



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:49 AM UTC

PDB ID : 1ZQ1 / pdb_00001zq1
Title : Structure of GatDE tRNA-Dependent Amidotransferase from *Pyrococcus abyssi*
Authors : Schmitt, E.; Panvert, M.; Blanquet, S.; Mechulam, Y.
Deposited on : 2005-05-18
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

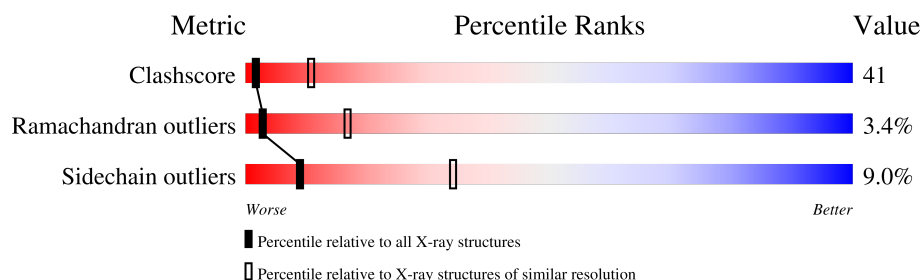
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

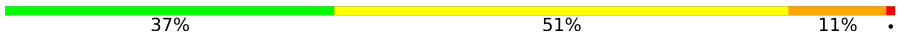
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	438	
1	B	438	
2	C	633	
2	D	633	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ASP	A	1000	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14869 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 Glutamyl-tRNA(Gln) amidotransferase subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	Se	0	0	0
			3406	2159	578	650	5	14			
1	B	437	Total	C	N	O	S	Se	0	0	0
			3406	2162	575	650	5	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9V0T9
A	36	MSE	MET	modified residue	UNP Q9V0T9
A	127	LEU	VAL	conflict	UNP Q9V0T9
A	149	MSE	MET	modified residue	UNP Q9V0T9
A	181	MSE	MET	modified residue	UNP Q9V0T9
A	191	MSE	MET	modified residue	UNP Q9V0T9
A	217	MSE	MET	modified residue	UNP Q9V0T9
A	225	MSE	MET	modified residue	UNP Q9V0T9
A	234	MSE	MET	modified residue	UNP Q9V0T9
A	237	MSE	MET	modified residue	UNP Q9V0T9
A	257	MSE	MET	modified residue	UNP Q9V0T9
A	362	MSE	MET	modified residue	UNP Q9V0T9
A	393	MSE	MET	modified residue	UNP Q9V0T9
A	403	MSE	MET	modified residue	UNP Q9V0T9
A	418	MSE	MET	modified residue	UNP Q9V0T9
A	419	MSE	MET	modified residue	UNP Q9V0T9
B	1	MSE	MET	modified residue	UNP Q9V0T9
B	36	MSE	MET	modified residue	UNP Q9V0T9
B	127	LEU	VAL	conflict	UNP Q9V0T9
B	149	MSE	MET	modified residue	UNP Q9V0T9
B	181	MSE	MET	modified residue	UNP Q9V0T9
B	191	MSE	MET	modified residue	UNP Q9V0T9
B	217	MSE	MET	modified residue	UNP Q9V0T9
B	225	MSE	MET	modified residue	UNP Q9V0T9
B	234	MSE	MET	modified residue	UNP Q9V0T9

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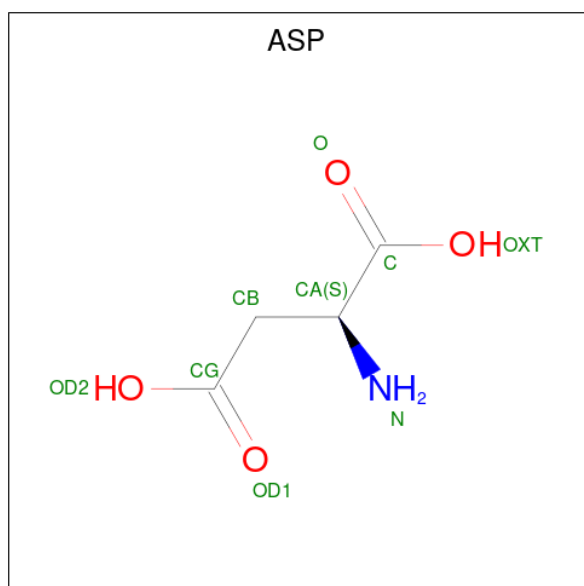
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Chain	Residue	Modelled	Actual	Comment	Reference
B	237	MSE	MET	modified residue	UNP Q9V0T9
B	257	MSE	MET	modified residue	UNP Q9V0T9
B	362	MSE	MET	modified residue	UNP Q9V0T9
B	393	MSE	MET	modified residue	UNP Q9V0T9
B	403	MSE	MET	modified residue	UNP Q9V0T9
B	418	MSE	MET	modified residue	UNP Q9V0T9
B	419	MSE	MET	modified residue	UNP Q9V0T9

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	508	Total	C	N	O	S	0	0	0
			4005	2543	700	755	7			
2	D	508	Total	C	N	O	S	0	0	0
			3966	2523	693	743	7			

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	24	Total 24	O 24	0	0
4	C	22	Total 22	O 22	0	0
4	D	10	Total 10	O 10	0	0

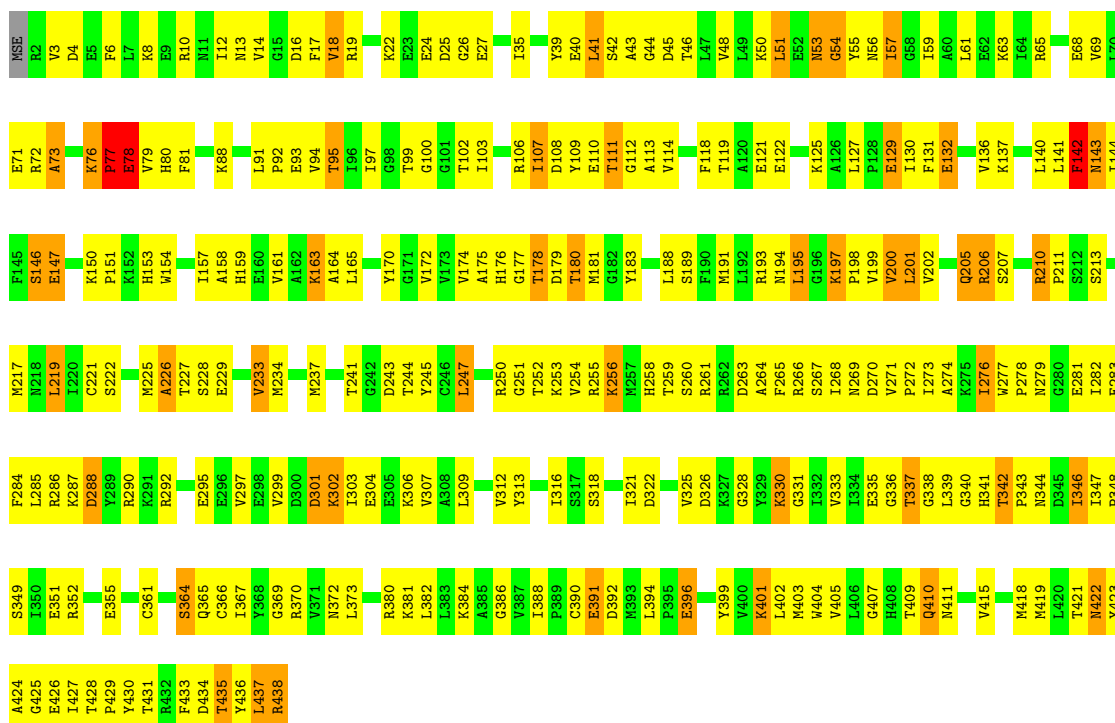
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

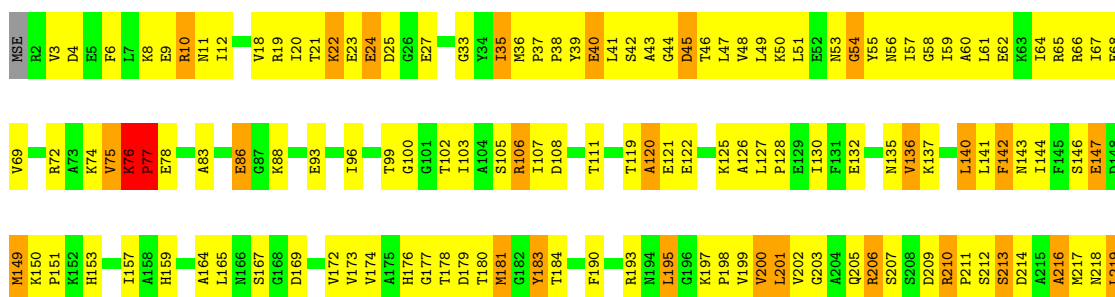
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit D

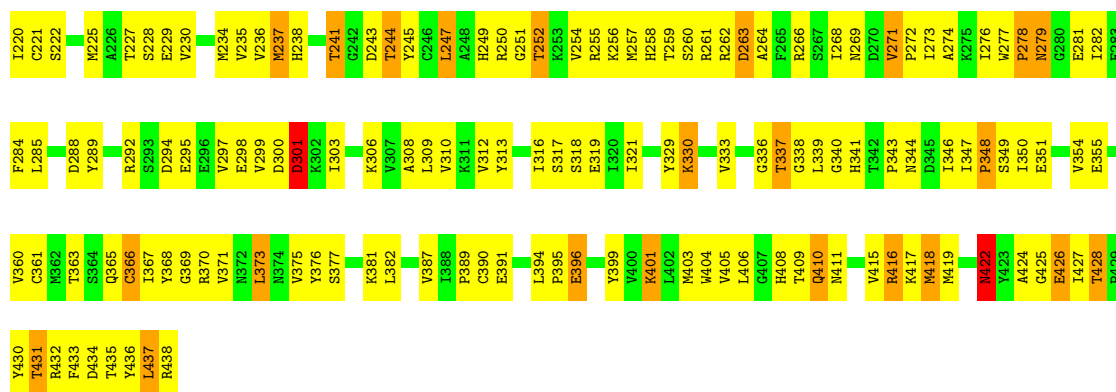
Chain A: 



• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit D

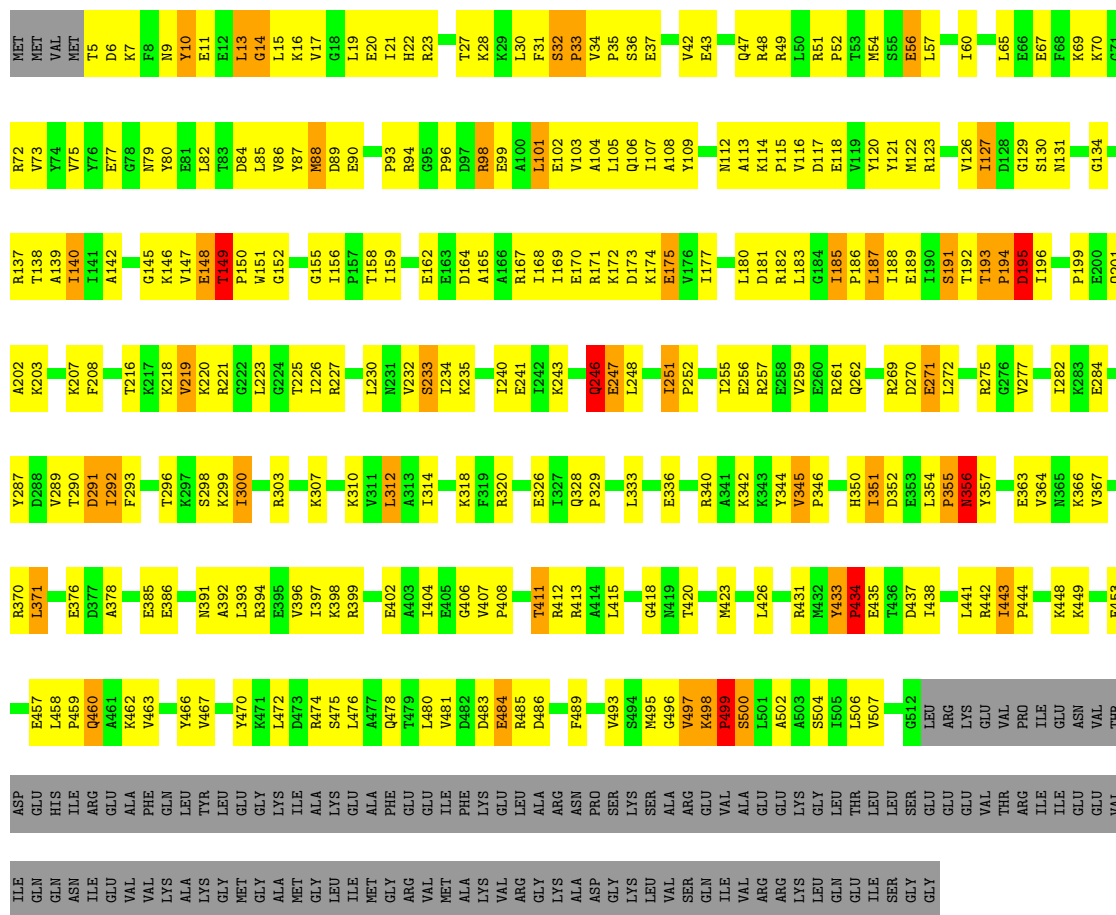
Chain B: 





• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain C: 36% 38% 6% 20%



• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain D: 34% 40% 5% 20%





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.70Å 138.20Å 134.40Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.9 (50.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14869	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3455	1.12	26/4651 (0.6%)
1	B	0.53	0/3455	1.10	22/4652 (0.5%)
2	C	0.48	0/4070	1.07	26/5497 (0.5%)
2	D	0.42	0/4031	0.99	18/5450 (0.3%)
All	All	0.49	0/15011	1.07	92/20250 (0.5%)

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASP	N-CA-C	-12.45	96.82	112.88
2	C	345	VAL	CA-C-N	8.53	129.36	119.47
2	C	345	VAL	C-N-CA	8.53	129.36	119.47
2	C	418	GLY	N-CA-C	-8.44	102.85	115.00
1	A	53	ASN	N-CA-C	-8.40	103.63	114.04
1	B	200	VAL	N-CA-C	8.03	119.66	107.77
2	D	129	GLY	N-CA-C	-7.96	103.55	115.00
1	B	210	ARG	CA-C-N	7.73	129.50	119.84
1	B	210	ARG	C-N-CA	7.73	129.50	119.84
1	B	106	ARG	N-CA-C	-7.59	99.23	110.46
1	B	229	GLU	N-CA-C	-7.56	103.62	112.92
2	C	88	MET	N-CA-C	-7.56	103.89	113.72
2	C	129	GLY	N-CA-C	-7.47	104.41	114.95
1	A	54	GLY	N-CA-C	-7.46	105.06	113.79
2	C	351	ILE	N-CA-C	7.45	119.11	110.62
2	D	445	ASP	N-CA-C	-7.32	103.29	111.71
1	B	262	ARG	N-CA-C	-7.28	103.66	112.54
1	A	200	VAL	N-CA-C	7.25	119.41	107.24
2	D	38	LEU	N-CA-C	-7.02	101.48	110.53
1	A	388	ILE	N-CA-C	6.99	113.92	107.56
2	C	127	ILE	N-CA-C	6.92	117.04	110.53
1	A	256	LYS	N-CA-C	-6.80	98.84	109.25
1	A	410	GLN	N-CA-C	-6.74	104.62	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	GLY	N-CA-C	-6.71	107.09	115.08
2	D	88	MET	N-CA-C	-6.65	103.64	113.61
1	A	132	GLU	N-CA-C	-6.60	103.83	112.41
2	D	407	VAL	N-CA-C	6.57	114.05	107.55
1	A	226	ALA	N-CA-C	-6.56	104.16	111.71
2	C	433	TYR	CA-C-N	6.54	128.02	119.84
2	C	433	TYR	C-N-CA	6.54	128.02	119.84
1	A	77	PRO	N-CA-C	6.46	125.78	112.47
2	C	32	SER	CA-C-N	6.44	127.89	119.84
2	C	32	SER	C-N-CA	6.44	127.89	119.84
1	B	310	VAL	N-CA-C	6.43	117.14	107.75
1	B	120	ALA	N-CA-C	-6.40	104.38	111.36
1	B	167	SER	N-CA-C	-6.32	104.45	111.71
2	D	30	LEU	N-CA-C	6.29	119.80	111.75
1	B	235	VAL	N-CA-C	-6.28	99.42	108.53
1	B	264	ALA	N-CA-C	6.26	124.14	110.80
1	A	301	ASP	N-CA-C	6.25	117.78	110.97
2	C	180	LEU	N-CA-C	6.20	120.11	112.54
2	D	198	HIS	CA-C-N	6.13	126.31	119.32
2	D	198	HIS	C-N-CA	6.13	126.31	119.32
2	D	32	SER	CA-C-N	6.10	127.46	119.84
2	D	32	SER	C-N-CA	6.10	127.46	119.84
2	C	30	LEU	N-CA-C	6.08	119.54	111.75
2	C	13	LEU	N-CA-C	-6.02	100.75	109.59
2	C	394	ARG	N-CA-C	-6.01	104.36	111.03
2	D	34	VAL	CA-C-N	6.01	126.95	119.98
2	D	34	VAL	C-N-CA	6.01	126.95	119.98
1	A	43	ALA	N-CA-C	-5.98	102.22	110.35
2	C	145	GLY	N-CA-C	-5.96	103.47	112.41
2	C	149	THR	N-CA-C	5.95	113.58	108.22
2	D	436	THR	N-CA-C	5.91	119.59	112.38
1	B	43	ALA	N-CA-C	5.82	118.70	110.50
1	B	136	VAL	N-CA-C	5.81	117.12	108.23
1	A	288	ASP	N-CA-C	5.81	118.33	109.62
1	A	422	ASN	N-CA-C	5.79	118.64	108.56
1	B	53	ASN	N-CA-C	-5.75	105.76	112.89
1	B	278	PRO	N-CA-C	-5.72	105.22	113.75
1	A	373	LEU	N-CA-C	5.71	119.32	112.93
1	A	205	GLN	N-CA-C	-5.66	105.48	112.90
1	A	76	LYS	CA-C-N	5.66	126.91	119.84
1	A	76	LYS	C-N-CA	5.66	126.91	119.84
1	B	301	ASP	N-CA-C	5.63	118.96	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	TYR	N-CA-C	-5.61	102.97	111.56
2	C	195	ASP	N-CA-C	5.58	120.36	113.50
1	A	364	SER	N-CA-C	5.54	118.43	109.40
2	D	61	ASP	CA-C-N	5.48	124.94	119.24
2	D	61	ASP	C-N-CA	5.48	124.94	119.24
2	D	465	ARG	N-CA-C	-5.48	106.27	113.12
2	D	502	ALA	N-CA-C	-5.41	105.07	110.97
1	B	76	LYS	N-CA-C	5.36	121.66	109.81
2	C	158	THR	N-CA-C	5.36	117.91	108.75
2	C	443	ILE	CA-C-N	5.34	125.26	119.76
2	C	443	ILE	C-N-CA	5.34	125.26	119.76
1	A	322	ASP	N-CA-C	-5.32	105.38	111.07
1	A	18	VAL	N-CA-C	5.29	116.53	108.80
2	C	251	ILE	CA-C-N	-5.29	113.08	118.85
2	C	251	ILE	C-N-CA	-5.29	113.08	118.85
1	A	285	LEU	N-CA-C	-5.21	106.32	113.30
1	B	422	ASN	N-CA-C	5.10	117.61	108.17
2	C	219	VAL	N-CA-C	-5.09	100.98	108.11
1	A	197	LYS	CA-C-N	5.09	125.24	119.90
1	A	197	LYS	C-N-CA	5.09	125.24	119.90
2	C	185	ILE	CA-C-N	5.09	125.00	119.76
2	C	185	ILE	C-N-CA	5.09	125.00	119.76
1	A	228	SER	N-CA-C	5.08	117.36	110.35
2	D	145	GLY	N-CA-C	-5.05	102.91	112.10
1	A	178	THR	N-CA-C	5.02	119.43	112.45
1	B	366	CYS	N-CA-C	-5.02	101.57	109.25
1	B	410	GLN	N-CA-C	-5.02	107.11	114.39

There are no chirality outliers.

There are no planarity outliers.

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	3406	0	3410	370	0
1	B	3406	0	3417	353	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4005	0	4058	296	0
2	D	3966	0	4003	299	0
3	A	9	0	3	4	0
3	B	9	0	3	1	0
4	A	12	0	0	0	0
4	B	24	0	0	0	0
4	C	22	0	0	0	0
4	D	10	0	0	0	0
All	All	14869	0	14894	1216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (1216) 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)
2:C:192:THR:HG22	2:C:193:THR:H	1.02	1.12
2:D:192:THR:HG22	2:D:193:THR:H	1.00	1.11
1:B:276:ILE:HG22	1:B:282:ILE:HG12	1.27	1.09
1:A:266:ARG:HD2	1:B:437:LEU:HD21	1.36	1.07
1:A:409:THR:HG22	1:A:411:ASN:H	1.18	1.05
1:A:76:LYS:HB2	1:A:77:PRO:CD	1.89	1.02
1:B:3:VAL:HA	1:B:61:LEU:HD11	1.40	1.02
1:A:76:LYS:CB	1:A:77:PRO:HD2	1.90	1.01
2:C:72:ARG:HG2	2:C:174:LYS:HA	1.39	1.01
1:A:221:CYS:HB3	1:A:276:ILE:HD12	1.40	1.00
1:A:76:LYS:HB2	1:A:77:PRO:HD2	1.01	0.99
1:A:380:ARG:HD2	1:B:40:GLU:HG2	1.45	0.97
1:A:3:VAL:HG22	1:A:61:LEU:HD11	1.46	0.96
1:A:402:LEU:HA	1:A:419:MSE:CE	1.97	0.95
2:C:149:THR:HG22	2:C:152:GLY:O	1.67	0.95
2:C:411:THR:HG22	2:C:426:LEU:HD23	1.48	0.95
2:C:20:GLU:OE2	2:C:191:SER:HB3	1.66	0.95
1:A:402:LEU:HA	1:A:419:MSE:HE3	1.48	0.94
2:C:192:THR:HG22	2:C:193:THR:N	1.80	0.93
1:B:433:PHE:HB2	2:C:88:MET:HE1	1.47	0.93
2:C:192:THR:CG2	2:C:193:THR:H	1.82	0.93
1:A:77:PRO:O	1:A:78:GLU:HB3	1.67	0.93
1:B:3:VAL:HG13	1:B:61:LEU:HD21	1.50	0.92
2:D:192:THR:HG22	2:D:193:THR:N	1.83	0.92
2:D:368:ILE:HG23	2:D:373:LEU:HB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:MSE:HE1	1:B:243:ASP:HB3	1.51	0.91
1:A:3:VAL:HG23	1:A:44:GLY:O	1.71	0.90
1:A:202:VAL:HG21	1:A:222:SER:CB	2.02	0.90
1:B:250:ARG:HD3	1:B:425:GLY:HA3	1.50	0.90
2:C:413:ARG:HB3	2:C:423:MET:HE2	1.54	0.89
2:D:207:LYS:HB2	2:D:248:LEU:HD21	1.55	0.88
2:C:98:ARG:CD	2:C:98:ARG:H	1.85	0.88
1:B:268:ILE:HG21	1:B:367:ILE:HG22	1.56	0.88
1:B:409:THR:HG22	1:B:411:ASN:H	1.37	0.88
2:C:293:PHE:HA	2:C:296:THR:HG23	1.52	0.88
2:D:502:ALA:O	2:D:506:LEU:HG	1.73	0.88
1:A:95:THR:HG21	1:A:164:ALA:HB1	1.55	0.88
1:B:103:ILE:HG21	1:B:219:LEU:HG	1.56	0.87
1:A:202:VAL:HG21	1:A:222:SER:HB3	1.55	0.87
1:A:50:LYS:HE3	1:A:56:ASN:HD21	1.38	0.87
1:A:108:ASP:OD1	1:A:110:GLU:HG2	1.75	0.87
2:C:106:GLN:HE21	2:C:216:THR:HG22	1.40	0.86
2:C:463:VAL:HG11	2:C:478:GLN:HE21	1.41	0.86
2:D:211:ASP:HB3	2:D:459:PRO:HD2	1.58	0.86
1:A:217:MSE:HE2	2:C:49:ARG:HH22	1.41	0.85
1:A:241:THR:O	2:C:48:ARG:NH1	2.08	0.85
2:D:411:THR:HG22	2:D:424:ARG:O	1.76	0.85
1:A:337:THR:HG22	1:A:341:HIS:HB2	1.57	0.84
1:B:165:LEU:HD13	1:B:172:VAL:HG23	1.58	0.84
1:A:165:LEU:HD23	1:A:297:VAL:HG21	1.59	0.84
1:B:119:THR:HG22	1:B:121:GLU:H	1.43	0.84
1:B:150:LYS:H	1:B:153:HIS:HD2	1.20	0.84
1:B:241:THR:HG22	2:D:48:ARG:HH12	1.41	0.84
2:D:409:GLU:HG2	2:D:426:LEU:HD22	1.60	0.84
1:A:125:LYS:HE3	2:C:60:ILE:HG12	1.60	0.84
1:A:150:LYS:H	1:A:153:HIS:HD2	1.24	0.84
2:D:72:ARG:HG2	2:D:174:LYS:HA	1.59	0.84
2:C:149:THR:HG23	2:C:151:TRP:H	1.43	0.83
2:C:257:ARG:HG3	2:C:257:ARG:HH11	1.41	0.83
1:B:344:ASN:HD22	1:B:381:LYS:NZ	1.75	0.83
2:D:340:ARG:NH1	2:D:399:ARG:HG2	1.94	0.83
1:A:409:THR:HG22	1:A:411:ASN:N	1.94	0.83
1:B:127:LEU:HD22	1:B:219:LEU:HD12	1.61	0.83
1:A:401:LYS:HD2	1:A:419:MSE:SE	2.28	0.83
2:D:193:THR:HB	2:D:195:ASP:OD1	1.79	0.82
2:D:355:PRO:HG2	2:D:361:GLN:HG2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:THR:HG23	2:D:162:GLU:HB3	1.60	0.82
2:D:289:VAL:HG13	2:D:292:ILE:HD12	1.61	0.82
1:B:69:VAL:HG11	1:B:72:ARG:HH11	1.44	0.82
1:A:78:GLU:O	1:A:78:GLU:HG3	1.81	0.81
2:D:472:LEU:H	2:D:472:LEU:HD23	1.45	0.81
1:B:241:THR:HG23	2:D:90:GLU:OE2	1.80	0.81
2:C:72:ARG:HG2	2:C:174:LYS:CA	2.09	0.81
2:D:240:ILE:HD12	2:D:262:GLN:HE21	1.44	0.81
1:B:313:TYR:H	1:B:316:ILE:HD11	1.45	0.81
1:B:100:GLY:HA2	1:B:143:ASN:HD22	1.46	0.80
1:B:217:MSE:HG3	1:B:278:PRO:HG3	1.64	0.80
1:B:59:ILE:HG21	1:B:64:ILE:HD11	1.62	0.80
2:D:192:THR:CG2	2:D:193:THR:H	1.86	0.80
2:C:22:HIS:HB2	2:C:227:ARG:HB2	1.61	0.80
1:A:18:VAL:HG13	1:A:68:GLU:O	1.82	0.80
1:A:313:TYR:CE1	1:A:316:ILE:HG12	2.15	0.80
1:A:336:GLY:O	1:A:365:GLN:HG3	1.81	0.80
1:B:303:ILE:HG22	1:B:404:TRP:HA	1.64	0.79
1:B:241:THR:O	2:D:48:ARG:NH1	2.15	0.79
2:D:149:THR:HG22	2:D:152:GLY:O	1.83	0.79
2:C:98:ARG:H	2:C:98:ARG:HD3	1.48	0.79
2:D:65:LEU:HD22	2:D:69:LYS:HE3	1.65	0.79
2:C:164:ASP:HB2	2:C:187:LEU:HD13	1.65	0.79
1:B:3:VAL:HG23	1:B:44:GLY:HA2	1.64	0.78
1:B:257:MSE:HE2	1:B:268:ILE:HD12	1.64	0.78
1:A:179:ASP:OD2	3:A:1000:ASP:HB3	1.84	0.78
1:A:179:ASP:OD1	1:B:337:THR:HG23	1.84	0.78
2:C:292:ILE:HD13	2:C:366:LYS:HB3	1.65	0.78
1:A:3:VAL:HG22	1:A:61:LEU:CD1	2.14	0.77
2:C:463:VAL:HG11	2:C:478:GLN:NE2	1.98	0.77
1:B:258:HIS:HD2	1:B:260:SER:H	1.29	0.77
1:A:258:HIS:HD2	1:A:261:ARG:H	1.30	0.77
2:C:293:PHE:HA	2:C:296:THR:CG2	2.15	0.76
2:D:138:THR:HG22	2:D:139:ALA:H	1.51	0.76
2:D:480:LEU:HD21	2:D:489:PHE:CG	2.21	0.76
1:A:193:ARG:HA	1:A:193:ARG:NE	2.01	0.76
2:C:287:TYR:CD2	2:C:371:LEU:HD22	2.20	0.76
1:B:337:THR:HG22	1:B:341:HIS:HB2	1.66	0.76
2:C:243:LYS:HB2	2:C:423:MET:HE1	1.68	0.76
1:B:221:CYS:HB3	1:B:276:ILE:CD1	2.16	0.75
1:A:217:MSE:HG3	1:A:278:PRO:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LYS:O	1:B:76:LYS:HG3	1.85	0.75
1:B:375:VAL:HG13	2:C:437:ASP:OD1	1.86	0.75
2:C:502:ALA:O	2:C:506:LEU:HG	1.86	0.75
1:A:370:ARG:HH11	1:A:391:GLU:HG3	1.51	0.75
1:B:126:ALA:C	1:B:127:LEU:HD12	2.10	0.75
1:B:88:LYS:H	1:B:135:ASN:HD21	1.31	0.75
2:D:243:LYS:HB2	2:D:423:MET:HE1	1.68	0.75
2:D:277:VAL:HG22	2:D:318:LYS:HD2	1.67	0.75
1:A:312:VAL:HA	1:A:316:ILE:HD11	1.67	0.75
1:B:318:SER:HB2	1:B:349:SER:HB3	1.68	0.75
1:A:146:SER:HB2	1:A:180:THR:H	1.51	0.75
2:C:14:GLY:H	2:C:235:LYS:HB2	1.50	0.75
2:D:457:GLU:CD	2:D:457:GLU:H	1.93	0.75
1:B:126:ALA:HB2	2:D:54:MET:CE	2.16	0.75
1:A:217:MSE:HE1	1:A:243:ASP:HB3	1.68	0.74
1:B:179:ASP:OD2	3:B:5000:ASP:HB3	1.87	0.74
1:B:344:ASN:HD22	1:B:381:LYS:HZ3	1.34	0.74
2:D:22:HIS:HB2	2:D:227:ARG:HB2	1.69	0.74
1:A:193:ARG:HA	1:A:193:ARG:HE	1.52	0.74
1:A:51:LEU:HD21	1:A:57:ILE:HD12	1.69	0.74
1:A:437:LEU:HD21	1:B:266:ARG:HD2	1.70	0.74
2:D:342:LYS:HA	2:D:345:VAL:O	1.87	0.74
1:B:165:LEU:HD23	1:B:297:VAL:HG21	1.69	0.74
2:C:221:ARG:HH22	2:C:484:GLU:CB	2.00	0.74
2:D:394:ARG:HA	2:D:397:ILE:HD12	1.69	0.74
1:B:150:LYS:H	1:B:153:HIS:CD2	2.05	0.73
2:C:193:THR:HB	2:C:195:ASP:OD1	1.88	0.73
1:A:180:THR:HG23	1:A:183:TYR:HB2	1.68	0.73
2:C:326:GLU:OE2	2:C:329:PRO:HA	1.88	0.73
2:D:498:LYS:CB	2:D:502:ALA:HB3	2.18	0.73
1:B:39:TYR:HD2	1:B:42:SER:HG	1.34	0.73
1:B:313:TYR:N	1:B:316:ILE:HD11	2.03	0.73
1:B:433:PHE:HB2	2:C:88:MET:CE	2.19	0.73
2:C:36:SER:HB2	2:C:185:ILE:HG12	1.69	0.73
2:C:314:ILE:HG12	2:C:393:LEU:HD22	1.71	0.73
2:D:85:LEU:HD23	2:D:88:MET:HE3	1.70	0.72
1:A:153:HIS:O	1:A:157:ILE:HG12	1.90	0.72
1:B:244:THR:HG22	1:B:277:TRP:CZ3	2.25	0.72
1:A:12:ILE:HG21	1:A:35:ILE:HD12	1.72	0.71
2:D:411:THR:HG21	2:D:424:ARG:HD2	1.70	0.71
2:D:234:ILE:HD11	2:D:259:VAL:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:CG	2:C:56:GLU:HG2	2.15	0.71
1:A:100:GLY:HA2	1:A:143:ASN:HD22	1.54	0.71
1:A:422:ASN:ND2	1:A:426:GLU:HG2	2.06	0.71
1:B:119:THR:HG22	1:B:121:GLU:N	2.05	0.71
2:D:324:GLY:O	2:D:332:ARG:HD3	1.89	0.71
2:C:103:VAL:HG22	2:C:218:LYS:HD2	1.73	0.71
2:C:138:THR:HG23	2:C:162:GLU:HB3	1.72	0.71
1:A:405:VAL:HB	1:A:419:MSE:CE	2.20	0.71
1:A:409:THR:CG2	1:A:411:ASN:H	2.01	0.70
1:B:141:LEU:HD23	1:B:157:ILE:HD13	1.73	0.70
2:D:465:ARG:HH21	2:D:466:TYR:HE2	1.37	0.70
2:D:54:MET:HG2	2:D:58:GLY:HA2	1.73	0.70
2:C:170:GLU:OE1	2:C:172:LYS:HE3	1.92	0.70
1:B:422:ASN:ND2	1:B:426:GLU:HG2	2.05	0.70
1:A:303:ILE:HG13	1:A:303:ILE:O	1.91	0.70
1:A:103:ILE:HG21	1:A:219:LEU:HG	1.73	0.70
1:A:401:LYS:C	1:A:419:MSE:HE1	2.17	0.70
2:C:70:LYS:HD2	2:C:72:ARG:HH21	1.56	0.70
2:D:207:LYS:CB	2:D:248:LEU:HD21	2.22	0.70
2:D:200:GLU:O	2:D:204:VAL:HG23	1.92	0.70
2:C:466:TYR:HB3	2:C:472:LEU:HD21	1.72	0.70
2:C:234:ILE:HD11	2:C:259:VAL:HG13	1.74	0.69
2:D:14:GLY:HA3	2:D:235:LYS:HG3	1.73	0.69
1:B:271:VAL:HG23	1:B:272:PRO:O	1.93	0.69
1:A:165:LEU:HD13	1:A:172:VAL:HG23	1.74	0.69
1:A:409:THR:HG22	1:A:410:GLN:N	2.07	0.69
1:B:258:HIS:CD2	1:B:260:SER:H	2.10	0.69
2:D:106:GLN:HE21	2:D:216:THR:HG22	1.58	0.69
1:B:176:HIS:HB3	1:B:181:MSE:HE2	1.73	0.69
2:D:393:LEU:O	2:D:397:ILE:HG13	1.92	0.69
1:B:18:VAL:HG12	1:B:19:ARG:N	2.08	0.69
1:A:313:TYR:CD1	1:A:316:ILE:HG12	2.28	0.69
1:B:127:LEU:HD21	1:B:216:ALA:HA	1.75	0.69
1:A:174:VAL:HB	1:A:201:LEU:HD13	1.75	0.68
1:A:176:HIS:HB3	1:A:181:MSE:HE2	1.75	0.68
2:D:65:LEU:CD2	2:D:69:LYS:HE3	2.23	0.68
2:D:96:PRO:HD2	2:D:441:LEU:HD12	1.74	0.68
2:D:282:ILE:HD11	2:D:404:ILE:HD11	1.75	0.68
2:D:28:LYS:HE3	2:D:33:PRO:HA	1.75	0.68
2:D:314:ILE:HG12	2:D:393:LEU:HD22	1.76	0.68
1:A:312:VAL:HA	1:A:316:ILE:CD1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:MSE:HE2	1:B:268:ILE:CD1	2.22	0.68
2:D:149:THR:HG21	2:D:201:GLN:HG3	1.75	0.68
1:A:88:LYS:HB2	1:A:91:LEU:HD12	1.74	0.68
1:A:259:THR:CG2	1:B:339:LEU:HD23	2.23	0.68
1:A:279:ASN:ND2	1:A:281:GLU:HG3	2.08	0.68
2:D:23:ARG:NE	2:D:226:ILE:HG12	2.09	0.68
1:A:258:HIS:CD2	1:A:261:ARG:H	2.13	0.67
1:B:227:THR:O	1:B:227:THR:HG22	1.94	0.67
1:B:299:VAL:HG12	1:B:300:ASP:N	2.08	0.67
2:D:23:ARG:HD3	2:D:226:ILE:HG23	1.75	0.67
2:D:296:THR:HG22	2:D:298:SER:H	1.60	0.67
1:B:77:PRO:O	1:B:78:GLU:HB3	1.93	0.67
1:B:76:LYS:CB	1:B:77:PRO:CD	2.72	0.67
1:A:244:THR:HG22	1:A:245:TYR:CD2	2.30	0.67
1:A:370:ARG:O	1:B:259:THR:HG21	1.93	0.67
1:A:422:ASN:HD21	1:A:427:ILE:H	1.40	0.67
2:D:392:ALA:O	2:D:396:VAL:HG23	1.93	0.67
1:A:313:TYR:O	1:A:316:ILE:HG13	1.95	0.67
1:A:259:THR:HG22	1:B:339:LEU:HD23	1.75	0.67
1:A:266:ARG:HD3	1:A:438:ARG:O	1.95	0.67
1:B:126:ALA:HB2	2:D:54:MET:HE3	1.75	0.67
2:D:89:ASP:HB2	2:D:132:VAL:HG12	1.75	0.67
1:A:158:ALA:HB2	1:A:191:MSE:HE3	1.77	0.66
1:B:108:ASP:CG	2:D:56:GLU:HG2	2.20	0.66
1:B:405:VAL:HA	1:B:418:MSE:CE	2.25	0.66
2:C:19:LEU:H	2:C:192:THR:HB	1.58	0.66
2:D:320:ARG:HH21	2:D:351:ILE:HD11	1.58	0.66
2:C:314:ILE:CG1	2:C:393:LEU:HD22	2.25	0.66
1:A:127:LEU:HD22	1:A:130:ILE:HG12	1.77	0.66
1:A:111:THR:HG22	1:A:113:ALA:H	1.60	0.66
1:B:125:LYS:HE3	2:D:60:ILE:HG12	1.76	0.66
1:B:432:ARG:O	1:B:435:THR:HG22	1.96	0.66
2:C:476:LEU:O	2:C:480:LEU:HG	1.95	0.66
1:B:434:ASP:HB3	2:C:80:TYR:CD2	2.31	0.66
1:A:225:MSE:HG2	1:A:276:ILE:HD13	1.79	0.65
1:A:301:ASP:O	1:A:303:ILE:HG23	1.96	0.65
1:A:405:VAL:CB	1:A:419:MSE:HE2	2.26	0.65
1:B:151:PRO:CG	1:B:403:MSE:HE1	2.26	0.65
2:C:356:ASN:HB3	2:C:357:TYR:CD1	2.31	0.65
1:A:312:VAL:HG11	1:A:343:PRO:HD3	1.78	0.65
1:A:433:PHE:HB2	2:D:88:MET:HE1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASP:HA	1:A:438:ARG:NH1	2.11	0.65
2:D:149:THR:HG23	2:D:151:TRP:H	1.61	0.65
1:B:69:VAL:HG11	1:B:72:ARG:NH1	2.12	0.65
2:C:463:VAL:HG21	2:C:478:GLN:NE2	2.12	0.65
1:A:402:LEU:HA	1:A:419:MSE:HE1	1.76	0.65
2:C:234:ILE:HD11	2:C:259:VAL:HA	1.77	0.65
1:A:50:LYS:HE2	1:A:54:GLY:O	1.96	0.65
1:A:405:VAL:CG2	1:A:419:MSE:HE2	2.27	0.65
1:B:6:PHE:CE2	1:B:61:LEU:HD22	2.32	0.65
1:B:195:LEU:HD11	1:B:199:VAL:HG23	1.79	0.65
2:C:28:LYS:HE3	2:C:33:PRO:HA	1.78	0.65
1:B:146:SER:HB2	1:B:180:THR:HB	1.79	0.65
1:A:405:VAL:HB	1:A:419:MSE:HE2	1.77	0.65
2:D:13:LEU:HB3	2:D:234:ILE:HG23	1.78	0.65
1:A:266:ARG:NH1	1:A:438:ARG:OXT	2.30	0.64
2:D:363:GLU:O	2:D:367:VAL:HG23	1.97	0.64
1:B:405:VAL:HA	1:B:418:MSE:HE3	1.78	0.64
1:A:158:ALA:HB2	1:A:191:MSE:CE	2.27	0.64
1:A:344:ASN:HD21	1:A:381:LYS:HD2	1.62	0.64
1:B:313:TYR:CE1	1:B:316:ILE:HG12	2.31	0.64
2:D:349:PHE:HA	2:D:353:GLU:OE2	1.97	0.64
1:A:427:ILE:HG22	1:A:428:THR:N	2.12	0.64
2:C:299:LYS:O	2:C:303:ARG:HG3	1.98	0.64
1:B:178:THR:HG21	1:B:205:GLN:OE1	1.97	0.64
1:B:409:THR:HG22	1:B:410:GLN:N	2.12	0.64
2:C:314:ILE:HD12	2:C:397:ILE:HD11	1.79	0.64
2:C:356:ASN:HB3	2:C:357:TYR:CE1	2.32	0.64
2:C:9:ASN:O	2:C:11:GLU:N	2.30	0.64
1:B:18:VAL:HG12	1:B:19:ARG:H	1.63	0.64
1:B:50:LYS:CE	1:B:56:ASN:HD21	2.10	0.64
1:A:146:SER:HB3	1:A:176:HIS:CE1	2.32	0.64
1:A:339:LEU:HD23	1:B:259:THR:CG2	2.28	0.64
1:B:140:LEU:C	1:B:140:LEU:HD12	2.23	0.64
2:C:277:VAL:HG21	2:C:318:LYS:HB2	1.78	0.64
1:A:6:PHE:HE1	1:A:10:ARG:HE	1.45	0.64
1:B:76:LYS:HB2	1:B:77:PRO:HD3	1.79	0.64
1:B:86:GLU:H	1:B:86:GLU:CD	2.05	0.64
2:C:240:ILE:HD12	2:C:262:GLN:NE2	2.13	0.64
2:C:246:GLN:HG2	2:C:247:GLU:H	1.62	0.64
2:D:353:GLU:HG2	2:D:354:LEU:HD23	1.80	0.64
1:A:22:LYS:NZ	1:A:24:GLU:HG2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LYS:CB	1:B:77:PRO:HD3	2.28	0.63
1:B:103:ILE:O	1:B:103:ILE:HG22	1.98	0.63
1:B:252:THR:CB	1:B:425:GLY:O	2.46	0.63
1:B:217:MSE:HE2	2:D:49:ARG:NH2	2.13	0.63
1:B:344:ASN:HA	1:B:347:ILE:HG12	1.80	0.63
2:C:310:LYS:HD2	2:C:386:GLU:HG3	1.80	0.63
1:A:51:LEU:N	1:A:51:LEU:HD12	2.14	0.63
1:A:422:ASN:ND2	1:A:427:ILE:H	1.96	0.63
1:B:225:MSE:SE	1:B:276:ILE:HG21	2.49	0.63
2:C:103:VAL:O	2:C:107:ILE:HG13	1.98	0.63
2:C:240:ILE:HD12	2:C:262:GLN:HE21	1.64	0.63
1:A:125:LYS:HB3	2:C:54:MET:HE3	1.80	0.63
2:D:350:HIS:CE1	2:D:353:GLU:HB3	2.34	0.63
2:D:126:VAL:HG21	2:D:131:ASN:ND2	2.14	0.63
1:B:252:THR:HB	1:B:425:GLY:O	1.99	0.63
1:A:93:GLU:HB3	1:A:137:LYS:HE3	1.80	0.63
1:A:351:GLU:O	1:A:355:GLU:HG3	1.98	0.63
1:A:92:PRO:HB3	1:A:170:TYR:CD2	2.34	0.62
1:A:270:ASP:OD2	1:A:286:ARG:NH2	2.32	0.62
2:C:98:ARG:H	2:C:98:ARG:NE	1.96	0.62
2:D:167:ARG:HG3	2:D:182:ARG:HD3	1.81	0.62
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.64	0.62
1:B:433:PHE:CB	2:C:88:MET:HE1	2.24	0.62
1:A:244:THR:HG22	1:A:245:TYR:HD2	1.62	0.62
1:A:347:ILE:HD12	1:A:382:LEU:HG	1.81	0.62
1:A:405:VAL:HG21	1:A:419:MSE:HE2	1.81	0.62
1:B:50:LYS:HE2	1:B:56:ASN:HD21	1.64	0.62
1:B:274:ALA:HB2	1:B:284:PHE:HA	1.81	0.62
1:B:303:ILE:HG13	1:B:303:ILE:O	1.99	0.62
1:A:205:GLN:HE22	1:A:256:LYS:CE	2.12	0.62
1:A:344:ASN:HA	1:A:347:ILE:HG12	1.82	0.62
1:B:12:ILE:CG2	1:B:35:ILE:HD12	2.30	0.62
1:B:409:THR:HG22	1:B:411:ASN:N	2.13	0.62
2:D:261:ARG:NH1	2:D:412:ARG:NE	2.48	0.62
2:D:167:ARG:NH1	2:D:181:ASP:OD2	2.33	0.62
1:A:54:GLY:O	2:C:122:MET:HE2	1.99	0.62
1:A:69:VAL:HG11	1:A:72:ARG:NH1	2.14	0.62
1:B:405:VAL:HG22	1:B:418:MSE:HE3	1.82	0.62
1:B:108:ASP:HA	2:D:56:GLU:HG2	1.81	0.61
2:D:14:GLY:H	2:D:235:LYS:H	1.47	0.61
2:D:251:ILE:HB	2:D:252:PRO:HD3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLU:CD	1:B:86:GLU:N	2.58	0.61
1:B:347:ILE:HB	1:B:348:PRO:HD3	1.80	0.61
1:A:195:LEU:HD22	1:A:197:LYS:O	2.00	0.61
1:A:225:MSE:HB3	1:A:234:MSE:HE1	1.82	0.61
1:A:259:THR:HG23	1:B:339:LEU:HA	1.81	0.61
1:B:217:MSE:CE	1:B:243:ASP:HB3	2.26	0.61
2:D:326:GLU:HA	2:D:332:ARG:HG2	1.81	0.61
1:B:76:LYS:HB2	1:B:77:PRO:CD	2.30	0.61
1:B:312:VAL:HA	1:B:316:ILE:CD1	2.30	0.61
2:C:65:LEU:CD2	2:C:69:LYS:HE3	2.29	0.61
2:C:289:VAL:HG11	2:C:367:VAL:HG22	1.82	0.61
2:D:93:PRO:HG3	2:D:137:ARG:NH1	2.14	0.61
1:A:225:MSE:CG	1:A:276:ILE:HD13	2.31	0.61
2:C:284:GLU:O	2:C:284:GLU:HG3	2.01	0.61
2:D:240:ILE:HD13	2:D:261:ARG:NH2	2.16	0.61
1:B:221:CYS:HB3	1:B:276:ILE:HD11	1.81	0.60
1:A:99:THR:HG23	1:A:142:PHE:HE1	1.66	0.60
1:B:252:THR:OG1	1:B:425:GLY:O	2.14	0.60
2:C:167:ARG:NH1	2:C:181:ASP:OD2	2.34	0.60
2:C:130:SER:HB2	2:C:165:ALA:HB1	1.81	0.60
2:D:221:ARG:HH22	2:D:484:GLU:CB	2.14	0.60
1:A:259:THR:HB	1:B:369:GLY:HA3	1.82	0.60
1:B:214:ASP:HB2	1:B:238:HIS:CE1	2.36	0.60
2:D:354:LEU:HB2	2:D:355:PRO:HA	1.83	0.60
1:A:109:TYR:CD2	2:C:431:ARG:HB3	2.37	0.60
1:A:205:GLN:OE1	1:A:205:GLN:HA	2.02	0.60
2:C:208:PHE:HE1	2:C:458:LEU:HD21	1.65	0.60
1:A:99:THR:HG22	1:A:99:THR:O	2.02	0.60
2:C:23:ARG:NE	2:C:226:ILE:HG12	2.16	0.60
2:D:495:MET:C	2:D:497:VAL:H	2.09	0.60
1:A:266:ARG:HD2	1:B:437:LEU:CD2	2.22	0.60
2:C:257:ARG:HG3	2:C:257:ARG:NH1	2.14	0.60
2:D:354:LEU:HD12	2:D:364:VAL:HG22	1.84	0.60
2:C:72:ARG:CG	2:C:174:LYS:HA	2.25	0.60
2:C:261:ARG:NH1	2:C:412:ARG:CZ	2.65	0.59
2:C:272:LEU:HD13	2:C:404:ILE:HG12	1.83	0.59
2:C:293:PHE:CD2	2:C:296:THR:HG21	2.36	0.59
1:A:200:VAL:HG12	1:A:202:VAL:HG23	1.84	0.59
1:B:3:VAL:CA	1:B:61:LEU:HD11	2.23	0.59
1:B:195:LEU:HD11	1:B:199:VAL:CG2	2.32	0.59
2:C:138:THR:HG22	2:C:139:ALA:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:LEU:O	2:C:397:ILE:HG13	2.02	0.59
1:A:39:TYR:O	1:A:41:LEU:N	2.34	0.59
1:B:312:VAL:HA	1:B:316:ILE:HD11	1.84	0.59
2:D:96:PRO:HG3	2:D:121:TYR:CE1	2.37	0.59
1:B:9:GLU:C	1:B:11:ASN:H	2.09	0.59
2:C:155:GLY:C	2:C:156:ILE:HD12	2.27	0.59
1:A:205:GLN:HE22	1:A:256:LYS:HE3	1.66	0.59
1:B:176:HIS:HE2	1:B:184:THR:HG1	1.48	0.59
2:D:105:LEU:HD21	2:D:443:ILE:HD13	1.84	0.59
1:A:159:HIS:CE1	1:A:299:VAL:HG11	2.37	0.59
1:B:416:ARG:O	1:B:417:LYS:C	2.46	0.59
2:D:85:LEU:HD23	2:D:88:MET:CE	2.33	0.59
2:C:15:LEU:HD12	2:C:16:LYS:N	2.18	0.59
1:A:18:VAL:CG1	1:A:19:ARG:N	2.65	0.59
1:B:313:TYR:CD1	1:B:316:ILE:HG12	2.37	0.59
1:A:274:ALA:HB2	1:A:284:PHE:HA	1.85	0.59
1:B:96:ILE:HA	1:B:173:VAL:O	2.03	0.59
1:A:12:ILE:HG21	1:A:35:ILE:CD1	2.32	0.58
1:A:342:THR:HG23	1:A:343:PRO:HD2	1.85	0.58
2:D:356:ASN:HB3	2:D:357:TYR:CD1	2.38	0.58
1:A:151:PRO:HG3	1:A:403:MSE:HE1	1.85	0.58
1:B:99:THR:O	1:B:99:THR:HG22	2.04	0.58
2:C:31:PHE:CE2	2:C:438:ILE:HG13	2.38	0.58
2:C:155:GLY:O	2:C:156:ILE:HD12	2.02	0.58
2:D:32:SER:O	2:D:34:VAL:N	2.33	0.58
2:D:231:ASN:HA	2:D:240:ILE:O	2.03	0.58
1:A:217:MSE:HE2	2:C:49:ARG:NH2	2.12	0.58
1:A:411:ASN:O	1:A:415:VAL:HG23	2.03	0.58
2:C:27:THR:OG1	2:C:186:PRO:HG2	2.03	0.58
2:C:168:ILE:HD11	2:C:171:ARG:HG2	1.85	0.58
2:D:31:PHE:CE2	2:D:438:ILE:HG12	2.39	0.58
1:A:250:ARG:HD3	1:A:425:GLY:HA3	1.85	0.58
2:C:77:GLU:OE1	2:C:169:ILE:HG13	2.03	0.58
2:C:87:TYR:CD2	2:C:183:LEU:HG	2.39	0.58
2:D:27:THR:HG21	2:D:100:ALA:N	2.19	0.58
1:B:3:VAL:HG23	1:B:44:GLY:CA	2.32	0.58
2:C:49:ARG:HG2	2:C:73:VAL:HG23	1.85	0.58
1:A:380:ARG:HD2	1:B:40:GLU:CG	2.28	0.58
1:B:125:LYS:HE2	2:D:58:GLY:O	2.03	0.58
2:C:43:GLU:OE1	2:C:79:ASN:HB2	2.04	0.58
2:C:47:GLN:HE21	2:C:73:VAL:HG21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:THR:HG22	2:D:139:ALA:N	2.17	0.58
2:D:282:ILE:HD12	2:D:401:ARG:HG2	1.85	0.58
1:A:146:SER:OG	3:A:1000:ASP:O	2.21	0.58
1:A:229:GLU:HA	1:A:292:ARG:HG2	1.86	0.58
1:A:435:THR:HG23	1:A:435:THR:O	2.03	0.58
1:B:347:ILE:HD12	1:B:382:LEU:HG	1.86	0.57
2:C:296:THR:HG22	2:C:363:GLU:CD	2.29	0.57
2:C:126:VAL:HG11	2:C:131:ASN:HD22	1.68	0.57
2:C:470:TYR:HD1	2:C:470:TYR:N	2.02	0.57
2:D:48:ARG:NH2	2:D:88:MET:O	2.37	0.57
1:B:250:ARG:O	1:B:254:VAL:HG23	2.04	0.57
2:D:167:ARG:HD3	2:D:181:ASP:OD1	2.04	0.57
1:A:195:LEU:CB	1:A:290:ARG:HH12	2.17	0.57
1:A:433:PHE:HB2	2:D:88:MET:CE	2.35	0.57
1:B:217:MSE:HG3	1:B:278:PRO:CG	2.34	0.57
2:C:350:HIS:HD2	2:C:352:ASP:H	1.52	0.57
2:D:498:LYS:O	2:D:499:PRO:C	2.46	0.57
1:A:225:MSE:HE3	1:A:234:MSE:HE1	1.87	0.57
1:B:127:LEU:HD22	1:B:219:LEU:CD1	2.33	0.57
2:C:402:GLU:HB3	2:C:408:PRO:HG3	1.87	0.57
1:A:333:VAL:HG21	1:A:399:TYR:HA	1.85	0.57
1:A:50:LYS:HE3	1:A:56:ASN:ND2	2.14	0.57
1:B:3:VAL:HG22	1:B:61:LEU:HG	1.87	0.57
1:B:218:ASN:ND2	1:B:237:MSE:HE1	2.20	0.57
2:C:413:ARG:CB	2:C:423:MET:HE2	2.29	0.57
2:C:470:TYR:N	2:C:470:TYR:CD1	2.73	0.57
1:A:51:LEU:C	1:A:53:ASN:H	2.13	0.56
1:A:95:THR:HG21	1:A:164:ALA:CB	2.31	0.56
1:A:384:LYS:HD2	1:B:41:LEU:HD13	1.87	0.56
2:C:246:GLN:H	2:C:246:GLN:CD	2.12	0.56
2:D:314:ILE:CG1	2:D:393:LEU:HD22	2.35	0.56
1:A:81:PHE:HB2	1:A:119:THR:HG21	1.85	0.56
1:B:99:THR:O	1:B:99:THR:CG2	2.53	0.56
1:A:195:LEU:HB3	1:A:290:ARG:NH1	2.21	0.56
1:A:269:ASN:ND2	1:A:392:ASP:HB2	2.20	0.56
1:A:342:THR:HG21	1:A:346:ILE:HG22	1.88	0.56
2:C:481:VAL:HA	2:C:486:ASP:HB3	1.86	0.56
2:D:325:ARG:O	2:D:332:ARG:HB3	2.06	0.56
2:C:293:PHE:CA	2:C:296:THR:HG23	2.32	0.56
1:B:39:TYR:O	1:B:40:GLU:C	2.48	0.56
1:B:225:MSE:HG2	1:B:276:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:HB	1:B:346:ILE:HD11	1.88	0.56
2:C:289:VAL:HG12	2:C:289:VAL:O	2.05	0.56
1:B:153:HIS:O	1:B:157:ILE:HG12	2.06	0.56
1:A:189:SER:HA	1:A:233:VAL:HG21	1.88	0.56
1:B:205:GLN:OE1	1:B:205:GLN:HA	2.06	0.56
1:B:317:SER:C	1:B:319:GLU:H	2.14	0.56
1:B:350:ILE:O	1:B:354:VAL:HG23	2.06	0.56
2:D:79:ASN:OD1	2:D:82:LEU:HB2	2.06	0.56
1:A:312:VAL:HG12	1:A:313:TYR:N	2.21	0.55
2:C:67:GLU:HG2	2:C:127:ILE:HG22	1.88	0.55
2:C:149:THR:HG21	2:C:201:GLN:HG3	1.88	0.55
2:C:98:ARG:O	2:C:102:GLU:HG3	2.07	0.55
2:C:234:ILE:CD1	2:C:259:VAL:HG13	2.36	0.55
2:C:354:LEU:HD13	2:C:364:VAL:HG22	1.88	0.55
2:C:412:ARG:HG2	2:C:412:ARG:HH11	1.71	0.55
2:D:296:THR:HG22	2:D:298:SER:N	2.20	0.55
1:B:299:VAL:CG1	1:B:300:ASP:N	2.70	0.55
1:A:3:VAL:CG2	1:A:61:LEU:HD11	2.31	0.55
1:A:202:VAL:HG21	1:A:222:SER:HB2	1.87	0.55
1:A:307:VAL:HG13	1:A:331:GLY:C	2.32	0.55
2:C:6:ASP:HB3	2:C:10:TYR:HE1	1.71	0.55
2:C:32:SER:O	2:C:34:VAL:N	2.35	0.55
2:C:79:ASN:HD21	2:C:82:LEU:HG	1.71	0.55
2:D:181:ASP:OD1	2:D:182:ARG:N	2.39	0.55
1:A:106:ARG:HD3	1:A:122:GLU:OE2	2.06	0.55
1:A:141:LEU:O	1:A:141:LEU:HD12	2.06	0.55
1:A:421:THR:HB	1:A:423:TYR:HE1	1.72	0.55
1:B:44:GLY:O	1:B:46:THR:N	2.40	0.55
1:B:409:THR:HG22	1:B:410:GLN:H	1.70	0.55
2:C:476:LEU:HD13	2:C:504:SER:CB	2.37	0.55
2:C:19:LEU:HD12	2:C:230:LEU:HD23	1.88	0.55
1:A:312:VAL:HG12	1:A:313:TYR:H	1.70	0.55
1:B:33:GLY:C	1:B:49:LEU:HD11	2.32	0.55
2:C:196:ILE:HG23	2:C:201:GLN:HG2	1.88	0.55
2:C:181:ASP:OD1	2:C:182:ARG:N	2.40	0.55
2:D:466:TYR:HB3	2:D:472:LEU:HD21	1.88	0.55
1:A:3:VAL:HG22	1:A:61:LEU:CG	2.37	0.55
1:A:18:VAL:HG12	1:A:19:ARG:N	2.20	0.55
1:B:106:ARG:HB3	2:D:55:SER:O	2.07	0.55
1:B:279:ASN:OD1	1:B:279:ASN:C	2.50	0.55
1:B:279:ASN:OD1	1:B:281:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:326:GLU:CA	2:D:332:ARG:HG2	2.36	0.55
3:A:1000:ASP:HB2	1:B:376:TYR:CE1	2.42	0.54
1:B:159:HIS:CE1	1:B:299:VAL:HG11	2.41	0.54
1:B:363:THR:HG21	1:B:395:PRO:HA	1.90	0.54
2:C:495:MET:C	2:C:497:VAL:H	2.13	0.54
1:B:24:GLU:O	1:B:27:GLU:HB2	2.07	0.54
1:B:205:GLN:HE22	1:B:256:LYS:HE3	1.72	0.54
1:A:430:TYR:CD2	2:D:34:VAL:HG22	2.42	0.54
1:B:214:ASP:O	1:B:218:ASN:ND2	2.40	0.54
1:B:274:ALA:CB	1:B:284:PHE:HA	2.37	0.54
1:A:158:ALA:CB	1:A:191:MSE:HE3	2.36	0.54
2:C:84:ASP:OD2	2:C:86:VAL:HB	2.07	0.54
2:D:166:ALA:HB2	2:D:183:LEU:HB2	1.88	0.54
2:D:261:ARG:NH1	2:D:412:ARG:CZ	2.70	0.54
1:A:179:ASP:HB3	1:B:337:THR:HG23	1.89	0.54
2:C:42:VAL:HG13	2:C:77:GLU:HB3	1.89	0.54
1:A:154:TRP:C	1:A:191:MSE:HE1	2.33	0.54
1:A:258:HIS:CD2	1:A:260:SER:H	2.26	0.54
1:B:64:ILE:HG21	1:B:67:ILE:HD11	1.89	0.54
2:D:312:LEU:HB2	2:D:393:LEU:HD11	1.89	0.54
1:A:195:LEU:CB	1:A:290:ARG:NH1	2.71	0.54
1:A:402:LEU:N	1:A:419:MSE:HE1	2.23	0.54
2:C:16:LYS:HB3	2:C:194:PRO:O	2.07	0.54
2:C:277:VAL:CG2	2:C:318:LYS:HD2	2.38	0.54
2:D:23:ARG:O	2:D:188:ILE:HG22	2.08	0.54
2:C:65:LEU:HD22	2:C:69:LYS:HE3	1.89	0.54
1:A:179:ASP:HB3	1:B:337:THR:CG2	2.38	0.54
1:A:342:THR:HG22	1:A:343:PRO:O	2.08	0.54
2:C:9:ASN:C	2:C:11:GLU:H	2.16	0.54
2:C:355:PRO:O	2:C:356:ASN:HB2	2.08	0.54
2:D:505:ILE:O	2:D:509:VAL:HB	2.08	0.54
1:B:217:MSE:HE2	2:D:49:ARG:HH22	1.73	0.54
2:C:96:PRO:HG3	2:C:121:TYR:CE1	2.44	0.54
1:A:339:LEU:HD23	1:B:259:THR:HG22	1.90	0.53
2:C:460:GLN:OE1	2:C:478:GLN:NE2	2.41	0.53
2:D:19:LEU:HB3	2:D:192:THR:OG1	2.08	0.53
1:A:178:THR:HG23	1:A:265:PHE:CE1	2.44	0.53
1:A:179:ASP:OD1	1:B:337:THR:CG2	2.55	0.53
1:A:263:ASP:CB	1:B:436:TYR:HE2	2.21	0.53
2:C:75:VAL:HB	2:C:177:ILE:HG12	1.89	0.53
2:D:299:LYS:O	2:D:303:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD11	2:C:140:ILE:HG21	1.90	0.53
1:B:361:CYS:HB3	1:B:390:CYS:SG	2.48	0.53
2:D:275:ARG:HD3	2:D:318:LYS:HB3	1.89	0.53
1:B:51:LEU:HD11	1:B:57:ILE:HD12	1.89	0.53
1:A:437:LEU:CD2	1:B:266:ARG:HD2	2.37	0.53
1:B:3:VAL:HG23	1:B:44:GLY:C	2.33	0.53
1:B:3:VAL:HG22	1:B:61:LEU:CD1	2.39	0.53
2:C:398:LYS:HE2	2:C:402:GLU:OE1	2.08	0.53
2:D:385:GLU:O	2:D:386:GLU:C	2.52	0.53
1:A:227:THR:O	1:A:227:THR:CG2	2.55	0.53
2:C:87:TYR:HD2	2:C:183:LEU:HG	1.74	0.53
2:D:457:GLU:CD	2:D:457:GLU:N	2.65	0.53
1:A:195:LEU:HB2	1:A:290:ARG:HH12	1.73	0.53
1:A:409:THR:HG22	1:A:410:GLN:H	1.71	0.53
1:B:200:VAL:HG22	1:B:234:MSE:HE3	1.89	0.53
1:B:268:ILE:O	1:B:269:ASN:HB2	2.08	0.53
2:C:312:LEU:HD23	2:C:312:LEU:N	2.24	0.53
2:C:457:GLU:CD	2:C:462:LYS:HG2	2.34	0.53
1:A:402:LEU:CA	1:A:419:MSE:HE1	2.38	0.53
2:C:241:GLU:CD	2:C:243:LYS:HE2	2.34	0.53
1:A:405:VAL:HG22	1:A:418:MSE:HE2	1.91	0.53
2:D:394:ARG:O	2:D:397:ILE:HB	2.07	0.53
1:A:205:GLN:HG2	1:A:261:ARG:O	2.08	0.53
1:B:93:GLU:OE1	1:B:137:LYS:HE3	2.09	0.53
2:D:147:VAL:HG23	2:D:156:ILE:HD11	1.91	0.53
2:D:157:PRO:HD2	2:D:191:SER:O	2.09	0.53
1:A:307:VAL:HG13	1:A:331:GLY:O	2.09	0.52
2:C:277:VAL:HG22	2:C:318:LYS:HD2	1.91	0.52
2:C:411:THR:O	2:C:423:MET:HB3	2.08	0.52
2:D:19:LEU:HD13	2:D:230:LEU:HD23	1.90	0.52
1:A:6:PHE:CE1	1:A:10:ARG:NE	2.77	0.52
1:B:21:THR:OG1	1:B:66:ARG:HB2	2.09	0.52
1:B:159:HIS:NE2	1:B:301:ASP:OD2	2.38	0.52
1:B:274:ALA:HA	1:B:285:LEU:HG	1.91	0.52
2:C:15:LEU:HD11	2:C:17:VAL:HG23	1.90	0.52
1:A:206:ARG:HG3	1:A:210:ARG:HD3	1.91	0.52
2:D:150:PRO:HB2	2:D:151:TRP:CE3	2.43	0.52
2:D:311:VAL:C	2:D:312:LEU:HD23	2.35	0.52
1:A:51:LEU:N	1:A:51:LEU:CD1	2.73	0.52
1:B:69:VAL:HG21	1:B:72:ARG:HH12	1.75	0.52
1:B:258:HIS:CE1	1:B:261:ARG:HD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:ASP:O	2:C:196:ILE:C	2.52	0.52
1:A:142:PHE:HD1	1:A:142:PHE:O	1.93	0.52
1:A:263:ASP:HB2	1:B:436:TYR:HE2	1.74	0.52
1:A:326:ASP:OD1	1:A:352:ARG:NH2	2.43	0.52
1:B:344:ASN:ND2	1:B:381:LYS:NZ	2.53	0.52
2:C:467:VAL:HG21	2:C:474:ARG:HG2	1.90	0.52
2:D:29:LYS:HD2	2:D:34:VAL:HB	1.92	0.52
2:D:29:LYS:HE2	2:D:183:LEU:O	2.10	0.52
1:A:258:HIS:HD2	1:A:260:SER:H	1.56	0.52
2:D:394:ARG:HA	2:D:397:ILE:CD1	2.40	0.52
1:A:330:LYS:HE3	1:A:330:LYS:HA	1.90	0.52
1:B:261:ARG:HH11	1:B:263:ASP:CB	2.23	0.52
2:D:231:ASN:HD22	2:D:239:ARG:HE	1.56	0.52
2:D:310:LYS:HD2	2:D:386:GLU:HG2	1.91	0.52
1:A:180:THR:CG2	1:A:180:THR:O	2.58	0.52
1:A:409:THR:CG2	1:A:410:GLN:N	2.72	0.52
1:B:22:LYS:HE2	1:B:24:GLU:HG2	1.91	0.52
1:B:83:ALA:HA	1:B:119:THR:HG23	1.92	0.52
2:D:36:SER:HB2	2:D:220:LYS:NZ	2.25	0.52
2:D:284:GLU:O	2:D:284:GLU:HG3	2.10	0.52
1:A:51:LEU:HD11	1:A:57:ILE:HB	1.92	0.52
1:A:303:ILE:HG22	1:A:404:TRP:HA	1.91	0.52
1:B:122:GLU:O	2:D:54:MET:HE1	2.10	0.52
1:B:176:HIS:ND1	1:B:177:GLY:N	2.58	0.52
1:B:317:SER:C	1:B:319:GLU:N	2.67	0.52
2:D:7:LYS:HG2	2:D:8:PHE:CE1	2.45	0.52
2:D:27:THR:OG1	2:D:186:PRO:HG2	2.10	0.52
1:A:271:VAL:HG22	1:A:272:PRO:HD2	1.91	0.52
1:A:347:ILE:N	1:A:348:PRO:CD	2.73	0.52
1:B:303:ILE:HG22	1:B:404:TRP:CA	2.39	0.52
2:D:360:SER:OG	2:D:363:GLU:HG3	2.10	0.52
1:A:3:VAL:HG13	1:A:61:LEU:HD21	1.92	0.51
1:A:51:LEU:CD2	1:A:57:ILE:HD12	2.38	0.51
1:A:76:LYS:CB	1:A:77:PRO:CD	2.66	0.51
1:A:141:LEU:HD23	1:A:157:ILE:HD13	1.93	0.51
1:B:165:LEU:CD1	1:B:172:VAL:HG23	2.37	0.51
2:D:72:ARG:HG2	2:D:174:LYS:CA	2.36	0.51
2:D:101:LEU:O	2:D:104:ALA:HB3	2.10	0.51
2:D:123:ARG:O	2:D:432:MET:HA	2.10	0.51
1:A:6:PHE:HE1	1:A:10:ARG:NE	2.08	0.51
1:A:130:ILE:HG13	1:A:131:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASN:O	1:B:415:VAL:HG23	2.09	0.51
1:A:14:VAL:O	1:A:14:VAL:HG13	2.11	0.51
1:B:249:HIS:HB3	1:B:254:VAL:HG22	1.93	0.51
1:B:351:GLU:O	1:B:355:GLU:HG3	2.10	0.51
2:C:257:ARG:HH11	2:C:257:ARG:CG	2.19	0.51
2:C:271:GLU:O	2:C:275:ARG:HG3	2.10	0.51
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.26	0.51
2:D:203:LYS:HD2	2:D:252:PRO:HG2	1.92	0.51
1:B:207:SER:OG	1:B:209:ASP:OD1	2.25	0.51
2:C:269:ARG:HG3	2:C:404:ILE:O	2.09	0.51
2:C:291:ASP:C	2:C:293:PHE:H	2.19	0.51
2:C:101:LEU:O	2:C:104:ALA:HB3	2.11	0.51
1:A:100:GLY:HA2	1:A:143:ASN:ND2	2.24	0.51
1:A:402:LEU:CA	1:A:419:MSE:CE	2.82	0.51
2:C:170:GLU:CD	2:C:172:LYS:HE3	2.35	0.51
2:C:275:ARG:HB3	2:C:318:LYS:HD3	1.92	0.51
1:B:130:ILE:HD12	1:B:136:VAL:HG21	1.92	0.51
1:B:165:LEU:HD13	1:B:172:VAL:CG2	2.37	0.51
1:B:221:CYS:HB3	1:B:276:ILE:HD12	1.88	0.51
1:A:107:ILE:HG22	1:A:114:VAL:HG13	1.92	0.51
1:A:330:LYS:HD3	1:A:410:GLN:OE1	2.11	0.51
2:C:88:MET:O	2:C:89:ASP:HB3	2.09	0.51
1:A:369:GLY:HA3	1:B:259:THR:HB	1.92	0.51
1:B:39:TYR:HD2	1:B:42:SER:OG	1.94	0.51
1:B:249:HIS:CB	1:B:254:VAL:HG22	2.40	0.51
1:B:330:LYS:HE2	1:B:410:GLN:OE1	2.11	0.51
2:D:123:ARG:HD3	2:D:135:PHE:CE2	2.46	0.51
2:D:180:LEU:O	2:D:181:ASP:C	2.54	0.51
1:A:146:SER:O	1:A:180:THR:HB	2.11	0.50
1:B:127:LEU:O	1:B:128:PRO:C	2.54	0.50
2:C:13:LEU:O	2:C:15:LEU:N	2.42	0.50
2:C:48:ARG:NH2	2:C:88:MET:O	2.44	0.50
2:D:156:ILE:HD12	2:D:156:ILE:N	2.25	0.50
2:D:242:ILE:HA	2:D:412:ARG:O	2.11	0.50
2:D:320:ARG:HB2	2:D:376:GLU:O	2.11	0.50
2:D:497:VAL:O	2:D:498:LYS:C	2.54	0.50
1:A:312:VAL:CA	1:A:316:ILE:HD11	2.40	0.50
2:C:93:PRO:HG3	2:C:137:ARG:NH1	2.26	0.50
2:D:166:ALA:HB1	2:D:179:ARG:O	2.12	0.50
1:A:103:ILE:HD11	1:A:175:ALA:HB1	1.94	0.50
1:A:423:TYR:CD1	1:A:423:TYR:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:LEU:HD12	2:D:251:ILE:HD12	1.94	0.50
1:A:22:LYS:HZ2	1:A:24:GLU:HG2	1.74	0.50
1:A:372:ASN:ND2	2:D:92:PRO:HB2	2.27	0.50
1:B:119:THR:HG22	1:B:120:ALA:N	2.26	0.50
1:B:190:PHE:CZ	1:B:401:LYS:HG3	2.47	0.50
2:C:98:ARG:CD	2:C:98:ARG:N	2.63	0.50
2:C:109:TYR:OH	2:C:448:LYS:HB3	2.11	0.50
2:C:156:ILE:HG22	2:C:156:ILE:O	2.11	0.50
2:D:311:VAL:O	2:D:312:LEU:HD23	2.12	0.50
2:D:345:VAL:HG12	2:D:347:GLY:H	1.76	0.50
2:D:476:LEU:O	2:D:480:LEU:HB2	2.12	0.50
1:A:253:LYS:O	1:A:267:SER:HA	2.12	0.50
1:B:150:LYS:N	1:B:153:HIS:HD2	1.98	0.50
1:B:408:HIS:HB2	1:B:418:MSE:HE2	1.93	0.50
2:D:374:SER:H	2:D:377:ASP:CG	2.20	0.50
2:D:390:LYS:O	2:D:394:ARG:HG3	2.12	0.50
2:D:498:LYS:O	2:D:500:SER:N	2.45	0.50
1:A:309:LEU:HB3	1:B:313:TYR:CD2	2.46	0.50
1:B:181:MSE:HE1	1:B:203:GLY:N	2.27	0.50
2:D:231:ASN:ND2	2:D:239:ARG:HE	2.09	0.50
2:D:415:LEU:HD11	2:D:421:GLU:HB2	1.94	0.50
1:A:227:THR:O	1:A:227:THR:HG22	2.10	0.50
1:A:259:THR:HG21	1:B:370:ARG:O	2.11	0.50
1:B:140:LEU:HD12	1:B:141:LEU:N	2.27	0.50
2:D:231:ASN:HD22	2:D:239:ARG:NE	2.10	0.50
2:D:495:MET:C	2:D:497:VAL:N	2.64	0.50
1:A:427:ILE:HG22	1:A:428:THR:H	1.76	0.50
1:B:51:LEU:HD21	1:B:57:ILE:HD12	1.93	0.50
1:B:174:VAL:HB	1:B:201:LEU:HD13	1.93	0.50
2:D:27:THR:HG1	2:D:186:PRO:HG2	1.75	0.50
1:A:161:VAL:O	1:A:165:LEU:HB2	2.12	0.49
1:A:210:ARG:NH2	2:C:123:ARG:NH2	2.60	0.49
2:D:149:THR:HG23	2:D:151:TRP:HE3	1.77	0.49
2:D:167:ARG:HG3	2:D:182:ARG:HB2	1.94	0.49
1:B:100:GLY:HA2	1:B:143:ASN:ND2	2.22	0.49
1:B:430:TYR:CD2	2:C:34:VAL:HG22	2.47	0.49
2:D:147:VAL:HG11	2:D:205:VAL:HA	1.94	0.49
2:D:498:LYS:CA	2:D:502:ALA:HB3	2.41	0.49
1:B:47:LEU:HD12	1:B:48:VAL:N	2.26	0.49
2:C:47:GLN:NE2	2:C:73:VAL:HG21	2.28	0.49
2:D:13:LEU:HB3	2:D:234:ILE:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:VAL:HG11	2:D:367:VAL:HG22	1.94	0.49
2:D:411:THR:HG23	2:D:411:THR:O	2.11	0.49
2:C:13:LEU:HB3	2:C:234:ILE:HG23	1.93	0.49
1:A:402:LEU:HD12	1:A:419:MSE:HE3	1.93	0.49
1:B:258:HIS:HD2	1:B:261:ARG:H	1.60	0.49
1:B:373:LEU:HD22	1:B:389:PRO:HB3	1.95	0.49
2:C:112:ASN:O	2:C:114:LYS:HE3	2.12	0.49
1:A:39:TYR:HD2	1:A:42:SER:HB2	1.77	0.49
1:A:53:ASN:HB3	1:A:55:TYR:HD1	1.77	0.49
1:A:127:LEU:HD13	1:A:219:LEU:CD1	2.43	0.49
1:B:195:LEU:HD22	1:B:197:LYS:H	1.78	0.49
2:C:495:MET:C	2:C:497:VAL:N	2.66	0.49
2:D:35:PRO:C	2:D:37:GLU:H	2.20	0.49
2:D:66:GLU:HG2	2:D:70:LYS:HE3	1.94	0.49
2:D:355:PRO:HG3	2:D:364:VAL:HG21	1.94	0.49
1:B:247:LEU:HD23	1:B:249:HIS:HE1	1.77	0.49
2:D:167:ARG:HG3	2:D:182:ARG:CB	2.42	0.49
2:D:289:VAL:HG12	2:D:289:VAL:O	2.12	0.49
1:B:126:ALA:O	2:D:51:ARG:NH2	2.46	0.49
1:B:250:ARG:CD	1:B:425:GLY:HA3	2.34	0.49
1:B:428:THR:CG2	1:B:430:TYR:O	2.60	0.49
2:C:149:THR:HG23	2:C:151:TRP:N	2.22	0.49
2:D:275:ARG:O	2:D:318:LYS:HD3	2.12	0.49
1:A:39:TYR:C	1:A:41:LEU:H	2.20	0.49
1:A:427:ILE:CG2	1:A:428:THR:N	2.76	0.49
1:B:210:ARG:NH2	2:D:123:ARG:NH2	2.60	0.49
1:B:12:ILE:HG21	1:B:35:ILE:HD12	1.93	0.49
1:B:18:VAL:CG1	1:B:19:ARG:N	2.75	0.49
2:C:240:ILE:HD13	2:C:261:ARG:NH2	2.27	0.49
2:D:67:GLU:HA	2:D:70:LYS:HD2	1.94	0.49
2:D:261:ARG:HH12	2:D:412:ARG:CZ	2.26	0.49
1:A:176:HIS:HD1	1:A:177:GLY:N	2.11	0.48
1:A:366:CYS:O	1:A:367:ILE:C	2.54	0.48
1:B:3:VAL:HG22	1:B:61:LEU:CG	2.43	0.48
1:B:18:VAL:HG13	1:B:68:GLU:O	2.12	0.48
2:D:193:THR:C	2:D:195:ASP:H	2.20	0.48
2:D:264:ASN:O	2:D:268:ILE:HG13	2.13	0.48
2:D:467:VAL:O	2:D:471:LYS:HA	2.13	0.48
1:A:217:MSE:HE2	1:A:278:PRO:HG2	1.95	0.48
1:A:421:THR:HB	1:A:423:TYR:CE1	2.48	0.48
1:B:9:GLU:HG2	1:B:10:ARG:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:HG21	1:B:399:TYR:HA	1.95	0.48
2:C:19:LEU:CD1	2:C:230:LEU:HD23	2.43	0.48
1:A:423:TYR:HD1	1:A:423:TYR:H	1.61	0.48
1:B:33:GLY:O	1:B:49:LEU:HD11	2.13	0.48
2:D:220:LYS:HB2	2:D:225:THR:HG21	1.95	0.48
1:B:370:ARG:HH11	2:C:94:ARG:CZ	2.26	0.48
1:B:436:TYR:CE1	1:B:437:LEU:HD13	2.48	0.48
2:C:208:PHE:CE1	2:C:458:LEU:HD21	2.47	0.48
2:C:292:ILE:HG22	2:C:292:ILE:O	2.13	0.48
1:A:181:MSE:SE	1:A:237:MSE:HE2	2.64	0.48
2:C:42:VAL:CG1	2:C:77:GLU:HB3	2.43	0.48
2:D:480:LEU:HD21	2:D:489:PHE:CD1	2.49	0.48
1:B:225:MSE:HA	1:B:228:SER:OG	2.12	0.48
2:C:173:ASP:O	2:C:174:LYS:HB2	2.11	0.48
2:C:291:ASP:C	2:C:293:PHE:N	2.71	0.48
2:D:240:ILE:HD12	2:D:262:GLN:NE2	2.19	0.48
1:A:245:TYR:HE1	1:A:247:LEU:CD1	2.26	0.48
1:A:313:TYR:CZ	1:A:316:ILE:HG12	2.49	0.48
1:B:23:GLU:CD	1:B:65:ARG:NH1	2.71	0.48
1:B:422:ASN:ND2	1:B:424:ALA:O	2.47	0.48
1:A:17:PHE:HB3	1:A:71:GLU:HB2	1.96	0.48
1:A:195:LEU:HD11	1:A:199:VAL:HG21	1.95	0.48
1:A:259:THR:HG21	1:B:370:ARG:C	2.38	0.48
2:C:207:LYS:HB2	2:C:248:LEU:HD21	1.96	0.48
1:A:270:ASP:CG	1:A:286:ARG:HH22	2.22	0.48
1:B:197:LYS:HG2	1:B:292:ARG:NH1	2.28	0.48
1:B:258:HIS:CD2	1:B:261:ARG:H	2.31	0.48
2:C:113:ALA:O	2:C:115:PRO:HD3	2.14	0.48
2:C:342:LYS:HA	2:C:345:VAL:O	2.14	0.48
2:C:344:TYR:CD1	2:C:391:ASN:HB3	2.48	0.48
2:D:19:LEU:HD13	2:D:230:LEU:CD2	2.44	0.48
2:D:107:ILE:HD13	2:D:213:LEU:CD2	2.44	0.48
1:A:176:HIS:ND1	1:A:177:GLY:N	2.62	0.47
2:D:290:THR:HA	2:D:311:VAL:HB	1.96	0.47
2:C:106:GLN:HE21	2:C:216:THR:CG2	2.21	0.47
2:D:371:LEU:N	2:D:371:LEU:HD23	2.29	0.47
2:D:385:GLU:C	2:D:385:GLU:OE1	2.57	0.47
1:A:22:LYS:HB2	1:A:63:LYS:O	2.14	0.47
1:A:217:MSE:CE	2:C:49:ARG:NH2	2.76	0.47
1:A:339:LEU:HA	1:B:259:THR:HG23	1.94	0.47
1:A:384:LYS:C	1:A:386:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:TYR:OH	2:D:138:THR:HG21	2.14	0.47
1:B:206:ARG:HG3	1:B:210:ARG:HD2	1.96	0.47
1:B:432:ARG:O	1:B:435:THR:CG2	2.61	0.47
2:C:320:ARG:HB2	2:C:376:GLU:O	2.13	0.47
1:A:282:ILE:HG12	1:A:283:GLU:N	2.29	0.47
1:A:337:THR:HG23	1:B:179:ASP:HB3	1.95	0.47
1:B:119:THR:HB	1:B:122:GLU:HG3	1.95	0.47
2:C:493:VAL:O	2:C:496:GLY:N	2.47	0.47
1:A:361:CYS:HB3	1:A:390:CYS:SG	2.54	0.47
1:A:429:PRO:O	2:D:94:ARG:NH2	2.48	0.47
1:B:48:VAL:HG22	2:D:120:TYR:CZ	2.48	0.47
1:B:230:VAL:HG22	1:B:289:TYR:CE1	2.50	0.47
2:C:65:LEU:HD23	2:C:65:LEU:O	2.14	0.47
2:C:99:GLU:O	2:C:103:VAL:HG23	2.15	0.47
2:D:345:VAL:HG23	2:D:392:ALA:HB2	1.96	0.47
1:A:108:ASP:O	1:A:112:GLY:N	2.42	0.47
1:A:147:GLU:OE2	3:A:1000:ASP:N	2.48	0.47
1:A:258:HIS:CD2	1:A:261:ARG:HG3	2.49	0.47
1:A:279:ASN:ND2	1:A:281:GLU:OE2	2.47	0.47
2:D:266:LEU:C	2:D:268:ILE:H	2.22	0.47
1:A:146:SER:HB3	1:A:176:HIS:HE1	1.76	0.47
1:A:337:THR:CG2	1:B:179:ASP:HB3	2.44	0.47
1:B:57:ILE:CG2	1:B:58:GLY:N	2.77	0.47
1:B:126:ALA:HB2	2:D:54:MET:HE1	1.95	0.47
1:B:234:MSE:HG2	1:B:273:ILE:HD12	1.96	0.47
2:C:292:ILE:HD13	2:C:366:LYS:C	2.38	0.47
2:D:107:ILE:HD13	2:D:213:LEU:HD22	1.97	0.47
2:D:334:GLY:O	2:D:337:PHE:HB2	2.15	0.47
2:D:374:SER:H	2:D:377:ASP:HB2	1.78	0.47
1:A:81:PHE:CB	1:A:119:THR:HG21	2.45	0.47
1:A:125:LYS:HE3	2:C:60:ILE:CG1	2.39	0.47
1:A:127:LEU:HD13	1:A:219:LEU:HD13	1.96	0.47
1:B:74:LYS:O	1:B:75:VAL:C	2.58	0.47
2:C:411:THR:CG2	2:C:426:LEU:HA	2.45	0.47
1:B:206:ARG:O	1:B:207:SER:C	2.56	0.47
1:B:422:ASN:HD22	1:B:426:GLU:HG2	1.80	0.47
2:D:167:ARG:CG	2:D:182:ARG:HD3	2.43	0.47
1:A:111:THR:HG22	1:A:113:ALA:N	2.30	0.47
1:A:144:ILE:CD1	1:A:153:HIS:CE1	2.97	0.47
1:A:211:PRO:HB2	2:C:134:GLY:HA3	1.97	0.47
1:A:255:ARG:HB2	1:A:394:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLY:O	2:D:122:MET:HE2	2.15	0.47
2:C:289:VAL:C	2:C:291:ASP:N	2.73	0.47
2:D:272:LEU:HD22	2:D:319:PHE:CE1	2.49	0.47
2:C:199:PRO:O	2:C:202:ALA:HB3	2.15	0.46
2:C:232:VAL:HG12	2:C:233:SER:H	1.79	0.46
1:A:16:ASP:OD2	1:A:73:ALA:N	2.42	0.46
1:A:306:LYS:HD2	1:A:328:GLY:O	2.15	0.46
1:B:3:VAL:HG22	1:B:61:LEU:HD11	1.98	0.46
1:B:193:ARG:HB2	1:B:298:GLU:O	2.15	0.46
2:C:116:VAL:O	2:C:443:ILE:HD12	2.16	0.46
2:D:457:GLU:OE1	2:D:462:LYS:HE3	2.15	0.46
1:A:409:THR:CG2	1:A:410:GLN:H	2.28	0.46
2:D:27:THR:HG21	2:D:100:ALA:CA	2.46	0.46
1:A:107:ILE:HD11	1:A:109:TYR:CZ	2.51	0.46
1:A:337:THR:HG23	1:B:179:ASP:OD1	2.15	0.46
1:B:12:ILE:HG22	1:B:35:ILE:HD12	1.97	0.46
2:D:126:VAL:HG21	2:D:131:ASN:HD22	1.77	0.46
2:D:351:ILE:CG2	2:D:378:ALA:HB1	2.45	0.46
1:A:25:ASP:OD1	1:A:25:ASP:O	2.32	0.46
1:A:263:ASP:HB2	1:B:436:TYR:CE2	2.50	0.46
1:B:370:ARG:NH1	2:C:94:ARG:CZ	2.78	0.46
2:C:474:ARG:O	2:C:475:SER:C	2.59	0.46
2:D:124:LYS:HA	2:D:432:MET:HG2	1.97	0.46
2:D:154:VAL:HG12	2:D:192:THR:HG23	1.97	0.46
2:D:245:VAL:HG13	2:D:254:ILE:HD12	1.98	0.46
2:D:266:LEU:C	2:D:268:ILE:N	2.71	0.46
1:A:244:THR:CG2	1:A:245:TYR:HD2	2.29	0.46
2:C:449:LYS:O	2:C:453:GLU:HG3	2.16	0.46
1:A:163:LYS:O	1:A:164:ALA:C	2.57	0.46
1:B:299:VAL:CG1	1:B:300:ASP:H	2.28	0.46
2:C:312:LEU:HB2	2:C:393:LEU:CD1	2.45	0.46
2:C:351:ILE:HG21	2:C:378:ALA:HB1	1.97	0.46
2:D:14:GLY:N	2:D:235:LYS:H	2.14	0.46
2:D:497:VAL:O	2:D:499:PRO:N	2.49	0.46
1:A:244:THR:CG2	1:A:245:TYR:CD2	2.97	0.46
1:A:428:THR:CG2	1:A:430:TYR:O	2.63	0.46
1:B:147:GLU:H	1:B:147:GLU:HG3	1.44	0.46
1:A:154:TRP:O	1:A:157:ILE:HB	2.16	0.46
1:B:130:ILE:C	1:B:132:GLU:H	2.23	0.46
1:B:164:ALA:HB1	1:B:169:ASP:OD2	2.16	0.46
2:C:9:ASN:C	2:C:11:GLU:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:497:VAL:O	2:C:498:LYS:C	2.59	0.46
1:B:151:PRO:HG2	1:B:403:MSE:HE1	1.97	0.46
1:B:225:MSE:O	1:B:228:SER:OG	2.34	0.46
1:B:261:ARG:NH1	1:B:263:ASP:CB	2.79	0.46
2:D:234:ILE:HG22	2:D:235:LYS:N	2.31	0.46
2:D:353:GLU:CG	2:D:354:LEU:HD23	2.45	0.46
1:A:69:VAL:HG11	1:A:72:ARG:HH11	1.81	0.45
1:B:176:HIS:NE2	1:B:184:THR:OG1	2.43	0.45
2:D:415:LEU:HD11	2:D:421:GLU:CB	2.46	0.45
1:A:259:THR:HG22	1:B:339:LEU:CD2	2.46	0.45
1:A:428:THR:HG22	1:A:430:TYR:H	1.81	0.45
1:B:257:MSE:CE	1:B:368:TYR:CE1	2.98	0.45
1:B:257:MSE:HE3	1:B:368:TYR:CE1	2.51	0.45
2:C:251:ILE:O	2:C:255:ILE:HG13	2.16	0.45
1:A:12:ILE:CG2	1:A:35:ILE:HD12	2.44	0.45
1:A:88:LYS:NZ	1:A:132:GLU:OE2	2.49	0.45
1:B:20:ILE:HA	1:B:66:ARG:O	2.16	0.45
1:B:313:TYR:H	1:B:316:ILE:CD1	2.24	0.45
1:B:408:HIS:HB2	1:B:418:MSE:CE	2.47	0.45
2:C:65:LEU:HD21	2:C:69:LYS:HE3	1.99	0.45
2:C:220:LYS:CB	2:C:225:THR:HG21	2.47	0.45
2:D:23:ARG:CD	2:D:226:ILE:HG12	2.46	0.45
1:A:210:ARG:HH21	2:C:123:ARG:NH2	2.14	0.45
1:B:336:GLY:O	1:B:365:GLN:HG3	2.16	0.45
2:C:234:ILE:HD11	2:C:259:VAL:CA	2.45	0.45
2:C:262:GLN:HG2	2:C:407:VAL:HG11	1.99	0.45
2:C:442:ARG:O	2:C:444:PRO:HD3	2.16	0.45
2:C:497:VAL:O	2:C:499:PRO:N	2.49	0.45
2:D:300:ILE:H	2:D:300:ILE:HG13	1.54	0.45
2:D:354:LEU:HB2	2:D:355:PRO:CA	2.45	0.45
2:D:423:MET:HB3	2:D:424:ARG:HG3	1.98	0.45
1:A:271:VAL:HG13	1:A:272:PRO:O	2.16	0.45
1:B:294:ASP:O	1:B:295:GLU:C	2.59	0.45
1:A:206:ARG:NH2	1:A:260:SER:O	2.40	0.45
1:B:396:GLU:CD	1:B:396:GLU:H	2.22	0.45
2:C:15:LEU:HD11	2:C:17:VAL:CG2	2.46	0.45
1:B:50:LYS:HE3	1:B:56:ASN:HD21	1.79	0.45
1:B:217:MSE:CE	2:D:49:ARG:NH2	2.79	0.45
1:A:198:PRO:HB2	1:A:226:ALA:HA	1.98	0.45
1:B:36:MSE:HE1	1:B:111:THR:O	2.17	0.45
1:B:409:THR:CG2	1:B:410:GLN:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLU:C	1:B:11:ASN:N	2.75	0.45
1:B:406:LEU:C	1:B:408:HIS:H	2.24	0.45
2:D:22:HIS:CE1	2:D:189:GLU:HG3	2.52	0.45
2:D:198:HIS:ND1	2:D:199:PRO:HD2	2.32	0.45
2:D:255:ILE:O	2:D:259:VAL:HG23	2.17	0.45
2:D:272:LEU:HD12	2:D:404:ILE:HA	1.99	0.45
1:A:22:LYS:HZ1	1:A:24:GLU:HG2	1.80	0.45
1:A:147:GLU:H	1:A:147:GLU:HG3	1.30	0.45
1:A:428:THR:HG22	1:A:430:TYR:N	2.32	0.45
2:C:257:ARG:NH1	2:C:257:ARG:CG	2.79	0.45
2:C:355:PRO:O	2:C:356:ASN:CB	2.65	0.45
2:C:459:PRO:O	2:C:462:LYS:HB2	2.16	0.45
2:D:269:ARG:HG3	2:D:404:ILE:O	2.17	0.45
1:A:97:ILE:HD12	1:A:161:VAL:HG22	1.99	0.44
1:A:245:TYR:HE1	1:A:247:LEU:HD13	1.81	0.44
1:A:304:GLU:OE2	1:A:306:LYS:HB2	2.17	0.44
2:C:67:GLU:HG2	2:C:127:ILE:CG2	2.46	0.44
2:C:123:ARG:HE	2:C:435:GLU:HA	1.82	0.44
2:C:282:ILE:HG22	2:C:397:ILE:HG23	1.99	0.44
2:C:292:ILE:CD1	2:C:366:LYS:HB3	2.40	0.44
2:C:480:LEU:HD13	2:C:489:PHE:CG	2.52	0.44
2:D:19:LEU:H	2:D:192:THR:HB	1.82	0.44
2:D:27:THR:O	2:D:36:SER:OG	2.33	0.44
1:A:119:THR:HG22	1:A:121:GLU:H	1.81	0.44
1:A:143:ASN:HD22	1:A:143:ASN:HA	1.59	0.44
1:A:225:MSE:SE	1:A:276:ILE:HG21	2.67	0.44
1:B:216:ALA:O	1:B:220:ILE:HG13	2.18	0.44
2:C:196:ILE:HD13	2:C:202:ALA:HA	1.98	0.44
2:C:232:VAL:HG12	2:C:233:SER:N	2.32	0.44
2:C:240:ILE:CD1	2:C:261:ARG:HH21	2.30	0.44
2:C:498:LYS:O	2:C:499:PRO:C	2.60	0.44
2:D:73:VAL:HG12	2:D:174:LYS:O	2.17	0.44
1:A:301:ASP:O	1:A:302:LYS:C	2.61	0.44
1:A:433:PHE:HD1	2:D:88:MET:HE1	1.83	0.44
1:B:25:ASP:C	1:B:27:GLU:H	2.25	0.44
1:B:217:MSE:HE2	1:B:278:PRO:HG2	1.99	0.44
1:B:245:TYR:HE1	1:B:247:LEU:HD13	1.82	0.44
1:B:247:LEU:HD23	1:B:249:HIS:CE1	2.51	0.44
1:B:344:ASN:ND2	1:B:381:LYS:HD2	2.32	0.44
1:B:346:ILE:O	1:B:347:ILE:C	2.60	0.44
2:C:203:LYS:HB2	2:C:252:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:GLN:HG3	2:D:225:THR:HG23	1.99	0.44
2:D:101:LEU:C	2:D:101:LEU:HD23	2.41	0.44
1:A:46:THR:HG21	2:C:118:GLU:OE1	2.16	0.44
1:A:109:TYR:CE2	2:C:431:ARG:HB3	2.52	0.44
1:B:193:ARG:HA	1:B:193:ARG:NE	2.32	0.44
1:B:236:VAL:HA	1:B:247:LEU:O	2.18	0.44
1:B:338:GLY:C	1:B:340:GLY:H	2.26	0.44
2:D:219:VAL:HG12	2:D:220:LYS:N	2.32	0.44
2:D:411:THR:O	2:D:423:MET:HB2	2.17	0.44
1:A:118:PHE:HD2	1:A:140:LEU:HD23	1.82	0.44
1:A:250:ARG:CD	1:A:425:GLY:HA3	2.47	0.44
1:B:60:ALA:O	1:B:61:LEU:C	2.60	0.44
2:C:20:GLU:OE2	2:C:191:SER:CB	2.53	0.44
2:C:85:LEU:HD23	2:C:88:MET:HE3	1.99	0.44
2:C:411:THR:HG22	2:C:426:LEU:HA	1.99	0.44
1:A:286:ARG:HG2	1:A:287:LYS:N	2.32	0.44
1:B:45:ASP:OD2	2:D:442:ARG:NH1	2.51	0.44
1:B:142:PHE:HD1	1:B:142:PHE:O	2.00	0.44
1:B:146:SER:HB2	1:B:180:THR:H	1.82	0.44
1:B:180:THR:HG23	1:B:183:TYR:HB2	2.00	0.44
2:C:220:LYS:HB2	2:C:225:THR:HG21	2.00	0.44
2:C:289:VAL:C	2:C:291:ASP:H	2.26	0.44
2:C:70:LYS:HD2	2:C:72:ARG:NH2	2.30	0.44
2:D:203:LYS:HB2	2:D:252:PRO:HG3	1.98	0.44
2:D:339:ASP:HB3	2:D:422:TYR:HB3	2.00	0.44
1:A:99:THR:O	1:A:99:THR:CG2	2.65	0.44
1:A:206:ARG:HB3	1:A:213:SER:HA	1.99	0.44
1:A:268:ILE:O	1:A:269:ASN:HB2	2.16	0.44
2:C:47:GLN:HE21	2:C:73:VAL:CG2	2.31	0.44
2:C:147:VAL:HG22	2:C:208:PHE:CD2	2.52	0.44
2:C:216:THR:O	2:C:218:LYS:HG2	2.18	0.44
2:D:56:GLU:H	2:D:56:GLU:HG3	1.45	0.44
2:D:154:VAL:CG1	2:D:192:THR:HG23	2.47	0.44
2:D:411:THR:HG22	2:D:424:ARG:C	2.41	0.44
1:A:144:ILE:HD13	1:A:153:HIS:CE1	2.53	0.44
1:A:207:SER:O	1:A:210:ARG:HG3	2.17	0.44
1:A:321:ILE:O	1:A:325:VAL:HG23	2.18	0.44
1:B:23:GLU:CD	1:B:65:ARG:HH12	2.26	0.44
1:B:277:TRP:O	1:B:278:PRO:C	2.60	0.44
2:C:31:PHE:HB3	2:C:93:PRO:HB2	1.99	0.44
2:C:105:LEU:O	2:C:108:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:406:GLY:O	2:C:408:PRO:HD3	2.18	0.44
2:D:34:VAL:HA	2:D:35:PRO:HD3	1.75	0.44
1:A:122:GLU:HA	2:C:54:MET:HE1	2.00	0.43
1:A:313:TYR:N	1:A:316:ILE:HD11	2.32	0.43
1:B:59:ILE:HG21	1:B:64:ILE:CD1	2.41	0.43
1:B:288:ASP:CG	1:B:288:ASP:O	2.61	0.43
1:B:312:VAL:HG11	1:B:343:PRO:HD3	2.00	0.43
1:B:370:ARG:HE	1:B:370:ARG:HB2	1.45	0.43
2:C:14:GLY:O	2:C:16:LYS:HG2	2.18	0.43
2:C:65:LEU:HD23	2:C:65:LEU:C	2.42	0.43
2:C:108:ALA:HA	2:C:159:ILE:CD1	2.48	0.43
2:C:240:ILE:CD1	2:C:261:ARG:NH2	2.80	0.43
1:A:286:ARG:HG3	1:A:288:ASP:OD1	2.18	0.43
1:A:391:GLU:HB3	1:A:392:ASP:H	1.51	0.43
2:C:33:PRO:HD2	2:C:94:ARG:HH21	1.83	0.43
2:C:174:LYS:O	2:C:175:GLU:HB2	2.18	0.43
2:D:93:PRO:HG2	2:D:438:ILE:HD13	2.00	0.43
1:A:318:SER:HB2	1:A:349:SER:HB3	2.00	0.43
1:A:433:PHE:CD1	2:D:88:MET:HE1	2.54	0.43
1:B:234:MSE:HG2	1:B:273:ILE:CD1	2.48	0.43
2:C:113:ALA:HB1	2:C:142:ALA:HB1	2.00	0.43
1:A:250:ARG:O	1:A:252:THR:N	2.51	0.43
1:B:217:MSE:HE1	1:B:243:ASP:CB	2.35	0.43
2:C:207:LYS:CB	2:C:248:LEU:HD21	2.49	0.43
2:C:351:ILE:CG2	2:C:378:ALA:HB1	2.48	0.43
1:A:271:VAL:HG22	1:A:272:PRO:CD	2.48	0.43
1:B:198:PRO:HG3	1:B:230:VAL:O	2.19	0.43
1:B:360:VAL:HG12	1:B:387:VAL:HG13	2.01	0.43
2:D:225:THR:O	2:D:225:THR:HG22	2.17	0.43
2:D:313:ALA:O	2:D:314:ILE:HD13	2.19	0.43
1:A:178:THR:HG21	1:A:205:GLN:OE1	2.19	0.43
2:C:5:THR:HG23	2:C:5:THR:O	2.18	0.43
2:C:168:ILE:HG23	2:C:168:ILE:O	2.17	0.43
2:C:354:LEU:HD13	2:C:364:VAL:CG2	2.48	0.43
2:C:412:ARG:HG2	2:C:412:ARG:NH1	2.33	0.43
2:D:36:SER:HB3	2:D:185:ILE:HG12	2.00	0.43
2:D:368:ILE:HA	2:D:373:LEU:HD12	2.00	0.43
1:A:46:THR:HA	1:A:59:ILE:O	2.19	0.43
1:A:181:MSE:HE1	1:A:202:VAL:C	2.43	0.43
1:A:194:ASN:OD1	1:A:295:GLU:HB3	2.18	0.43
1:A:427:ILE:CG2	1:A:428:THR:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ILE:HG22	1:B:282:ILE:CG1	2.20	0.43
1:B:292:ARG:HH11	1:B:292:ARG:CG	2.31	0.43
2:C:51:ARG:HA	2:C:52:PRO:HD3	1.92	0.43
2:C:269:ARG:NH2	2:C:270:ASP:OD1	2.43	0.43
2:C:314:ILE:HG13	2:C:393:LEU:HD22	2.00	0.43
2:D:296:THR:HG23	2:D:363:GLU:OE2	2.19	0.43
2:D:465:ARG:NH2	2:D:466:TYR:HE2	2.09	0.43
1:A:12:ILE:HG22	1:A:13:ASN:N	2.34	0.43
1:A:178:THR:HG23	1:A:265:PHE:HE1	1.83	0.43
1:B:108:ASP:HA	2:D:56:GLU:CG	2.45	0.43
2:D:9:ASN:O	2:D:11:GLU:N	2.52	0.43
2:D:130:SER:HB2	2:D:165:ALA:HB1	2.01	0.43
1:A:200:VAL:HG12	1:A:202:VAL:CG2	2.49	0.43
1:A:225:MSE:CE	1:A:234:MSE:HE1	2.48	0.43
1:A:346:ILE:O	1:A:346:ILE:CG2	2.66	0.43
1:B:177:GLY:O	1:B:181:MSE:HB2	2.19	0.43
2:C:292:ILE:HD13	2:C:366:LYS:CB	2.41	0.43
1:A:194:ASN:O	1:A:297:VAL:HA	2.19	0.43
2:C:98:ARG:HD3	2:C:98:ARG:N	2.24	0.43
2:C:291:ASP:O	2:C:293:PHE:N	2.52	0.43
2:D:240:ILE:HD13	2:D:261:ARG:HH21	1.84	0.43
2:D:470:TYR:HB2	2:D:472:LEU:HD22	2.01	0.43
2:D:345:VAL:HG21	2:D:382:VAL:CG1	2.49	0.42
2:D:351:ILE:HG21	2:D:378:ALA:CB	2.49	0.42
2:D:374:SER:C	2:D:376:GLU:H	2.27	0.42
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.87	0.42
1:A:253:LYS:NZ	1:A:392:ASP:OD2	2.53	0.42
1:B:37:PRO:HA	1:B:38:PRO:HD3	1.80	0.42
1:B:244:THR:HG22	1:B:277:TRP:CH2	2.54	0.42
2:C:21:ILE:HA	2:C:227:ARG:O	2.19	0.42
2:C:35:PRO:C	2:C:37:GLU:H	2.27	0.42
2:C:303:ARG:O	2:C:307:LYS:HG3	2.20	0.42
2:C:483:ASP:C	2:C:485:ARG:H	2.27	0.42
2:D:93:PRO:HG2	2:D:438:ILE:CD1	2.49	0.42
2:D:216:THR:O	2:D:217:LYS:C	2.62	0.42
1:A:384:LYS:C	1:A:386:GLY:N	2.76	0.42
1:B:50:LYS:HE2	1:B:56:ASN:ND2	2.33	0.42
1:A:342:THR:CG2	1:A:346:ILE:HG22	2.48	0.42
1:A:401:LYS:CD	1:A:419:MSE:SE	3.12	0.42
1:B:6:PHE:CE1	1:B:10:ARG:NE	2.87	0.42
1:B:247:LEU:HB3	1:B:249:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:TYR:O	1:B:316:ILE:HG13	2.19	0.42
2:C:103:VAL:HG22	2:C:218:LYS:CD	2.46	0.42
2:C:116:VAL:HG12	2:C:117:ASP:N	2.33	0.42
2:C:277:VAL:CG2	2:C:318:LYS:HB2	2.46	0.42
1:A:4:ASP:OD1	1:A:8:LYS:HE3	2.19	0.42
1:A:125:LYS:HB3	2:C:54:MET:CE	2.49	0.42
1:A:307:VAL:HG22	1:A:331:GLY:HA3	2.01	0.42
1:B:18:VAL:CG1	1:B:19:ARG:H	2.28	0.42
1:B:144:ILE:CG2	1:B:149:MSE:HE3	2.50	0.42
1:B:406:LEU:C	1:B:408:HIS:N	2.78	0.42
2:C:31:PHE:HA	2:C:94:ARG:O	2.18	0.42
2:C:344:TYR:CE1	2:C:391:ASN:HB3	2.55	0.42
2:C:345:VAL:HA	2:C:346:PRO:HD3	1.70	0.42
2:D:5:THR:O	2:D:5:THR:HG23	2.20	0.42
1:A:179:ASP:CG	1:B:337:THR:HG23	2.43	0.42
1:A:245:TYR:C	1:A:245:TYR:CD1	2.97	0.42
2:C:483:ASP:O	2:C:485:ARG:N	2.53	0.42
2:D:57:LEU:HD12	2:D:57:LEU:H	1.85	0.42
2:D:164:ASP:HB2	2:D:187:LEU:HD13	2.02	0.42
1:A:261:ARG:O	1:A:264:ALA:HB2	2.19	0.42
1:A:428:THR:HG21	1:A:430:TYR:O	2.20	0.42
1:B:210:ARG:O	1:B:212:SER:N	2.52	0.42
1:B:230:VAL:HG22	1:B:289:TYR:CD1	2.55	0.42
2:C:23:ARG:HD3	2:C:226:ILE:HG23	2.01	0.42
2:C:340:ARG:HG3	2:C:399:ARG:HG2	2.01	0.42
2:C:433:TYR:HA	2:C:434:PRO:HD3	1.92	0.42
2:D:44:PHE:CD1	2:D:44:PHE:C	2.98	0.42
2:D:67:GLU:HG2	2:D:127:ILE:CG2	2.50	0.42
2:D:141:ILE:HD12	2:D:161:LEU:HB2	2.01	0.42
2:D:170:GLU:OE1	2:D:172:LYS:HE3	2.20	0.42
1:A:48:VAL:HG22	2:C:120:TYR:CZ	2.55	0.42
1:A:436:TYR:CE1	1:B:258:HIS:HB2	2.55	0.42
1:B:61:LEU:O	1:B:62:GLU:C	2.62	0.42
1:B:321:ILE:HD12	1:B:346:ILE:CG2	2.49	0.42
2:D:140:ILE:HG12	2:D:158:THR:CG2	2.49	0.42
2:D:466:TYR:O	2:D:472:LEU:HD23	2.20	0.42
1:A:94:VAL:O	1:A:94:VAL:HG23	2.19	0.42
1:A:260:SER:HB3	1:B:339:LEU:HD21	2.02	0.42
1:A:344:ASN:C	1:A:346:ILE:H	2.27	0.42
1:B:218:ASN:ND2	1:B:237:MSE:CE	2.83	0.42
1:B:225:MSE:CG	1:B:276:ILE:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ARG:NH1	2:C:94:ARG:NH1	2.68	0.42
2:D:107:ILE:O	2:D:111:LEU:HG	2.20	0.42
2:D:304:VAL:HG12	2:D:309:GLY:HA3	2.01	0.42
2:D:493:VAL:O	2:D:496:GLY:N	2.48	0.42
1:A:277:TRP:CD1	1:A:277:TRP:N	2.87	0.42
1:A:309:LEU:HB3	1:B:313:TYR:CE2	2.55	0.42
1:B:202:VAL:O	1:B:202:VAL:HG13	2.20	0.42
2:C:289:VAL:HG13	2:C:292:ILE:HD12	2.01	0.42
2:C:300:ILE:H	2:C:300:ILE:HG13	1.33	0.42
1:A:79:VAL:HG12	1:A:80:HIS:N	2.35	0.41
1:A:261:ARG:NH2	1:B:436:TYR:HB3	2.35	0.41
1:B:250:ARG:HD3	1:B:425:GLY:CA	2.35	0.41
1:B:401:LYS:HD3	1:B:419:MSE:SE	2.69	0.41
1:A:170:TYR:CZ	1:A:292:ARG:NH2	2.88	0.41
1:A:258:HIS:NE2	1:A:261:ARG:HG3	2.36	0.41
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.85	0.41
1:B:431:THR:HG22	1:B:435:THR:HG21	2.02	0.41
2:C:470:TYR:HB2	2:C:472:LEU:HD23	2.02	0.41
2:D:14:GLY:CA	2:D:235:LYS:HG3	2.47	0.41
2:D:320:ARG:HB2	2:D:376:GLU:C	2.45	0.41
2:D:345:VAL:HG21	2:D:382:VAL:HG11	2.02	0.41
1:A:103:ILE:HG22	1:A:103:ILE:O	2.20	0.41
1:B:38:PRO:O	1:B:39:TYR:C	2.63	0.41
1:B:210:ARG:NH2	2:D:123:ARG:HH22	2.18	0.41
1:B:277:TRP:C	1:B:279:ASN:N	2.75	0.41
2:C:356:ASN:HD22	2:C:357:TYR:H	1.69	0.41
2:D:289:VAL:O	2:D:290:THR:C	2.62	0.41
1:A:183:TYR:CE2	1:A:396:GLU:HB3	2.56	0.41
1:A:302:LYS:HB3	1:A:407:GLY:O	2.21	0.41
1:B:272:PRO:HB2	1:B:285:LEU:HD12	2.01	0.41
2:C:310:LYS:NZ	2:C:386:GLU:OE2	2.48	0.41
2:D:31:PHE:HE2	2:D:438:ILE:HG12	1.83	0.41
2:D:501:LEU:O	2:D:505:ILE:CB	2.69	0.41
1:A:108:ASP:CG	1:A:111:THR:HB	2.45	0.41
1:A:154:TRP:O	1:A:191:MSE:HE1	2.20	0.41
1:A:279:ASN:HD22	1:A:281:GLU:HG3	1.82	0.41
1:B:12:ILE:HG21	1:B:35:ILE:CD1	2.50	0.41
1:B:205:GLN:HG2	1:B:261:ARG:O	2.21	0.41
2:C:277:VAL:O	2:C:404:ILE:HG21	2.20	0.41
2:C:328:GLN:O	2:C:329:PRO:C	2.60	0.41
2:D:70:LYS:HD3	2:D:72:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:PHE:HE1	2:D:458:LEU:CD2	2.34	0.41
2:D:219:VAL:CG1	2:D:220:LYS:N	2.82	0.41
2:D:354:LEU:HA	2:D:355:PRO:C	2.46	0.41
1:A:150:LYS:H	1:A:153:HIS:CD2	2.16	0.41
1:A:154:TRP:HZ3	1:A:403:MSE:CE	2.32	0.41
1:A:206:ARG:NH1	2:C:90:GLU:HA	2.35	0.41
1:A:274:ALA:CB	1:A:284:PHE:HA	2.48	0.41
1:A:277:TRP:HD1	1:A:281:GLU:O	2.02	0.41
1:B:100:GLY:HA3	1:B:144:ILE:H	1.85	0.41
1:B:436:TYR:C	1:B:438:ARG:H	2.27	0.41
2:C:21:ILE:O	2:C:189:GLU:HA	2.21	0.41
2:C:150:PRO:HB2	2:C:151:TRP:CE3	2.55	0.41
2:D:101:LEU:C	2:D:101:LEU:CD2	2.94	0.41
2:D:109:TYR:C	2:D:111:LEU:N	2.76	0.41
2:D:397:ILE:O	2:D:398:LYS:C	2.63	0.41
1:B:140:LEU:C	1:B:140:LEU:CD1	2.93	0.41
1:B:318:SER:HB2	1:B:349:SER:CB	2.43	0.41
2:C:310:LYS:HD2	2:C:386:GLU:HB2	2.02	0.41
2:C:392:ALA:O	2:C:396:VAL:HG23	2.21	0.41
2:C:498:LYS:O	2:C:500:SER:N	2.54	0.41
2:D:31:PHE:O	2:D:32:SER:HB2	2.20	0.41
2:D:99:GLU:O	2:D:100:ALA:C	2.63	0.41
1:B:244:THR:HB	1:B:245:TYR:H	1.34	0.41
2:C:6:ASP:HB3	2:C:10:TYR:CE1	2.53	0.41
2:D:116:VAL:HG12	2:D:118:GLU:H	1.84	0.41
2:D:277:VAL:HG12	2:D:278:LYS:N	2.35	0.41
2:D:277:VAL:CG2	2:D:318:LYS:HB2	2.51	0.41
1:A:22:LYS:HZ1	1:A:24:GLU:CG	2.34	0.41
1:A:188:LEU:O	1:A:189:SER:C	2.64	0.41
1:A:210:ARG:HH21	2:C:123:ARG:CZ	2.33	0.41
1:A:259:THR:HG23	1:B:339:LEU:HD23	1.99	0.41
1:A:338:GLY:C	1:A:340:GLY:H	2.29	0.41
1:A:433:PHE:CB	2:D:88:MET:HE1	2.49	0.41
1:B:25:ASP:OD1	1:B:25:ASP:O	2.39	0.41
1:B:51:LEU:HD21	1:B:57:ILE:CD1	2.51	0.41
1:B:344:ASN:ND2	1:B:381:LYS:CD	2.83	0.41
1:B:426:GLU:HG2	1:B:427:ILE:H	1.86	0.41
2:C:7:LYS:HD2	2:C:256:GLU:OE2	2.21	0.41
2:C:32:SER:HA	2:C:33:PRO:HD3	1.88	0.41
2:C:43:GLU:HB3	2:C:80:TYR:CE1	2.56	0.41
2:C:65:LEU:CD2	2:C:65:LEU:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:169:ILE:HB	2:C:177:ILE:HG22	2.03	0.41
2:C:289:VAL:O	2:C:291:ASP:N	2.53	0.41
2:C:291:ASP:OD2	2:C:370:ARG:NH1	2.54	0.41
2:C:298:SER:OG	2:C:300:ILE:HD12	2.21	0.41
2:D:17:VAL:O	2:D:196:ILE:HB	2.20	0.41
2:D:32:SER:HA	2:D:33:PRO:HD3	1.88	0.41
2:D:149:THR:CG2	2:D:152:GLY:O	2.63	0.41
2:D:293:PHE:O	2:D:294:GLU:C	2.63	0.41
1:A:229:GLU:HA	1:A:292:ARG:CG	2.51	0.41
1:A:370:ARG:HB2	1:A:392:ASP:HB3	2.03	0.41
2:C:23:ARG:HD2	2:C:225:THR:O	2.22	0.41
2:C:188:ILE:HG23	2:C:188:ILE:O	2.21	0.41
2:C:333:LEU:O	2:C:336:GLU:HB2	2.22	0.41
2:D:188:ILE:O	2:D:188:ILE:HG23	2.21	0.41
2:D:275:ARG:HH11	2:D:318:LYS:C	2.29	0.41
2:D:509:VAL:O	2:D:510:LEU:C	2.64	0.41
1:A:129:GLU:H	1:A:129:GLU:CD	2.28	0.40
1:A:342:THR:HG23	1:A:343:PRO:CD	2.51	0.40
1:A:424:ALA:C	1:A:426:GLU:H	2.29	0.40
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.75	0.40
2:C:463:VAL:HG11	2:C:478:GLN:HG2	2.03	0.40
2:D:216:THR:C	2:D:218:LYS:N	2.78	0.40
1:B:39:TYR:HB2	2:D:440:PRO:HG2	2.02	0.40
1:B:430:TYR:CE2	2:C:34:VAL:HG22	2.55	0.40
2:C:147:VAL:HG22	2:C:208:PHE:HD2	1.86	0.40
1:A:151:PRO:HA	1:A:154:TRP:CE3	2.57	0.40
1:A:170:TYR:CE1	1:A:292:ARG:CZ	3.04	0.40
1:B:8:LYS:O	1:B:9:GLU:C	2.64	0.40
1:B:241:THR:CG2	2:D:90:GLU:OE2	2.62	0.40
1:B:308:ALA:HB2	1:B:329:TYR:CE2	2.56	0.40
2:D:208:PHE:HE1	2:D:458:LEU:HD21	1.87	0.40
2:D:374:SER:H	2:D:377:ASP:CB	2.35	0.40
1:A:179:ASP:CB	1:B:337:THR:HG23	2.51	0.40
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.86	0.40
1:A:313:TYR:CD2	1:B:309:LEU:HB3	2.57	0.40
1:B:206:ARG:HB3	1:B:213:SER:HA	2.03	0.40
2:C:138:THR:HG22	2:C:139:ALA:H	1.86	0.40
2:C:146:LYS:HE3	2:C:148:GLU:OE1	2.21	0.40
1:A:244:THR:HG22	1:A:245:TYR:N	2.37	0.40
1:A:277:TRP:O	1:A:278:PRO:C	2.64	0.40
2:D:25:LEU:HD21	2:D:188:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:ILE:HG12	2:D:431:ARG:O	2.21	0.40
2:D:261:ARG:HH12	2:D:412:ARG:NE	2.16	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/438 (99%)	374 (86%)	49 (11%)	12 (3%)	4	21
1	B	435/438 (99%)	366 (84%)	56 (13%)	13 (3%)	3	19
2	C	506/633 (80%)	434 (86%)	54 (11%)	18 (4%)	2	16
2	D	506/633 (80%)	428 (85%)	57 (11%)	21 (4%)	2	13
All	All	1882/2142 (88%)	1602 (85%)	216 (12%)	64 (3%)	3	17

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	77	PRO
1	A	78	GLU
1	A	163	LYS
1	A	251	GLY
1	B	40	GLU
1	B	45	ASP
1	B	75	VAL
1	B	76	LYS
1	B	77	PRO
2	C	10	TYR
2	C	499	PRO
2	D	246	GLN

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Mol	Chain	Res	Type
2	D	386	GLU
2	D	499	PRO
1	A	27	GLU
1	A	41	LEU
1	B	251	GLY
2	C	175	GLU
2	C	223	LEU
2	C	484	GLU
2	C	500	SER
2	C	507	VAL
2	D	10	TYR
2	D	372	ASN
2	D	497	VAL
2	D	500	SER
1	A	73	ALA
1	A	302	LYS
1	B	10	ARG
1	B	181	MSE
1	B	213	SER
1	B	416	ARG
2	C	33	PRO
2	C	356	ASN
2	C	498	LYS
2	D	217	LYS
2	D	223	LEU
2	D	484	GLU
2	D	498	LYS
1	A	26	GLY
1	A	142	PHE
1	B	211	PRO
2	C	14	GLY
2	C	290	THR
2	C	355	PRO
2	C	434	PRO
2	C	497	VAL
2	D	33	PRO
2	D	128	ASP
2	D	300	ILE
2	D	356	ASN
2	D	454	ASN
2	D	507	VAL
1	B	216	ALA

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Mol	Chain	Res	Type
1	B	418	MSE
2	C	246	GLN
2	D	144	ASP
1	A	129	GLU
2	C	194	PRO
2	C	292	ILE
2	D	434	PRO
2	D	194	PRO
2	D	329	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/357 (102%)	329 (90%)	37 (10%)	7	29
1	B	367/357 (103%)	323 (88%)	44 (12%)	5	22
2	C	421/548 (77%)	392 (93%)	29 (7%)	14	45
2	D	412/548 (75%)	381 (92%)	31 (8%)	12	41
All	All	1566/1810 (86%)	1425 (91%)	141 (9%)	9	34

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	57	ILE
1	A	77	PRO
1	A	78	GLU
1	A	95	THR
1	A	102	THR
1	A	107	ILE
1	A	111	THR
1	A	136	VAL
1	A	142	PHE
1	A	143	ASN
1	A	146	SER

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Mol	Chain	Res	Type
1	A	147	GLU
1	A	180	THR
1	A	195	LEU
1	A	201	LEU
1	A	206	ARG
1	A	210	ARG
1	A	219	LEU
1	A	233	VAL
1	A	247	LEU
1	A	254	VAL
1	A	273	ILE
1	A	276	ILE
1	A	330	LYS
1	A	335	GLU
1	A	337	THR
1	A	342	THR
1	A	346	ILE
1	A	364	SER
1	A	391	GLU
1	A	396	GLU
1	A	401	LYS
1	A	431	THR
1	A	435	THR
1	A	437	LEU
1	A	438	ARG
1	B	4	ASP
1	B	22	LYS
1	B	24	GLU
1	B	35	ILE
1	B	77	PRO
1	B	86	GLU
1	B	102	THR
1	B	105	SER
1	B	107	ILE
1	B	140	LEU
1	B	142	PHE
1	B	147	GLU
1	B	149	MSE
1	B	195	LEU
1	B	201	LEU
1	B	206	ARG
1	B	219	LEU

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Mol	Chain	Res	Type
1	B	222	SER
1	B	237	MSE
1	B	241	THR
1	B	244	THR
1	B	247	LEU
1	B	252	THR
1	B	263	ASP
1	B	271	VAL
1	B	279	ASN
1	B	301	ASP
1	B	306	LYS
1	B	330	LYS
1	B	337	THR
1	B	348	PRO
1	B	366	CYS
1	B	371	VAL
1	B	373	LEU
1	B	377	SER
1	B	391	GLU
1	B	394	LEU
1	B	396	GLU
1	B	401	LYS
1	B	422	ASN
1	B	426	GLU
1	B	428	THR
1	B	431	THR
1	B	437	LEU
2	C	56	GLU
2	C	57	LEU
2	C	98	ARG
2	C	101	LEU
2	C	140	ILE
2	C	148	GLU
2	C	149	THR
2	C	187	LEU
2	C	191	SER
2	C	193	THR
2	C	195	ASP
2	C	219	VAL
2	C	233	SER
2	C	246	GLN
2	C	247	GLU

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Mol	Chain	Res	Type
2	C	271	GLU
2	C	291	ASP
2	C	300	ILE
2	C	312	LEU
2	C	356	ASN
2	C	371	LEU
2	C	385	GLU
2	C	411	THR
2	C	415	LEU
2	C	420	THR
2	C	434	PRO
2	C	441	LEU
2	C	460	GLN
2	C	499	PRO
2	D	36	SER
2	D	48	ARG
2	D	51	ARG
2	D	56	GLU
2	D	57	LEU
2	D	65	LEU
2	D	101	LEU
2	D	110	LEU
2	D	140	ILE
2	D	148	GLU
2	D	149	THR
2	D	158	THR
2	D	168	ILE
2	D	232	VAL
2	D	246	GLN
2	D	247	GLU
2	D	271	GLU
2	D	354	LEU
2	D	356	ASN
2	D	371	LEU
2	D	385	GLU
2	D	386	GLU
2	D	415	LEU
2	D	417	ASP
2	D	424	ARG
2	D	426	LEU
2	D	436	THR
2	D	441	LEU

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Mol	Chain	Res	Type
2	D	457	GLU
2	D	472	LEU
2	D	499	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	135	ASN
1	A	143	ASN
1	A	153	HIS
1	A	218	ASN
1	A	258	HIS
1	A	279	ASN
1	A	344	ASN
1	A	422	ASN
1	B	56	ASN
1	B	135	ASN
1	B	143	ASN
1	B	153	HIS
1	B	258	HIS
1	B	344	ASN
1	B	365	GLN
1	B	408	HIS
1	B	422	ASN
2	C	22	HIS
2	C	47	GLN
2	C	79	ASN
2	C	106	GLN
2	C	131	ASN
2	C	228	GLN
2	C	231	ASN
2	C	262	GLN
2	C	350	HIS
2	C	356	ASN
2	C	372	ASN
2	C	391	ASN
2	C	478	GLN
2	D	22	HIS
2	D	106	GLN
2	D	131	ASN
2	D	246	GLN

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Mol	Chain	Res	Type
2	D	262	GLN
2	D	350	HIS
2	D	356	ASN
2	D	478	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ASP	B	5000	-	7,8,8	1.19	1 (14%)	6,10,10	1.16	1 (16%)
3	ASP	A	1000	-	7,8,8	1.16	1 (14%)	6,10,10	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	B	5000	-	-	4/8/8/8	-
3	ASP	A	1000	-	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	ASP	OXT-C	-2.26	1.23	1.30
3	B	5000	ASP	OXT-C	-2.24	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5000	ASP	OXT-C-O	-2.11	119.30	124.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	ASP	O-C-CA-N
3	B	5000	ASP	O-C-CA-N
3	A	1000	ASP	OXT-C-CA-N
3	B	5000	ASP	OXT-C-CA-N
3	A	1000	ASP	OXT-C-CA-CB
3	B	5000	ASP	OXT-C-CA-CB
3	A	1000	ASP	O-C-CA-CB
3	B	5000	ASP	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5000	ASP	1	0
3	A	1000	ASP	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.