1	B	454	LEU
1	B	458	LEU
1	B	475	ILE
1	B	485	PRO
1	B	488	THR

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Mol	Chain	Res	Type
1	B	490	ASN
1	B	492	PHE
1	B	493	LYS
1	B	497	LYS
1	B	500	ASN
1	B	503	VAL
1	B	505	ASP
1	B	506	GLU
1	B	509	LEU
1	B	510	GLU
1	B	520	HIS
1	B	526	ILE
1	B	541	LEU
1	B	543	LYS
1	B	547	LEU
1	B	569	LYS
1	B	582	ILE
1	B	613	ARG
1	C	39	THR
1	C	49	GLN
1	C	58	ASP
1	C	65	LYS
1	C	74	LEU
1	C	77	ASP
1	C	82	ASN
1	C	86	LEU
1	C	90	THR
1	C	129	THR
1	C	142	SER
1	C	144	GLU
1	C	193	ARG
1	C	215	ASP
1	C	224	GLN
1	C	299	MET
1	C	318	LEU
1	C	326	LEU
1	C	334	LEU
1	C	364	THR
1	C	366	ARG
1	C	371	GLN
1	C	383	LEU
1	C	384	GLU

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Mol	Chain	Res	Type
1	C	392	LEU
1	C	405	PHE
1	C	426	ARG
1	C	454	LEU
1	C	458	LEU
1	C	475	ILE
1	C	482	SER
1	C	486	GLN
1	C	488	THR
1	C	490	ASN
1	C	493	LYS
1	C	497	LYS
1	C	505	ASP
1	C	506	GLU
1	C	508	THR
1	C	509	LEU
1	C	510	GLU
1	C	512	LEU
1	C	522	TRP
1	C	527	ASN
1	C	543	LYS
1	C	547	LEU
1	C	569	LYS
1	C	582	ILE
1	C	613	ARG
1	D	38	LEU
1	D	39	THR
1	D	49	GLN
1	D	58	ASP
1	D	65	LYS
1	D	74	LEU
1	D	77	ASP
1	D	86	LEU
1	D	90	THR
1	D	129	THR
1	D	142	SER
1	D	144	GLU
1	D	193	ARG
1	D	209	GLU
1	D	224	GLN
1	D	284	ARG
1	D	299	MET

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Mol	Chain	Res	Type
1	D	318	LEU
1	D	326	LEU
1	D	334	LEU
1	D	364	THR
1	D	366	ARG
1	D	371	GLN
1	D	383	LEU
1	D	384	GLU
1	D	392	LEU
1	D	405	PHE
1	D	426	ARG
1	D	428	ARG
1	D	454	LEU
1	D	458	LEU
1	D	475	ILE
1	D	482	SER
1	D	485	PRO
1	D	488	THR
1	D	490	ASN
1	D	492	PHE
1	D	493	LYS
1	D	497	LYS
1	D	500	ASN
1	D	502	LEU
1	D	503	VAL
1	D	505	ASP
1	D	510	GLU
1	D	512	LEU
1	D	543	LYS
1	D	569	LYS
1	D	582	ILE
1	D	613	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	132	ASN
1	A	168	GLN
1	A	301	ASN
1	A	337	ASN
1	A	376	GLN

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	414	GLN
1	A	457	ASN
1	A	498	GLN
1	A	500	ASN
1	A	511	GLN
1	A	524	HIS
1	A	528	ASN
1	A	549	ASN
1	B	104	GLN
1	B	132	ASN
1	B	168	GLN
1	B	301	ASN
1	B	371	GLN
1	B	376	GLN
1	B	391	GLN
1	B	498	GLN
1	B	500	ASN
1	B	524	HIS
1	B	549	ASN
1	B	557	HIS
1	C	104	GLN
1	C	132	ASN
1	C	168	GLN
1	C	245	HIS
1	C	301	ASN
1	C	337	ASN
1	C	391	GLN
1	C	414	GLN
1	C	457	ASN
1	C	464	ASN
1	C	498	GLN
1	C	500	ASN
1	C	501	GLN
1	C	524	HIS
1	C	549	ASN
1	C	557	HIS
1	D	132	ASN
1	D	168	GLN
1	D	207	ASN
1	D	246	GLN
1	D	301	ASN

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Mol	Chain	Res	Type
1	D	337	ASN
1	D	379	ASN
1	D	391	GLN
1	D	414	GLN
1	D	457	ASN
1	D	486	GLN
1	D	498	GLN
1	D	500	ASN
1	D	511	GLN
1	D	549	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	587/605 (97%)	-0.12	11 (1%)	67	68	7, 25, 67, 83	0
1	B	581/605 (96%)	0.02	31 (5%)	27	25	9, 25, 74, 87	0
1	C	581/605 (96%)	0.03	25 (4%)	36	34	7, 27, 74, 86	0
1	D	582/605 (96%)	0.05	25 (4%)	36	34	8, 27, 76, 89	0
All	All	2331/2420 (96%)	-0.01	92 (3%)	40	39	7, 26, 73, 89	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	571	VAL	7.3
1	D	605	ALA	7.1
1	B	596	ALA	6.5
1	B	595	LEU	6.3
1	D	541	LEU	5.4
1	D	568	TYR	5.3
1	C	505	ASP	5.0
1	B	505	ASP	4.9
1	C	568	TYR	4.9
1	B	569	LYS	4.3
1	D	504	THR	4.2
1	D	606	VAL	4.2
1	A	509	LEU	4.1
1	B	571	VAL	4.1
1	B	504	THR	4.0
1	B	568	TYR	3.9
1	D	567	ASP	3.7
1	C	547	LEU	3.7
1	D	602	LYS	3.7
1	B	501	GLN	3.6
1	C	504	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	532	ASP	3.5
1	C	541	LEU	3.5
1	B	508	THR	3.4
1	C	545	PHE	3.4
1	C	508	THR	3.3
1	B	503	VAL	3.3
1	D	505	ASP	3.2
1	B	567	ASP	3.1
1	C	605	ALA	3.0
1	B	570	GLU	3.0
1	D	604	TRP	3.0
1	B	532	ASP	3.0
1	D	570	GLU	2.9
1	D	566	ALA	2.9
1	D	601	SER	2.9
1	C	627	VAL	2.8
1	A	403	ASP	2.8
1	A	545	PHE	2.8
1	B	601	SER	2.7
1	B	556	ALA	2.7
1	B	591	LEU	2.7
1	B	403	ASP	2.7
1	B	629	LYS	2.7
1	D	596	ALA	2.6
1	B	608	VAL	2.6
1	B	605	ALA	2.5
1	C	503	VAL	2.5
1	A	534	ASP	2.5
1	D	576	ALA	2.5
1	D	627	VAL	2.5
1	A	508	THR	2.5
1	C	606	VAL	2.4
1	D	569	LYS	2.4
1	B	502	LEU	2.4
1	D	499	ILE	2.4
1	C	507	LEU	2.4
1	B	600	GLU	2.4
1	C	502	LEU	2.3
1	D	532	ASP	2.3
1	C	566	ALA	2.3
1	C	509	LEU	2.3
1	D	507	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	503	VAL	2.3
1	A	595	LEU	2.3
1	B	531	VAL	2.3
1	B	627	VAL	2.3
1	C	487	PRO	2.2
1	A	505	ASP	2.2
1	D	510	GLU	2.2
1	C	562	LEU	2.2
1	A	627	VAL	2.2
1	D	591	LEU	2.2
1	D	559	TRP	2.2
1	C	597	LYS	2.1
1	C	569	LYS	2.1
1	A	540	ASN	2.1
1	B	604	TRP	2.1
1	C	623	THR	2.1
1	B	564	VAL	2.1
1	B	509	LEU	2.1
1	B	615	GLY	2.1
1	A	615	GLY	2.1
1	B	507	LEU	2.1
1	D	198	LYS	2.1
1	B	618	GLY	2.1
1	A	531	VAL	2.0
1	C	596	ALA	2.0
1	B	561	LEU	2.0
1	C	602	LYS	2.0
1	C	601	SER	2.0
1	D	564	VAL	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	701	1/1	0.88	0.20	2.66	24,24,24,24	1
2	ZN	D	701	1/1	0.97	0.12	-1.32	28,28,28,28	1
2	ZN	A	701	1/1	0.98	0.09	-3.10	9,9,9,9	1
2	ZN	C	701	1/1	0.96	0.08	-4.06	15,15,15,15	1

6.5 Other polymers ⓘ

There are no such residues in this entry.