



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 2ABR / pdb_00002abr
Title : Structure of D280A arginine deiminase with L-arginine forming a S-alkylthiuronium reaction intermediate
Authors : Galkin, A.; Lu, X.; Dunaway-Mariano, D.; Herzberg, O.
Deposited on : 2005-07-15
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

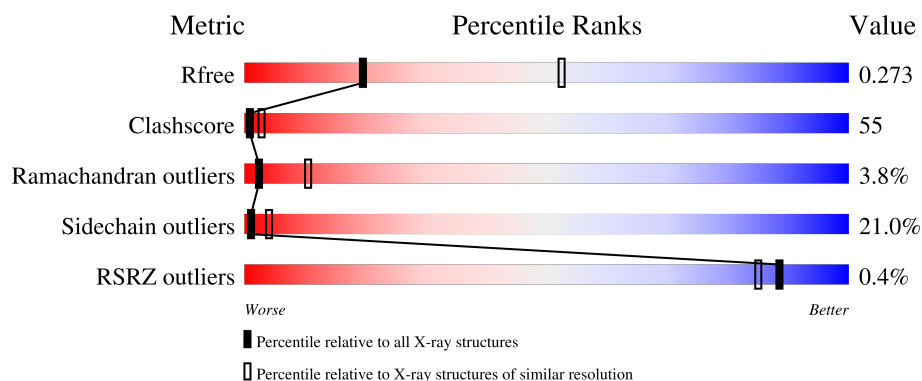
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	418	 29% 51% 15% . .
1	B	418	 31% 51% 15% . .
1	C	418	 30% 49% 16% . .
1	D	418	 31% 52% 13% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12637 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 Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3151	1994	549	591	17			
1	B	406	Total	C	N	O	S	0	0	0
			3174	2008	553	596	17			
1	C	403	Total	C	N	O	S	0	0	0
			3158	1998	550	593	17			
1	D	402	Total	C	N	O	S	0	0	0
			3154	1996	552	589	17			

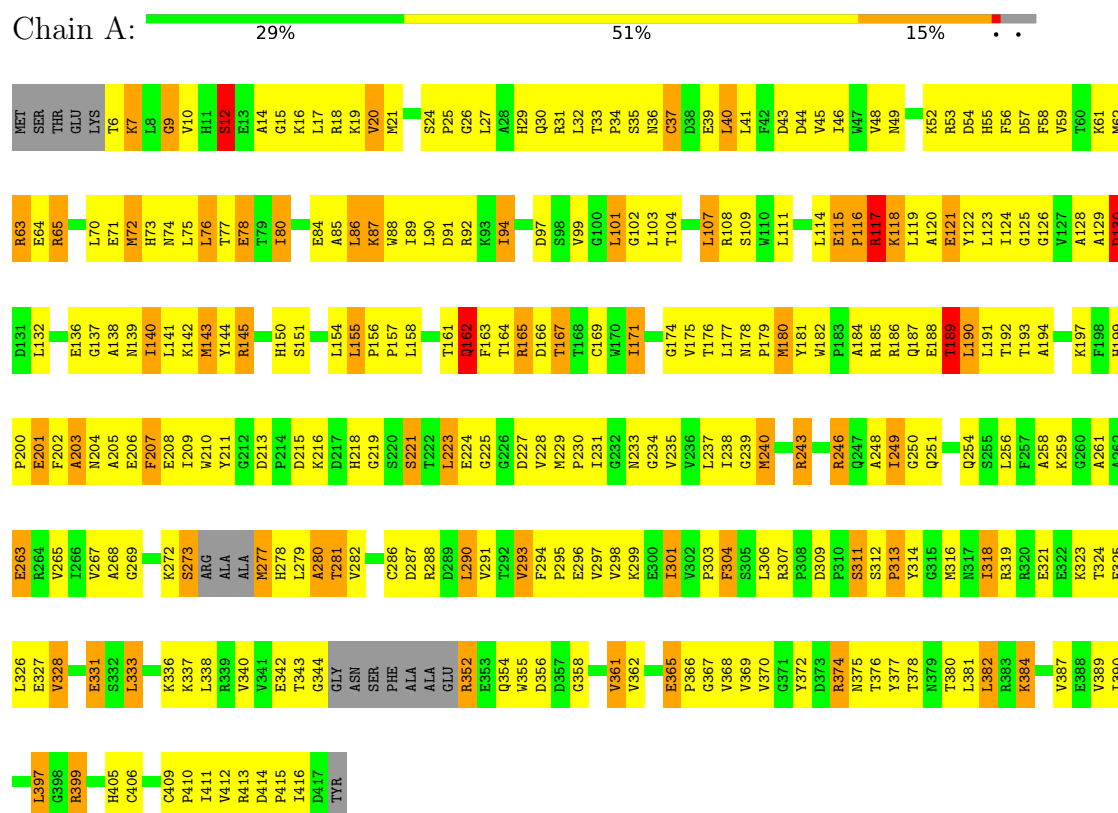
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ALA	ASP	engineered mutation	UNP P13981
A	406	CYR	CYS	modified residue	UNP P13981
B	280	ALA	ASP	engineered mutation	UNP P13981
B	406	CYR	CYS	modified residue	UNP P13981
C	280	ALA	ASP	engineered mutation	UNP P13981
C	406	CYR	CYS	modified residue	UNP P13981
D	280	ALA	ASP	engineered mutation	UNP P13981
D	406	CYR	CYS	modified residue	UNP P13981

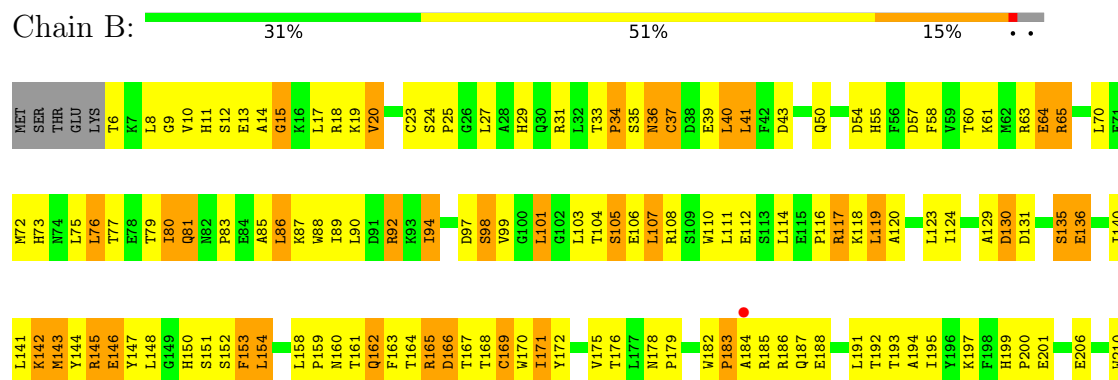
3 Residue-property plots

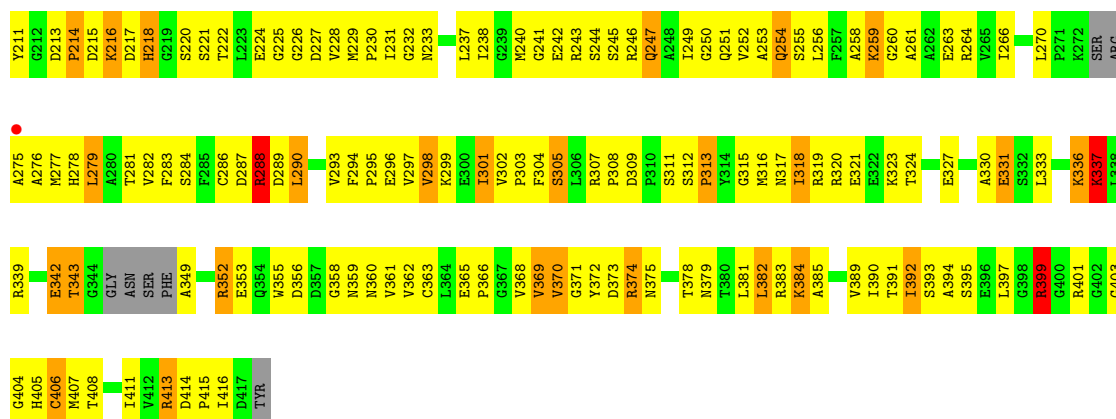
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



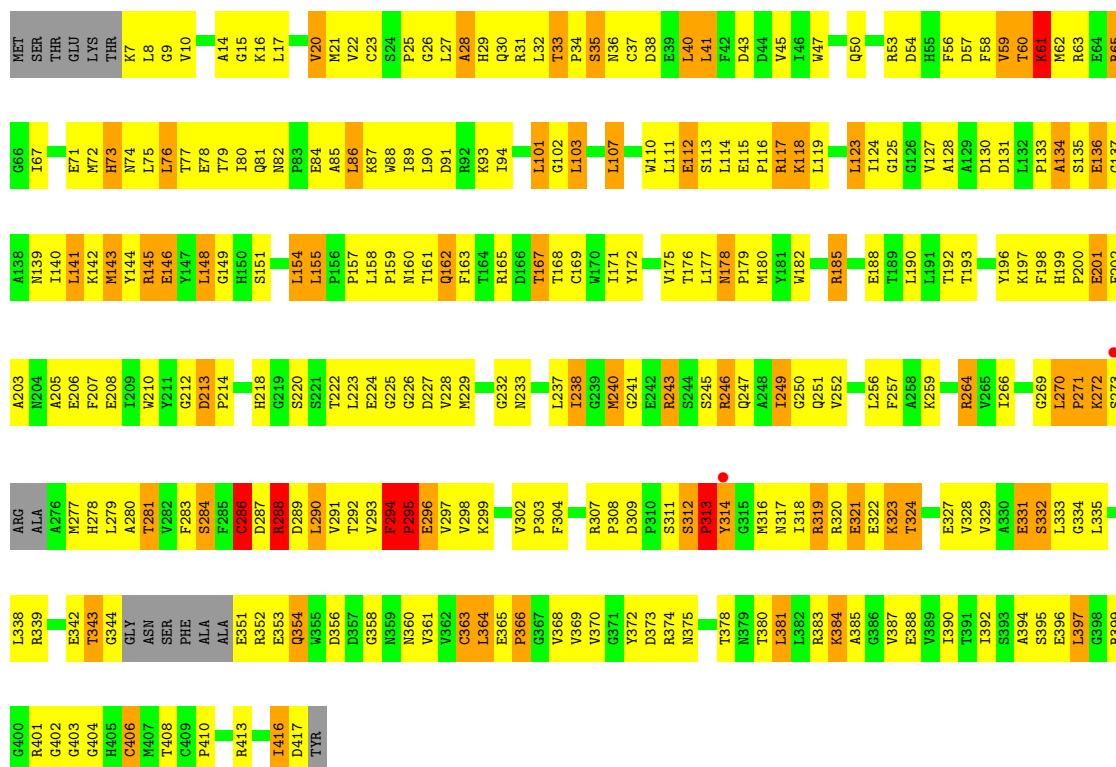
• Molecule 1: Arginine deiminase





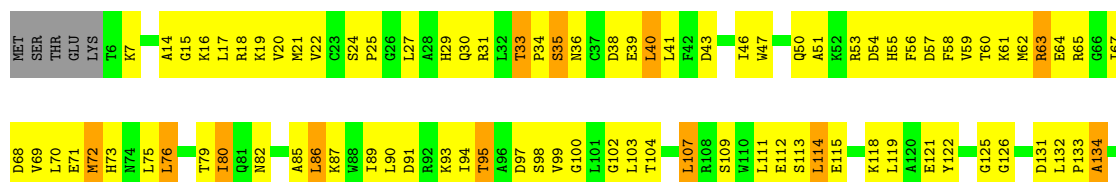
• Molecule 1: Arginine deiminase

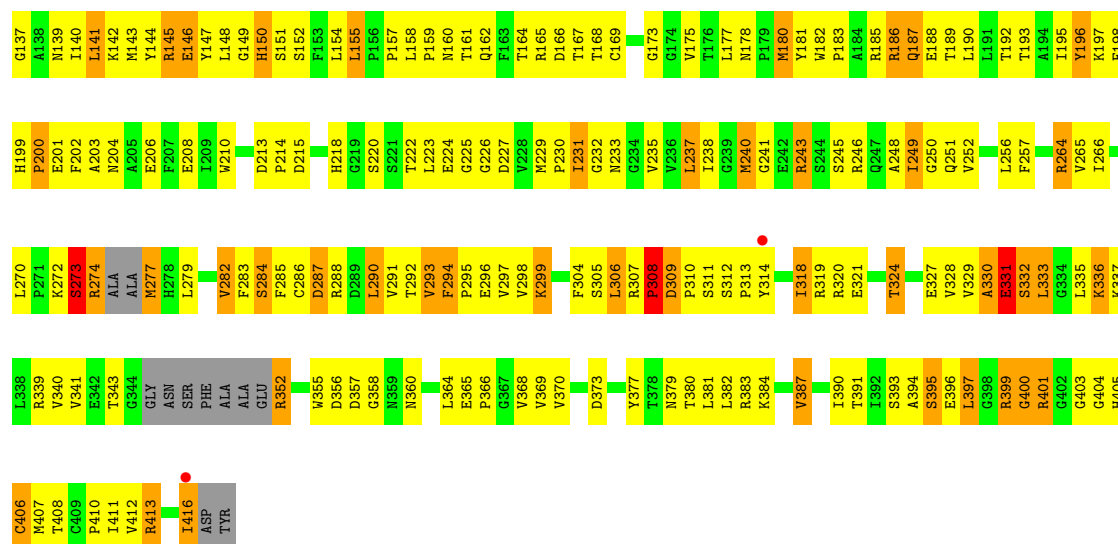
Chain C: 30% 49% 16% . .



• Molecule 1: Arginine deiminase

Chain D: 31% 52% 13% . .





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 120.60Å 147.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 95.7 (20.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.274 0.212 , 0.273	Depositor DCC
R_{free} test set	1715 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12637	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7701e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.61	0/3199	0.98	8/4336 (0.2%)
1	B	0.62	0/3222	0.96	7/4368 (0.2%)
1	C	0.61	0/3206	1.01	9/4345 (0.2%)
1	D	0.59	0/3202	0.98	8/4339 (0.2%)
All	All	0.61	0/12829	0.98	32/17388 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLN	OE1-CD-NE2	-9.48	113.12	122.60
1	C	354	GLN	OE1-CD-NE2	-9.04	113.56	122.60
1	C	270	LEU	O-C-N	7.44	128.19	121.35
1	B	153	PHE	N-CA-C	7.12	120.02	108.63
1	B	81	GLN	CG-CD-NE2	6.79	126.58	116.40
1	A	37	CYS	N-CA-C	-6.74	105.06	113.28
1	A	340	VAL	N-CA-C	6.56	117.57	108.12
1	D	307	ARG	O-C-N	6.55	125.90	121.71
1	C	313	PRO	CB-CA-C	6.43	122.16	111.56
1	C	286	CYS	N-CA-C	-6.35	105.42	113.43
1	C	354	GLN	CG-CD-NE2	6.27	125.80	116.40
1	D	204	ASN	N-CA-C	6.07	121.74	113.97
1	D	206	GLU	N-CA-C	6.00	118.50	108.96
1	D	200	PRO	CA-N-CD	-5.97	103.64	112.00
1	D	231	ILE	N-CA-C	-5.78	105.48	113.00
1	D	399	ARG	N-CA-C	-5.62	105.68	112.54
1	A	9	GLY	N-CA-C	5.52	117.53	110.96
1	B	343	THR	CB-CA-C	-5.51	108.43	116.53
1	A	304	PHE	CA-C-N	-5.51	114.42	122.19
1	A	304	PHE	C-N-CA	-5.51	114.42	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	ASN	N-CA-C	5.44	116.80	109.24
1	B	370	VAL	N-CA-C	5.39	115.61	107.80
1	A	87	LYS	N-CA-C	-5.32	104.94	111.75
1	D	309	ASP	CA-C-N	-5.20	113.43	119.47
1	D	309	ASP	C-N-CA	-5.20	113.43	119.47
1	A	89	ILE	CB-CA-C	-5.19	105.22	112.02
1	B	399	ARG	N-CA-C	-5.13	106.99	113.20
1	C	284	SER	N-CA-C	5.09	116.70	108.26
1	C	89	ILE	CB-CA-C	-5.07	105.37	112.02
1	B	36	ASN	N-CA-C	-5.06	105.81	112.94
1	C	294	PHE	O-C-N	5.06	125.33	121.23
1	A	389	VAL	N-CA-C	5.03	114.72	106.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3151	0	3139	361	0
1	B	3174	0	3160	313	0
1	C	3158	0	3143	365	0
1	D	3154	0	3148	405	0
All	All	12637	0	12590	1383	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 55.

All (1383) 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:A:180:MET:HE1	1:A:224:GLU:CG	1.55	1.36
1:D:43:ASP:CB	1:D:401:ARG:HH12	1.37	1.36
1:D:43:ASP:HB2	1:D:401:ARG:NH1	1.55	1.20
1:D:14:ALA:O	1:D:366:PRO:HD3	1.39	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:MET:HE3	1:A:279:LEU:HD23	1.23	1.17
1:D:352:ARG:HB3	1:D:352:ARG:NH1	1.59	1.17
1:A:306:LEU:HD13	1:A:318:ILE:HG23	1.21	1.17
1:C:199:HIS:CD2	1:C:200:PRO:HD2	1.80	1.17
1:D:413:ARG:HG3	1:D:413:ARG:HH11	1.10	1.13
1:D:186:ARG:HH11	1:D:186:ARG:CG	1.61	1.13
1:B:242:GLU:HB2	1:B:275:ALA:HA	1.26	1.13
1:B:293:VAL:HG13	1:B:298:VAL:CG2	1.78	1.12
1:C:319:ARG:HG2	1:C:319:ARG:NH1	1.46	1.12
1:A:115:GLU:N	1:A:115:GLU:OE1	1.81	1.12
1:D:76:LEU:O	1:D:80:ILE:HG12	1.50	1.12
1:B:64:GLU:OE2	1:B:64:GLU:HA	1.40	1.11
1:B:17:LEU:HD13	1:B:413:ARG:NH1	1.66	1.11
1:C:319:ARG:HH11	1:C:319:ARG:CG	1.61	1.11
1:A:65:ARG:HH11	1:A:65:ARG:HB3	1.14	1.10
1:B:90:LEU:HD22	1:B:94:ILE:HD11	1.34	1.10
1:A:180:MET:HE1	1:A:224:GLU:HG3	1.26	1.10
1:D:186:ARG:HH11	1:D:186:ARG:HG2	1.08	1.10
1:A:180:MET:CE	1:A:224:GLU:HG3	1.83	1.08
1:D:352:ARG:HB3	1:D:352:ARG:HH11	0.93	1.08
1:B:293:VAL:HG13	1:B:298:VAL:HG21	1.10	1.06
1:D:76:LEU:HD22	1:D:80:ILE:HD11	1.05	1.05
1:A:272:LYS:O	1:A:273:SER:HB3	1.51	1.05
1:A:180:MET:HE1	1:A:224:GLU:HG2	1.39	1.04
1:D:401:ARG:HG2	1:D:401:ARG:HH11	1.24	1.02
1:B:242:GLU:HB2	1:B:275:ALA:CA	1.89	1.02
1:D:273:SER:O	1:D:274:ARG:HB2	1.55	1.02
1:D:76:LEU:CD2	1:D:80:ILE:HD11	1.88	1.01
1:B:70:LEU:HB3	1:B:75:LEU:HD11	1.42	1.01
1:D:352:ARG:NH1	1:D:352:ARG:CB	2.22	1.00
1:A:229:MET:CE	1:A:279:LEU:HD23	1.91	1.00
1:B:142:LYS:HD2	1:B:145:ARG:NH2	1.75	1.00
1:D:274:ARG:HA	1:D:274:ARG:HE	1.27	1.00
1:B:167:THR:O	1:B:168:THR:CG2	2.09	0.99
1:A:115:GLU:CD	1:A:115:GLU:H	1.68	0.99
1:D:43:ASP:HB2	1:D:401:ARG:HH12	0.84	0.99
1:C:167:THR:C	1:C:178:ASN:HD22	1.70	0.99
1:D:183:PRO:HA	1:D:186:ARG:HD2	1.42	0.98
1:A:180:MET:HE3	1:A:180:MET:HA	1.44	0.97
1:B:399:ARG:HG2	1:B:399:ARG:HH11	1.28	0.97
1:C:102:GLY:C	1:C:103:LEU:HD12	1.89	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:CE	1:D:149:GLY:HA3	1.94	0.97
1:D:111:LEU:O	1:D:114:LEU:HB2	1.64	0.97
1:A:293:VAL:HB	1:A:298:VAL:HG21	1.43	0.97
1:D:352:ARG:HH11	1:D:352:ARG:CB	1.77	0.97
1:A:25:PRO:HA	1:A:29:HIS:CE1	1.98	0.97
1:D:401:ARG:HH11	1:D:401:ARG:CG	1.78	0.96
1:A:224:GLU:OE1	1:A:243:ARG:HD3	1.65	0.96
1:D:76:LEU:HD22	1:D:80:ILE:CD1	1.95	0.96
1:A:180:MET:CE	1:A:224:GLU:CG	2.40	0.96
1:A:272:LYS:HE2	1:D:149:GLY:HA3	1.48	0.96
1:D:293:VAL:CG1	1:D:298:VAL:HG21	1.94	0.96
1:B:17:LEU:HD13	1:B:413:ARG:HH12	1.28	0.95
1:C:107:LEU:HD21	1:C:127:VAL:HG11	1.48	0.95
1:A:103:LEU:HD13	1:A:154:LEU:CD1	1.96	0.95
1:D:169:CYS:SG	1:D:225:GLY:HA2	2.06	0.95
1:C:295:PRO:HD2	1:C:343:THR:O	1.66	0.95
1:A:101:LEU:HD13	1:A:102:GLY:H	1.32	0.95
1:A:229:MET:HE3	1:A:279:LEU:CD2	1.96	0.94
1:C:137:GLY:HA2	1:C:140:ILE:HD12	1.47	0.94
1:C:101:LEU:HD12	1:C:102:GLY:N	1.83	0.94
1:A:86:LEU:CD1	1:A:90:LEU:HG	1.98	0.94
1:A:228:VAL:HG22	1:A:238:ILE:HG12	1.45	0.94
1:C:140:ILE:HA	1:C:143:MET:HE2	1.46	0.93
1:C:360:ASN:ND2	1:C:406:CYR:SG	2.40	0.93
1:D:114:LEU:HD12	1:D:119:LEU:HA	1.50	0.93
1:C:199:HIS:CD2	1:C:200:PRO:CD	2.52	0.93
1:D:399:ARG:O	1:D:400:GLY:O	1.87	0.93
1:B:101:LEU:HD11	1:C:316:MET:CE	1.99	0.93
1:A:32:LEU:HD23	1:A:40:LEU:HD23	1.49	0.92
1:B:293:VAL:CG1	1:B:298:VAL:HG21	1.99	0.92
1:D:292:THR:O	1:D:293:VAL:HG22	1.69	0.92
1:B:167:THR:O	1:B:168:THR:HG22	1.68	0.92
1:D:17:LEU:HD21	1:D:20:VAL:HG11	1.52	0.91
1:A:229:MET:CE	1:A:279:LEU:CD2	2.49	0.91
1:D:328:VAL:O	1:D:332:SER:HB3	1.69	0.91
1:A:240:MET:HB2	1:A:249:ILE:CD1	2.00	0.91
1:B:360:ASN:OD1	1:B:406:CYR:SG	2.28	0.91
1:C:32:LEU:HD23	1:C:40:LEU:HD23	1.53	0.91
1:A:174:GLY:HA3	1:A:210:TRP:CE2	2.06	0.90
1:D:231:ILE:HD13	1:D:237:LEU:HD21	1.49	0.90
1:D:43:ASP:CB	1:D:401:ARG:NH1	2.21	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ARG:HG3	1:D:413:ARG:NH1	1.74	0.90
1:D:292:THR:C	1:D:293:VAL:HG23	1.97	0.90
1:C:117:ARG:HD2	1:C:117:ARG:O	1.72	0.89
1:A:399:ARG:HG2	1:B:399:ARG:HE	1.35	0.89
1:C:76:LEU:O	1:C:80:ILE:HG12	1.73	0.89
1:C:154:LEU:N	1:C:154:LEU:HD23	1.87	0.89
1:D:292:THR:O	1:D:293:VAL:CG2	2.21	0.89
1:D:293:VAL:O	1:D:295:PRO:HD3	1.73	0.88
1:D:257:PHE:CE2	1:D:308:PRO:HD3	2.08	0.88
1:D:186:ARG:HG2	1:D:186:ARG:NH1	1.82	0.88
1:D:274:ARG:HA	1:D:274:ARG:NE	1.84	0.88
1:A:144:TYR:CZ	1:D:240:MET:HE1	2.08	0.88
1:B:217:ASP:O	1:B:218:HIS:HB2	1.70	0.88
1:C:14:ALA:O	1:C:366:PRO:HD3	1.72	0.88
1:C:240:MET:HE2	1:C:246:ARG:HB3	1.55	0.88
1:D:343:THR:HG22	1:D:357:ASP:HA	1.55	0.87
1:A:171:ILE:HG23	1:A:230:PRO:HB3	1.54	0.87
1:C:107:LEU:HD11	1:C:155:LEU:HD22	1.55	0.87
1:B:294:PHE:CD2	1:B:297:VAL:HG23	2.08	0.87
1:C:77:THR:HG23	1:C:116:PRO:O	1.73	0.87
1:A:31:ARG:HG2	1:A:31:ARG:HH11	1.38	0.86
1:B:309:ASP:O	1:B:315:GLY:HA2	1.76	0.86
1:D:43:ASP:HB3	1:D:401:ARG:HH12	1.40	0.86
1:C:294:PHE:CE1	1:C:297:VAL:HG23	2.10	0.86
1:D:292:THR:C	1:D:293:VAL:CG2	2.49	0.85
1:D:231:ILE:HD11	1:D:235:VAL:CG1	2.06	0.85
1:D:43:ASP:HA	1:D:401:ARG:HH22	1.41	0.85
1:C:28:ALA:CA	1:C:125:GLY:HA2	2.06	0.85
1:B:242:GLU:CB	1:B:275:ALA:HA	2.05	0.85
1:A:269:GLY:HA3	1:D:148:LEU:CD1	2.07	0.85
1:D:306:LEU:HD12	1:D:318:ILE:HB	1.58	0.85
1:A:86:LEU:HD12	1:A:90:LEU:HG	1.57	0.84
1:D:41:LEU:HD11	1:D:182:TRP:CD1	2.12	0.84
1:C:101:LEU:C	1:C:101:LEU:CD1	2.50	0.84
1:B:124:ILE:HG23	1:B:161:THR:HG21	1.59	0.84
1:C:294:PHE:HE1	1:C:296:GLU:HG2	1.42	0.84
1:D:413:ARG:HH11	1:D:413:ARG:CG	1.90	0.84
1:D:72:MET:HE2	1:D:192:THR:OG1	1.76	0.84
1:D:343:THR:HG21	1:D:358:GLY:H	1.39	0.84
1:D:17:LEU:HD11	1:D:20:VAL:CG1	2.08	0.84
1:D:199:HIS:CE1	1:D:201:GLU:HB2	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:CD1	1:B:413:ARG:NH1	2.41	0.83
1:B:101:LEU:HD11	1:C:316:MET:HE3	1.60	0.83
1:C:295:PRO:HG3	1:C:342:GLU:HB2	1.60	0.83
1:D:293:VAL:HG13	1:D:298:VAL:HG21	1.59	0.83
1:A:72:MET:HE2	1:A:192:THR:OG1	1.79	0.82
1:D:237:LEU:N	1:D:237:LEU:HD23	1.94	0.82
1:D:14:ALA:O	1:D:366:PRO:CD	2.27	0.82
1:D:401:ARG:HB2	1:D:406:CYR:H32	1.59	0.82
1:C:28:ALA:HA	1:C:125:GLY:HA2	1.60	0.82
1:A:240:MET:HE2	1:A:246:ARG:CB	2.08	0.82
1:D:20:VAL:HG21	1:D:62:MET:HE1	1.61	0.82
1:C:294:PHE:CE1	1:C:296:GLU:HG2	2.15	0.82
1:B:294:PHE:HD2	1:B:297:VAL:CG2	1.93	0.81
1:C:364:LEU:HD12	1:C:368:VAL:CG1	2.09	0.81
1:C:229:MET:HB2	1:C:237:LEU:HB2	1.62	0.81
1:C:313:PRO:HB2	1:C:314:TYR:CE1	2.15	0.81
1:A:240:MET:HE2	1:A:246:ARG:HB2	1.60	0.81
1:B:295:PRO:HG3	1:B:342:GLU:HB3	1.59	0.81
1:B:242:GLU:HB2	1:B:275:ALA:C	2.04	0.81
1:A:240:MET:HB2	1:A:249:ILE:HD12	1.62	0.81
1:B:336:LYS:O	1:B:337:LYS:HB3	1.79	0.81
1:C:137:GLY:O	1:C:141:LEU:HD23	1.80	0.81
1:C:312:SER:CB	1:C:316:MET:O	2.29	0.80
1:B:142:LYS:CD	1:B:145:ARG:HH22	1.94	0.80
1:C:85:ALA:HB2	1:C:198:PHE:CD1	2.17	0.80
1:D:343:THR:CG2	1:D:357:ASP:HA	2.11	0.80
1:A:103:LEU:HD13	1:A:154:LEU:HD11	1.65	0.79
1:D:186:ARG:CG	1:D:186:ARG:NH1	2.33	0.79
1:A:269:GLY:HA3	1:D:148:LEU:HD11	1.64	0.79
1:A:169:CYS:O	1:A:175:VAL:HG23	1.82	0.79
1:C:257:PHE:CZ	1:C:308:PRO:HD3	2.18	0.79
1:A:290:LEU:HD22	1:A:291:VAL:N	1.96	0.79
1:C:85:ALA:HB2	1:C:198:PHE:CG	2.18	0.79
1:D:231:ILE:HD11	1:D:235:VAL:HG11	1.65	0.79
1:B:167:THR:O	1:B:168:THR:HG23	1.83	0.78
1:A:21:MET:HE1	1:A:192:THR:HG23	1.65	0.78
1:D:107:LEU:HD22	1:D:107:LEU:O	1.82	0.78
1:B:245:SER:O	1:B:249:ILE:HG13	1.83	0.78
1:C:312:SER:HB2	1:C:316:MET:O	1.84	0.78
1:D:257:PHE:CZ	1:D:308:PRO:HD3	2.19	0.78
1:A:80:ILE:HD11	1:A:120:ALA:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ILE:HG22	1:D:86:LEU:HG	1.64	0.78
1:A:213:ASP:OD1	1:A:215:ASP:HB2	1.84	0.78
1:B:142:LYS:CD	1:B:145:ARG:NH2	2.47	0.78
1:A:272:LYS:HG2	1:D:149:GLY:O	1.83	0.78
1:A:381:LEU:HA	1:A:384:LYS:HG3	1.65	0.78
1:D:43:ASP:CA	1:D:401:ARG:HH22	1.97	0.78
1:D:103:LEU:HD11	1:D:141:LEU:HD22	1.66	0.78
1:D:309:ASP:OD1	1:D:312:SER:HB2	1.84	0.78
1:A:65:ARG:HB3	1:A:65:ARG:NH1	1.97	0.78
1:D:273:SER:OG	1:D:274:ARG:N	2.15	0.78
1:D:343:THR:HG21	1:D:358:GLY:N	1.99	0.78
1:B:185:ARG:O	1:B:188:GLU:HB2	1.84	0.77
1:B:169:CYS:O	1:B:175:VAL:HG23	1.83	0.77
1:C:117:ARG:HD2	1:C:117:ARG:C	2.06	0.77
1:D:293:VAL:HG12	1:D:298:VAL:HG21	1.66	0.77
1:D:231:ILE:CD1	1:D:237:LEU:HD21	2.13	0.77
1:B:70:LEU:HD22	1:B:75:LEU:HD21	1.65	0.77
1:C:290:LEU:CD2	1:C:291:VAL:N	2.47	0.77
1:B:294:PHE:CD2	1:B:297:VAL:CG2	2.67	0.77
1:B:365:GLU:HG2	1:B:368:VAL:HB	1.66	0.77
1:C:199:HIS:CG	1:C:200:PRO:CD	2.67	0.77
1:B:167:THR:C	1:B:168:THR:HG23	2.09	0.77
1:C:168:THR:HA	1:C:178:ASN:ND2	2.00	0.77
1:D:306:LEU:CD1	1:D:318:ILE:HB	2.13	0.77
1:C:288:ARG:NH1	1:C:416:ILE:HG22	1.98	0.76
1:D:286:CYS:HB2	1:D:290:LEU:HD13	1.66	0.76
1:B:166:ASP:HB3	1:B:226:GLY:H	1.50	0.76
1:C:290:LEU:HD23	1:C:291:VAL:H	1.50	0.76
1:D:294:PHE:CD2	1:D:297:VAL:HG23	2.20	0.76
1:A:76:LEU:HD22	1:A:80:ILE:HD13	1.67	0.76
1:D:193:THR:HG21	1:D:214:PRO:HG2	1.65	0.76
1:A:231:ILE:HD12	1:A:333:LEU:HD13	1.68	0.76
1:A:356:ASP:OD1	1:A:356:ASP:O	2.03	0.76
1:D:286:CYS:HB2	1:D:290:LEU:CD1	2.16	0.76
1:C:286:CYS:SG	1:C:292:THR:HG23	2.26	0.76
1:D:166:ASP:HB3	1:D:180:MET:HE1	1.68	0.75
1:A:32:LEU:CD2	1:A:40:LEU:HD23	2.16	0.75
1:C:240:MET:CE	1:C:246:ARG:HB3	2.16	0.75
1:A:411:ILE:HG22	1:A:412:VAL:HG23	1.68	0.75
1:C:158:LEU:O	1:C:161:THR:HG23	1.85	0.75
1:C:353:GLU:OE2	1:C:353:GLU:HA	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ASP:HB2	1:C:375:ASN:OD1	1.86	0.75
1:A:107:LEU:HD11	1:A:155:LEU:HD21	1.69	0.75
1:A:365:GLU:HB2	1:A:366:PRO:HD2	1.68	0.75
1:C:23:CYS:HB3	1:C:162:GLN:HA	1.70	0.74
1:A:24:SER:HA	1:A:55:HIS:CE1	2.21	0.74
1:C:8:LEU:HD12	1:C:205:ALA:HB1	1.68	0.74
1:C:167:THR:C	1:C:178:ASN:ND2	2.44	0.74
1:D:94:ILE:CD1	1:D:107:LEU:HD13	2.18	0.74
1:C:101:LEU:HD12	1:C:101:LEU:C	2.09	0.74
1:D:76:LEU:O	1:D:80:ILE:CG1	2.32	0.74
1:A:272:LYS:HE3	1:D:149:GLY:HA3	1.68	0.74
1:A:355:TRP:CZ2	1:B:34:PRO:HG2	2.23	0.74
1:D:18:ARG:HG3	1:D:18:ARG:HH11	1.52	0.73
1:B:349:ALA:N	1:B:352:ARG:HH21	1.85	0.73
1:D:240:MET:HB2	1:D:249:ILE:HD12	1.69	0.73
1:C:293:VAL:O	1:C:295:PRO:HD3	1.88	0.73
1:D:72:MET:CE	1:D:192:THR:OG1	2.36	0.73
1:A:71:GLU:HG3	1:A:73:HIS:H	1.53	0.73
1:D:16:LYS:HD2	1:D:18:ARG:HH12	1.53	0.73
1:A:202:PHE:O	1:A:204:ASN:N	2.22	0.73
1:D:178:ASN:HB3	1:D:223:LEU:O	1.88	0.73
1:D:365:GLU:CD	1:D:368:VAL:HG21	2.14	0.73
1:A:343:THR:HG21	1:A:378:THR:OG1	1.88	0.72
1:B:97:ASP:HB3	1:C:218:HIS:O	1.89	0.72
1:D:157:PRO:O	1:D:159:PRO:HD2	1.89	0.72
1:C:321:GLU:HA	1:C:321:GLU:OE1	1.88	0.72
1:A:99:VAL:HG21	1:A:107:LEU:HD12	1.69	0.72
1:B:14:ALA:O	1:B:366:PRO:HD3	1.89	0.72
1:B:264:ARG:NH1	1:B:305:SER:OG	2.22	0.72
1:A:86:LEU:HD11	1:A:90:LEU:HG	1.70	0.72
1:D:257:PHE:CG	1:D:308:PRO:HG3	2.23	0.72
1:A:101:LEU:CD1	1:A:101:LEU:N	2.52	0.72
1:B:17:LEU:CD1	1:B:413:ARG:HH12	2.02	0.72
1:C:365:GLU:HG2	1:C:368:VAL:HB	1.70	0.72
1:A:101:LEU:HD13	1:A:102:GLY:N	2.03	0.72
1:A:158:LEU:HD21	1:A:187:GLN:HB2	1.72	0.72
1:A:206:GLU:O	1:A:207:PHE:HB3	1.89	0.72
1:A:365:GLU:HB2	1:A:366:PRO:CD	2.19	0.72
1:D:27:LEU:HD21	1:D:31:ARG:HH21	1.55	0.71
1:D:273:SER:O	1:D:274:ARG:CB	2.37	0.71
1:B:41:LEU:HD23	1:B:184:ALA:CB	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:CD1	1:B:333:LEU:HD21	2.19	0.71
1:B:57:ASP:OD1	1:B:61:LYS:HE3	1.89	0.71
1:C:178:ASN:HB2	1:C:180:MET:HE3	1.72	0.71
1:D:55:HIS:O	1:D:58:PHE:HB3	1.90	0.71
1:D:257:PHE:CD2	1:D:308:PRO:HD3	2.25	0.71
1:A:27:LEU:HD12	1:A:27:LEU:O	1.89	0.71
1:B:64:GLU:OE2	1:B:64:GLU:CA	2.29	0.71
1:B:167:THR:C	1:B:168:THR:CG2	2.62	0.71
1:B:302:VAL:HB	1:C:148:LEU:HD21	1.73	0.71
1:A:169:CYS:SG	1:A:225:GLY:HA2	2.30	0.70
1:A:312:SER:OG	1:A:313:PRO:HD2	1.91	0.70
1:D:54:ASP:HB3	1:D:397:LEU:HD22	1.73	0.70
1:D:139:ASN:O	1:D:143:MET:N	2.24	0.70
1:B:318:ILE:HG23	1:B:318:ILE:O	1.90	0.70
1:C:125:GLY:O	1:C:157:PRO:HB3	1.91	0.70
1:D:57:ASP:OD1	1:D:61:LYS:HE3	1.91	0.70
1:B:182:TRP:C	1:B:184:ALA:H	1.98	0.70
1:D:59:VAL:HG12	1:D:60:THR:N	2.05	0.70
1:C:185:ARG:O	1:C:188:GLU:HB2	1.91	0.70
1:B:247:GLN:N	1:B:247:GLN:OE1	2.25	0.70
1:B:282:VAL:HB	1:B:294:PHE:HB3	1.73	0.70
1:C:199:HIS:HD2	1:C:201:GLU:H	1.38	0.70
1:B:107:LEU:HD13	1:B:107:LEU:C	2.17	0.69
1:A:97:ASP:HB3	1:D:218:HIS:O	1.90	0.69
1:A:223:LEU:HD22	1:A:224:GLU:N	2.06	0.69
1:A:248:ALA:O	1:A:250:GLY:N	2.24	0.69
1:C:290:LEU:HD22	1:C:291:VAL:N	2.08	0.69
1:A:94:ILE:HD13	1:A:107:LEU:HD13	1.74	0.69
1:C:31:ARG:HD2	1:C:157:PRO:HG3	1.73	0.69
1:C:320:ARG:HG2	1:C:320:ARG:HH11	1.57	0.69
1:D:365:GLU:CD	1:D:368:VAL:CG2	2.65	0.69
1:A:180:MET:HE3	1:A:224:GLU:HG3	1.73	0.69
1:C:178:ASN:OD1	1:C:223:LEU:HD12	1.91	0.69
1:C:199:HIS:NE2	1:C:200:PRO:HD2	2.08	0.69
1:D:277:MET:O	1:D:277:MET:CG	2.40	0.69
1:A:33:THR:HG22	1:A:36:ASN:CG	2.18	0.69
1:D:330:ALA:O	1:D:332:SER:N	2.25	0.69
1:D:336:LYS:HD2	1:D:336:LYS:O	1.93	0.69
1:A:314:TYR:HE1	1:A:316:MET:O	1.76	0.69
1:B:94:ILE:HG21	1:B:107:LEU:HD12	1.75	0.69
1:D:139:ASN:O	1:D:143:MET:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:PRO:CG	1:C:342:GLU:HB2	2.22	0.69
1:B:72:MET:CE	1:B:164:THR:HG22	2.23	0.69
1:D:24:SER:HB3	1:D:55:HIS:ND1	2.08	0.69
1:D:318:ILE:O	1:D:319:ARG:HD3	1.91	0.69
1:A:25:PRO:HA	1:A:29:HIS:HE1	1.56	0.68
1:A:21:MET:HE1	1:A:192:THR:CG2	2.23	0.68
1:D:186:ARG:HH11	1:D:186:ARG:HG3	1.57	0.68
1:B:61:LYS:O	1:B:65:ARG:HG3	1.92	0.68
1:C:331:GLU:O	1:C:333:LEU:N	2.26	0.68
1:C:257:PHE:CG	1:C:308:PRO:HG3	2.29	0.68
1:D:70:LEU:HB3	1:D:75:LEU:HD11	1.75	0.68
1:A:65:ARG:HH11	1:A:65:ARG:CB	1.99	0.68
1:A:101:LEU:N	1:A:101:LEU:HD12	2.07	0.68
1:B:86:LEU:CD2	1:B:90:LEU:HG	2.24	0.68
1:C:107:LEU:HD11	1:C:155:LEU:CD2	2.21	0.68
1:B:79:THR:O	1:B:81:GLN:N	2.26	0.68
1:A:229:MET:HE1	1:A:279:LEU:HG	1.76	0.68
1:A:248:ALA:O	1:A:249:ILE:C	2.36	0.68
1:B:80:ILE:O	1:B:80:ILE:HG22	1.94	0.68
1:C:272:LYS:C	1:C:272:LYS:HD2	2.17	0.68
1:C:399:ARG:HH21	1:D:396:GLU:CD	2.02	0.68
1:D:43:ASP:HB2	1:D:401:ARG:CZ	2.24	0.67
1:A:362:VAL:C	1:A:369:VAL:HG23	2.19	0.67
1:C:85:ALA:O	1:C:88:TRP:HB3	1.94	0.67
1:D:56:PHE:O	1:D:57:ASP:C	2.35	0.67
1:B:33:THR:HG23	1:B:36:ASN:ND2	2.09	0.67
1:B:73:HIS:CD2	1:B:124:ILE:HD12	2.29	0.67
1:B:370:VAL:HG22	1:B:390:ILE:HB	1.75	0.67
1:C:21:MET:O	1:C:22:VAL:CG1	2.43	0.67
1:C:240:MET:HB2	1:C:249:ILE:HD12	1.75	0.67
1:D:82:ASN:OD1	1:D:82:ASN:C	2.37	0.67
1:B:182:TRP:O	1:B:184:ALA:N	2.27	0.67
1:C:23:CYS:HA	1:C:71:GLU:OE2	1.94	0.67
1:C:85:ALA:HA	1:C:198:PHE:CZ	2.30	0.67
1:C:399:ARG:NH2	1:D:396:GLU:CD	2.52	0.67
1:A:178:ASN:HB3	1:A:223:LEU:O	1.94	0.67
1:B:399:ARG:HG2	1:B:399:ARG:NH1	2.06	0.67
1:C:141:LEU:HD22	1:C:141:LEU:N	2.10	0.67
1:C:154:LEU:N	1:C:154:LEU:CD2	2.57	0.67
1:A:74:ASN:O	1:A:77:THR:HB	1.95	0.67
1:D:394:ALA:O	1:D:396:GLU:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:HD13	1:D:118:LYS:HG2	1.77	0.67
1:D:294:PHE:CE2	1:D:297:VAL:HG23	2.30	0.67
1:A:86:LEU:HD12	1:A:86:LEU:O	1.95	0.66
1:B:90:LEU:HD22	1:B:94:ILE:CD1	2.19	0.66
1:B:360:ASN:ND2	1:B:405:HIS:HB3	2.10	0.66
1:C:163:PHE:CE2	1:C:406:CYR:HC2	2.29	0.66
1:D:27:LEU:HA	1:D:30:GLN:HE21	1.59	0.66
1:D:264:ARG:NH1	1:D:305:SER:OG	2.28	0.66
1:A:54:ASP:HB2	1:A:397:LEU:HD22	1.77	0.66
1:B:246:ARG:HG2	1:B:247:GLN:OE1	1.95	0.66
1:B:323:LYS:HB3	1:B:327:GLU:OE1	1.95	0.66
1:D:227:ASP:O	1:D:238:ILE:HA	1.95	0.66
1:D:401:ARG:NH1	1:D:401:ARG:CG	2.46	0.66
1:A:54:ASP:HB2	1:A:397:LEU:CD2	2.26	0.66
1:C:331:GLU:O	1:C:334:GLY:N	2.26	0.66
1:A:107:LEU:O	1:A:107:LEU:HD22	1.96	0.66
1:C:141:LEU:N	1:C:141:LEU:CD2	2.59	0.66
1:C:290:LEU:HD23	1:C:291:VAL:N	2.08	0.66
1:C:343:THR:OG1	1:C:344:GLY:N	2.23	0.66
1:D:360:ASN:ND2	1:D:405:HIS:HB3	2.10	0.66
1:C:154:LEU:O	1:C:155:LEU:HD13	1.96	0.65
1:D:309:ASP:OD1	1:D:312:SER:CB	2.43	0.65
1:A:279:LEU:C	1:A:281:THR:H	2.02	0.65
1:A:314:TYR:CD2	1:D:102:GLY:HA2	2.32	0.65
1:A:88:TRP:HZ3	1:A:194:ALA:HB2	1.60	0.65
1:D:18:ARG:HH11	1:D:18:ARG:CG	2.08	0.65
1:A:303:PRO:HG3	1:A:328:VAL:HG21	1.78	0.65
1:B:94:ILE:CG2	1:B:107:LEU:HD12	2.26	0.65
1:C:140:ILE:HG22	1:C:144:TYR:CE2	2.32	0.65
1:C:162:GLN:O	1:C:162:GLN:HG2	1.96	0.65
1:A:356:ASP:OD1	1:A:356:ASP:C	2.39	0.65
1:C:85:ALA:O	1:C:88:TRP:N	2.29	0.65
1:C:302:VAL:HG12	1:C:304:PHE:CE2	2.31	0.65
1:A:174:GLY:HA3	1:A:210:TRP:CZ2	2.32	0.65
1:C:9:GLY:HA2	1:C:172:TYR:O	1.97	0.65
1:D:94:ILE:CD1	1:D:107:LEU:CD1	2.75	0.65
1:D:223:LEU:C	1:D:223:LEU:HD23	2.22	0.65
1:D:240:MET:HB2	1:D:249:ILE:CD1	2.26	0.65
1:A:229:MET:CE	1:A:279:LEU:HG	2.27	0.65
1:B:282:VAL:O	1:B:293:VAL:HA	1.97	0.65
1:D:306:LEU:HD12	1:D:318:ILE:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ASN:O	1:D:383:ARG:HD2	1.96	0.65
1:D:89:ILE:HG22	1:D:90:LEU:HD23	1.78	0.65
1:A:31:ARG:HG2	1:A:31:ARG:NH1	2.12	0.64
1:D:331:GLU:O	1:D:331:GLU:HG2	1.97	0.64
1:D:336:LYS:HD2	1:D:336:LYS:C	2.22	0.64
1:A:59:VAL:HG12	1:A:63:ARG:NH1	2.11	0.64
1:A:293:VAL:HG23	1:A:294:PHE:N	2.10	0.64
1:B:142:LYS:HD3	1:B:145:ARG:HH22	1.62	0.64
1:B:140:ILE:HD11	1:C:318:ILE:HG21	1.79	0.64
1:B:211:TYR:HB3	1:B:252:VAL:HG22	1.78	0.64
1:B:231:ILE:HD12	1:B:333:LEU:HD21	1.79	0.64
1:C:168:THR:CA	1:C:178:ASN:ND2	2.61	0.64
1:C:182:TRP:HE1	1:C:243:ARG:HH11	1.46	0.64
1:C:399:ARG:NH2	1:D:396:GLU:OE1	2.29	0.64
1:A:278:HIS:O	1:A:281:THR:HB	1.96	0.64
1:C:135:SER:O	1:C:139:ASN:HB2	1.97	0.64
1:D:63:ARG:C	1:D:65:ARG:H	2.06	0.64
1:B:290:LEU:HD23	1:B:339:ARG:O	1.98	0.64
1:D:365:GLU:OE1	1:D:368:VAL:HG21	1.98	0.64
1:D:80:ILE:CG2	1:D:86:LEU:HG	2.27	0.64
1:A:36:ASN:C	1:A:36:ASN:OD1	2.39	0.63
1:A:174:GLY:HA3	1:A:210:TRP:NE1	2.13	0.63
1:C:21:MET:O	1:C:22:VAL:HG12	1.98	0.63
1:D:383:ARG:HA	1:D:387:VAL:O	1.96	0.63
1:D:17:LEU:HD11	1:D:20:VAL:HG13	1.80	0.63
1:A:88:TRP:CZ3	1:A:194:ALA:HB2	2.33	0.63
1:A:169:CYS:O	1:A:175:VAL:CG2	2.46	0.63
1:D:43:ASP:C	1:D:43:ASP:OD1	2.40	0.63
1:A:356:ASP:HB2	1:A:375:ASN:OD1	1.98	0.63
1:B:238:ILE:HG22	1:B:249:ILE:HD13	1.80	0.63
1:B:349:ALA:N	1:B:352:ARG:NH2	2.47	0.63
1:C:27:LEU:O	1:C:30:GLN:N	2.29	0.63
1:C:314:TYR:N	1:C:314:TYR:CD1	2.65	0.63
1:C:380:THR:O	1:C:384:LYS:HB2	1.99	0.63
1:A:72:MET:CE	1:A:192:THR:OG1	2.46	0.63
1:D:80:ILE:HG21	1:D:119:LEU:HD23	1.80	0.63
1:B:294:PHE:CE2	1:B:297:VAL:HG23	2.33	0.63
1:C:17:LEU:HD21	1:C:20:VAL:HG11	1.80	0.63
1:B:80:ILE:O	1:B:80:ILE:CG2	2.47	0.63
1:C:90:LEU:HD22	1:C:94:ILE:HD11	1.81	0.63
1:C:140:ILE:HA	1:C:143:MET:CE	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASP:HA	1:B:225:GLY:HA3	1.80	0.62
1:A:102:GLY:HA2	1:D:314:TYR:CE2	2.33	0.62
1:A:101:LEU:HD12	1:A:101:LEU:H	1.64	0.62
1:B:9:GLY:HA2	1:B:172:TYR:O	1.98	0.62
1:B:211:TYR:CB	1:B:252:VAL:HG22	2.30	0.62
1:A:142:LYS:HB3	1:A:145:ARG:HH21	1.65	0.62
1:A:116:PRO:O	1:A:118:LYS:N	2.33	0.62
1:A:86:LEU:HD12	1:A:86:LEU:C	2.24	0.62
1:A:124:ILE:HG23	1:A:161:THR:HG21	1.82	0.62
1:A:399:ARG:CG	1:B:399:ARG:HE	2.11	0.62
1:A:304:PHE:CE1	1:D:144:TYR:CE1	2.87	0.62
1:B:161:THR:O	1:B:163:PHE:N	2.33	0.62
1:B:222:THR:O	1:B:244:SER:HA	1.99	0.62
1:C:34:PRO:HD3	1:C:45:VAL:HG21	1.81	0.62
1:C:168:THR:HA	1:C:178:ASN:HD21	1.64	0.62
1:C:179:PRO:O	1:C:222:THR:HA	2.00	0.62
1:A:290:LEU:HD22	1:A:290:LEU:C	2.25	0.61
1:C:111:LEU:C	1:C:113:SER:N	2.58	0.61
1:D:187:GLN:OE1	1:D:187:GLN:HA	2.00	0.61
1:A:303:PRO:CG	1:A:328:VAL:HG21	2.30	0.61
1:B:403:GLY:O	1:B:407:MET:HG3	1.99	0.61
1:C:245:SER:O	1:C:249:ILE:HG13	2.00	0.61
1:D:223:LEU:HD23	1:D:224:GLU:N	2.15	0.61
1:D:352:ARG:NH1	1:D:352:ARG:HB2	2.12	0.61
1:C:323:LYS:HB3	1:C:327:GLU:CB	2.30	0.61
1:C:381:LEU:HD23	1:C:381:LEU:N	2.16	0.61
1:C:293:VAL:HG13	1:C:298:VAL:HG21	1.83	0.61
1:D:20:VAL:HG12	1:D:410:PRO:HA	1.81	0.61
1:A:229:MET:CE	1:A:279:LEU:CG	2.78	0.61
1:D:167:THR:C	1:D:168:THR:HG23	2.25	0.61
1:C:364:LEU:HD12	1:C:368:VAL:HG12	1.83	0.61
1:A:55:HIS:O	1:A:59:VAL:HG23	1.99	0.61
1:D:22:VAL:HA	1:D:164:THR:HG21	1.83	0.61
1:D:330:ALA:C	1:D:332:SER:H	2.07	0.61
1:C:178:ASN:HB3	1:C:223:LEU:O	2.01	0.61
1:C:240:MET:HE2	1:C:246:ARG:CB	2.30	0.61
1:A:231:ILE:HD11	1:A:235:VAL:HG11	1.83	0.61
1:A:202:PHE:C	1:A:204:ASN:H	2.09	0.60
1:A:304:PHE:CZ	1:D:144:TYR:CE1	2.89	0.60
1:D:352:ARG:CB	1:D:352:ARG:CZ	2.78	0.60
1:B:145:ARG:HG2	1:B:146:GLU:N	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:SER:O	1:C:249:ILE:CG1	2.49	0.60
1:D:19:LYS:HD3	1:D:70:LEU:HD11	1.84	0.60
1:D:25:PRO:HA	1:D:29:HIS:CE1	2.36	0.60
1:D:304:PHE:CE1	1:D:320:ARG:HG3	2.36	0.60
1:B:79:THR:C	1:B:81:GLN:H	2.10	0.60
1:B:98:SER:OG	1:B:99:VAL:HG23	2.02	0.60
1:C:27:LEU:O	1:C:29:HIS:N	2.34	0.60
1:D:63:ARG:O	1:D:65:ARG:N	2.34	0.60
1:D:141:LEU:HD23	1:D:154:LEU:HD21	1.83	0.60
1:D:27:LEU:HA	1:D:30:GLN:NE2	2.17	0.60
1:A:362:VAL:O	1:A:369:VAL:HG23	2.00	0.60
1:A:40:LEU:O	1:A:41:LEU:HB2	2.00	0.60
1:A:91:ASP:OD1	1:A:108:ARG:NH1	2.34	0.60
1:B:72:MET:HE1	1:B:164:THR:HG22	1.82	0.60
1:B:73:HIS:NE2	1:B:124:ILE:HD12	2.17	0.60
1:B:99:VAL:HG12	1:B:103:LEU:HB2	1.84	0.60
1:B:231:ILE:HG21	1:B:237:LEU:CD1	2.30	0.60
1:C:111:LEU:C	1:C:113:SER:H	2.08	0.60
1:C:111:LEU:O	1:C:113:SER:N	2.35	0.60
1:A:17:LEU:HD21	1:A:20:VAL:CG1	2.32	0.60
1:C:169:CYS:SG	1:C:225:GLY:HA2	2.42	0.60
1:B:110:TRP:O	1:B:111:LEU:C	2.45	0.60
1:B:240:MET:HE1	1:C:144:TYR:CE1	2.37	0.59
1:C:33:THR:O	1:C:36:ASN:N	2.35	0.59
1:C:168:THR:CA	1:C:178:ASN:HD21	2.15	0.59
1:D:223:LEU:HD12	1:D:252:VAL:HG21	1.84	0.59
1:A:286:CYS:HB2	1:A:290:LEU:CD1	2.32	0.59
1:C:17:LEU:HD21	1:C:20:VAL:CG1	2.32	0.59
1:C:264:ARG:HD3	1:C:307:ARG:NH2	2.16	0.59
1:B:242:GLU:OE1	1:B:276:ALA:HA	2.02	0.59
1:A:41:LEU:HD11	1:A:182:TRP:CG	2.38	0.59
1:A:116:PRO:O	1:A:117:ARG:C	2.46	0.59
1:C:319:ARG:HG2	1:C:319:ARG:HH11	0.67	0.59
1:D:103:LEU:CD1	1:D:141:LEU:CD2	2.81	0.59
1:D:158:LEU:O	1:D:160:ASN:N	2.35	0.59
1:D:330:ALA:C	1:D:332:SER:N	2.58	0.59
1:B:304:PHE:CE1	1:B:320:ARG:HG3	2.37	0.59
1:C:303:PRO:HB2	1:C:321:GLU:HB2	1.85	0.59
1:C:312:SER:O	1:C:314:TYR:N	2.36	0.59
1:D:17:LEU:HD21	1:D:20:VAL:CG1	2.31	0.59
1:A:137:GLY:O	1:A:140:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASP:O	1:A:238:ILE:HA	2.03	0.59
1:D:145:ARG:HA	1:D:150:HIS:H	1.66	0.59
1:A:75:LEU:HA	1:A:78:GLU:HG3	1.84	0.59
1:A:192:THR:O	1:A:193:THR:C	2.46	0.59
1:A:223:LEU:HD22	1:A:224:GLU:H	1.68	0.59
1:A:280:ALA:HB1	1:A:405:HIS:ND1	2.17	0.59
1:B:17:LEU:HB2	1:B:413:ARG:HH12	1.68	0.59
1:B:312:SER:OG	1:B:313:PRO:HD2	2.02	0.59
1:C:33:THR:O	1:C:34:PRO:C	2.45	0.59
1:C:54:ASP:O	1:C:57:ASP:HB3	2.02	0.59
1:D:199:HIS:ND1	1:D:201:GLU:HB2	2.17	0.59
1:D:287:ASP:HB2	1:D:290:LEU:CB	2.33	0.59
1:B:33:THR:HG23	1:B:36:ASN:HD21	1.66	0.58
1:C:78:GLU:CD	1:C:199:HIS:HE1	2.11	0.58
1:C:128:ALA:HB3	1:C:131:ASP:OD2	2.03	0.58
1:A:304:PHE:CE1	1:D:144:TYR:HE1	2.21	0.58
1:D:20:VAL:CG2	1:D:62:MET:HE1	2.33	0.58
1:D:103:LEU:CD1	1:D:141:LEU:HD22	2.32	0.58
1:D:243:ARG:NH2	1:D:406:CYR:O1	2.36	0.58
1:B:15:GLY:HA3	1:B:414:ASP:O	2.03	0.58
1:B:182:TRP:C	1:B:184:ALA:N	2.59	0.58
1:C:27:LEU:HA	1:C:30:GLN:OE1	2.03	0.58
1:C:290:LEU:HD23	1:C:339:ARG:O	2.03	0.58
1:C:331:GLU:HG3	1:C:332:SER:N	2.18	0.58
1:D:111:LEU:O	1:D:119:LEU:HD13	2.03	0.58
1:D:169:CYS:SG	1:D:225:GLY:CA	2.89	0.58
1:A:25:PRO:CA	1:A:29:HIS:CE1	2.83	0.58
1:D:133:PRO:O	1:D:134:ALA:C	2.44	0.58
1:D:225:GLY:C	1:D:227:ASP:H	2.12	0.58
1:A:70:LEU:HD13	1:A:75:LEU:HD11	1.85	0.58
1:B:238:ILE:CG2	1:B:249:ILE:HD13	2.34	0.58
1:B:399:ARG:HH11	1:B:399:ARG:CG	2.07	0.58
1:D:401:ARG:CB	1:D:406:CYR:H32	2.30	0.58
1:B:217:ASP:O	1:B:218:HIS:CB	2.45	0.58
1:C:77:THR:CG2	1:C:116:PRO:O	2.49	0.58
1:C:158:LEU:N	1:C:159:PRO:CD	2.67	0.58
1:A:180:MET:HE3	1:A:180:MET:CA	2.19	0.58
1:C:287:ASP:O	1:C:288:ARG:C	2.46	0.58
1:D:76:LEU:CD2	1:D:80:ILE:CD1	2.67	0.58
1:B:29:HIS:NE2	1:B:159:PRO:O	2.37	0.58
1:A:84:GLU:O	1:A:88:TRP:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:HA	1:A:249:ILE:HB	1.86	0.58
1:B:210:TRP:CH2	1:B:261:ALA:HB2	2.39	0.58
1:B:216:LYS:HD3	1:B:218:HIS:CD2	2.39	0.58
1:D:95:THR:HG23	1:D:98:SER:OG	2.04	0.58
1:D:284:SER:O	1:D:291:VAL:HG12	2.04	0.58
1:B:251:GLN:C	1:B:253:ALA:N	2.60	0.57
1:D:22:VAL:CA	1:D:164:THR:HG21	2.33	0.57
1:C:199:HIS:CG	1:C:200:PRO:HD2	2.29	0.57
1:C:372:TYR:CG	1:C:394:ALA:HB2	2.39	0.57
1:D:43:ASP:CA	1:D:401:ARG:NH2	2.67	0.57
1:D:294:PHE:CD2	1:D:297:VAL:CG2	2.87	0.57
1:C:101:LEU:C	1:C:101:LEU:HD13	2.27	0.57
1:C:213:ASP:OD1	1:C:213:ASP:C	2.47	0.57
1:D:160:ASN:HB3	1:D:185:ARG:NE	2.18	0.57
1:C:154:LEU:HD23	1:C:154:LEU:H	1.70	0.57
1:C:199:HIS:CD2	1:C:201:GLU:H	2.21	0.57
1:B:171:ILE:HG23	1:B:230:PRO:HG3	1.86	0.57
1:C:331:GLU:CG	1:C:332:SER:N	2.67	0.57
1:A:248:ALA:O	1:A:251:GLN:N	2.38	0.57
1:A:295:PRO:HG3	1:A:342:GLU:CD	2.29	0.57
1:A:358:GLY:HA3	1:A:378:THR:HG21	1.87	0.57
1:C:27:LEU:HB3	1:C:125:GLY:HA3	1.86	0.57
1:D:16:LYS:CD	1:D:18:ARG:HH12	2.17	0.57
1:D:17:LEU:HB2	1:D:413:ARG:HH12	1.70	0.57
1:D:285:PHE:HA	1:D:291:VAL:HG12	1.86	0.57
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.15	0.57
1:B:77:THR:HG23	1:B:117:ARG:HA	1.87	0.57
1:B:221:SER:OG	1:B:247:GLN:HB2	2.05	0.57
1:C:158:LEU:HB3	1:C:161:THR:HG23	1.86	0.57
1:A:167:THR:HG21	1:A:188:GLU:HB2	1.85	0.57
1:C:278:HIS:O	1:C:281:THR:HG22	2.05	0.57
1:D:229:MET:HE1	1:D:283:PHE:O	2.05	0.57
1:C:323:LYS:HB3	1:C:327:GLU:HB3	1.86	0.56
1:D:293:VAL:O	1:D:295:PRO:CD	2.50	0.56
1:A:202:PHE:C	1:A:204:ASN:N	2.62	0.56
1:A:355:TRP:CH2	1:B:34:PRO:HG2	2.41	0.56
1:B:88:TRP:NE1	1:B:92:ARG:NH2	2.53	0.56
1:C:27:LEU:HD21	1:C:31:ARG:NH2	2.20	0.56
1:C:43:ASP:HB2	1:C:401:ARG:HH21	1.68	0.56
1:D:63:ARG:NH1	1:D:63:ARG:HG2	2.20	0.56
1:B:166:ASP:CG	1:B:278:HIS:HE1	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ILE:HA	1:B:230:PRO:HG3	1.87	0.56
1:B:279:LEU:C	1:B:281:THR:H	2.11	0.56
1:C:27:LEU:O	1:C:28:ALA:C	2.48	0.56
1:C:115:GLU:HB2	1:C:118:LYS:HZ2	1.71	0.56
1:A:25:PRO:HG3	1:A:162:GLN:OE1	2.04	0.56
1:A:237:LEU:O	1:A:238:ILE:HG13	2.05	0.56
1:B:33:THR:O	1:B:37:CYS:HB3	2.05	0.56
1:C:240:MET:HB2	1:C:249:ILE:CD1	2.36	0.56
1:D:181:TYR:HA	1:D:222:THR:HG21	1.87	0.56
1:D:401:ARG:NH1	1:D:401:ARG:HG2	2.07	0.56
1:B:229:MET:HE1	1:B:283:PHE:HD2	1.71	0.56
1:D:137:GLY:O	1:D:140:ILE:HG13	2.06	0.56
1:A:218:HIS:O	1:A:219:GLY:C	2.48	0.56
1:B:241:GLY:HA3	1:B:270:LEU:HD12	1.88	0.56
1:B:360:ASN:CG	1:B:406:CYR:SG	2.88	0.56
1:C:329:VAL:HG12	1:C:338:LEU:HD11	1.88	0.56
1:D:72:MET:O	1:D:73:HIS:C	2.48	0.56
1:A:331:GLU:O	1:A:331:GLU:HG2	2.06	0.56
1:D:158:LEU:O	1:D:161:THR:HG23	2.07	0.56
1:A:56:PHE:O	1:A:57:ASP:C	2.49	0.55
1:A:267:VAL:HB	1:A:304:PHE:HB2	1.88	0.55
1:B:298:VAL:O	1:B:301:ILE:HG13	2.06	0.55
1:B:358:GLY:HA3	1:B:378:THR:HG21	1.86	0.55
1:A:297:VAL:O	1:A:301:ILE:HG22	2.06	0.55
1:B:318:ILE:HG21	1:C:140:ILE:HD13	1.88	0.55
1:C:145:ARG:O	1:C:145:ARG:HG2	2.04	0.55
1:C:313:PRO:C	1:C:314:TYR:CD1	2.84	0.55
1:D:252:VAL:O	1:D:256:LEU:HG	2.07	0.55
1:D:287:ASP:HB2	1:D:290:LEU:HB2	1.88	0.55
1:D:366:PRO:CG	1:D:416:ILE:HD11	2.35	0.55
1:A:279:LEU:C	1:A:281:THR:N	2.65	0.55
1:B:36:ASN:O	1:B:40:LEU:HB2	2.07	0.55
1:D:94:ILE:HD12	1:D:107:LEU:HD13	1.88	0.55
1:D:160:ASN:HB2	1:D:188:GLU:OE2	2.06	0.55
1:D:286:CYS:SG	1:D:292:THR:HG23	2.46	0.55
1:A:75:LEU:HD22	1:A:199:HIS:CD2	2.42	0.55
1:B:94:ILE:HD13	1:B:107:LEU:CD1	2.37	0.55
1:C:103:LEU:HD12	1:C:103:LEU:N	2.20	0.55
1:C:302:VAL:HG12	1:C:304:PHE:HE2	1.71	0.55
1:C:320:ARG:HG2	1:C:320:ARG:NH1	2.18	0.55
1:A:18:ARG:HB2	1:A:412:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:CG1	1:A:63:ARG:NH1	2.70	0.55
1:C:140:ILE:HG22	1:C:144:TYR:CZ	2.41	0.55
1:B:356:ASP:OD1	1:B:356:ASP:C	2.49	0.55
1:C:395:SER:HB3	1:D:395:SER:HB3	1.89	0.55
1:D:233:ASN:CG	1:D:233:ASN:O	2.50	0.55
1:A:33:THR:OG1	1:A:34:PRO:HD2	2.07	0.55
1:A:268:ALA:HB1	1:A:301:ILE:CD1	2.36	0.55
1:C:364:LEU:HD12	1:C:368:VAL:HG11	1.88	0.55
1:D:27:LEU:HB3	1:D:125:GLY:HA3	1.89	0.55
1:D:140:ILE:HA	1:D:143:MET:CB	2.36	0.55
1:A:269:GLY:CA	1:D:148:LEU:HD13	2.36	0.55
1:B:12:SER:HA	1:B:230:PRO:O	2.07	0.55
1:D:277:MET:O	1:D:277:MET:HG2	2.07	0.55
1:A:62:MET:O	1:A:64:GLU:N	2.40	0.55
1:B:23:CYS:HB2	1:B:72:MET:HE3	1.89	0.55
1:B:358:GLY:O	1:B:361:VAL:HG13	2.07	0.55
1:C:26:GLY:O	1:C:27:LEU:C	2.50	0.55
1:D:57:ASP:OD1	1:D:61:LYS:CE	2.54	0.55
1:D:141:LEU:O	1:D:142:LYS:C	2.49	0.55
1:A:19:LYS:HD2	1:A:411:ILE:CG2	2.38	0.54
1:B:77:THR:HG21	1:B:117:ARG:HG2	1.88	0.54
1:A:9:GLY:O	1:A:412:VAL:HA	2.08	0.54
1:A:34:PRO:HD3	1:A:45:VAL:HG21	1.88	0.54
1:B:148:LEU:HD11	1:C:269:GLY:HA3	1.88	0.54
1:B:231:ILE:HG21	1:B:237:LEU:HD12	1.89	0.54
1:D:57:ASP:CG	1:D:61:LYS:HE3	2.32	0.54
1:D:141:LEU:C	1:D:143:MET:N	2.60	0.54
1:D:240:MET:HG3	1:D:241:GLY:N	2.22	0.54
1:A:86:LEU:HD11	1:A:90:LEU:CG	2.37	0.54
1:B:70:LEU:CB	1:B:75:LEU:HD11	2.29	0.54
1:C:33:THR:N	1:C:36:ASN:OD1	2.40	0.54
1:C:127:VAL:HG12	1:C:127:VAL:O	2.06	0.54
1:C:240:MET:HG2	1:C:241:GLY:N	2.21	0.54
1:C:284:SER:HB2	1:C:292:THR:OG1	2.07	0.54
1:C:396:GLU:OE2	1:D:399:ARG:NH2	2.41	0.54
1:D:17:LEU:HD11	1:D:20:VAL:HG12	1.86	0.54
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.72	0.54
1:A:246:ARG:NE	1:D:141:LEU:HD11	2.22	0.54
1:A:370:VAL:HA	1:A:390:ILE:O	2.07	0.54
1:B:293:VAL:HG13	1:B:298:VAL:CB	2.36	0.54
1:B:356:ASP:OD1	1:B:356:ASP:O	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ARG:HG2	1:C:387:VAL:O	2.07	0.54
1:D:168:THR:HG21	1:D:192:THR:HG21	1.88	0.54
1:A:115:GLU:N	1:A:115:GLU:CD	2.46	0.54
1:B:70:LEU:HB3	1:B:75:LEU:CD1	2.29	0.54
1:B:161:THR:C	1:B:163:PHE:N	2.66	0.54
1:B:352:ARG:HD2	1:B:355:TRP:HA	1.89	0.54
1:D:43:ASP:OD1	1:D:43:ASP:O	2.26	0.54
1:D:167:THR:C	1:D:168:THR:CG2	2.81	0.54
1:C:404:GLY:O	1:C:408:THR:HG23	2.07	0.54
1:A:240:MET:HE2	1:A:246:ARG:HB3	1.87	0.54
1:B:13:GLU:C	1:B:413:ARG:HE	2.16	0.54
1:C:111:LEU:HA	1:C:114:LEU:HD12	1.89	0.54
1:C:133:PRO:O	1:C:134:ALA:C	2.51	0.54
1:A:361:VAL:HB	1:A:369:VAL:HG21	1.90	0.54
1:C:158:LEU:CB	1:C:161:THR:HG23	2.39	0.54
1:B:246:ARG:CZ	1:C:141:LEU:HD11	2.38	0.53
1:C:33:THR:HB	1:C:36:ASN:CG	2.32	0.53
1:C:312:SER:C	1:C:314:TYR:H	2.17	0.53
1:A:24:SER:CA	1:A:55:HIS:CE1	2.90	0.53
1:A:55:HIS:O	1:A:58:PHE:HB3	2.06	0.53
1:A:73:HIS:CD2	1:A:124:ILE:HD12	2.42	0.53
1:A:324:THR:O	1:A:327:GLU:N	2.42	0.53
1:C:257:PHE:CE2	1:C:308:PRO:HD3	2.43	0.53
1:D:140:ILE:HA	1:D:143:MET:HB2	1.91	0.53
1:A:21:MET:HB3	1:A:409:CYS:HB3	1.89	0.53
1:A:306:LEU:CD1	1:A:318:ILE:HG23	2.15	0.53
1:C:85:ALA:HA	1:C:198:PHE:CE1	2.43	0.53
1:C:294:PHE:HD1	1:C:294:PHE:O	1.91	0.53
1:D:14:ALA:C	1:D:366:PRO:HD3	2.24	0.53
1:A:180:MET:HE1	1:A:224:GLU:CD	2.29	0.53
1:A:314:TYR:CE1	1:A:316:MET:O	2.61	0.53
1:C:252:VAL:HG12	1:C:256:LEU:HD11	1.90	0.53
1:D:397:LEU:HG	1:D:407:MET:SD	2.48	0.53
1:A:138:ALA:O	1:A:141:LEU:HB2	2.09	0.53
1:A:268:ALA:HB1	1:A:301:ILE:HD11	1.91	0.53
1:A:294:PHE:HE1	1:A:344:GLY:C	2.16	0.53
1:B:161:THR:O	1:B:162:GLN:C	2.51	0.53
1:D:33:THR:O	1:D:35:SER:N	2.41	0.53
1:D:312:SER:OG	1:D:313:PRO:HD2	2.08	0.53
1:D:401:ARG:HB2	1:D:406:CYR:C3	2.34	0.53
1:C:28:ALA:CB	1:C:125:GLY:HA2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:O	1:A:104:THR:C	2.51	0.53
1:A:122:TYR:O	1:A:126:GLY:N	2.39	0.53
1:C:93:LYS:HE3	1:C:155:LEU:HG	1.91	0.53
1:C:160:ASN:HB3	1:C:185:ARG:CZ	2.38	0.53
1:C:197:LYS:HE3	1:C:198:PHE:CZ	2.43	0.53
1:D:294:PHE:HD2	1:D:297:VAL:CG2	2.22	0.53
1:A:188:GLU:O	1:A:191:LEU:N	2.42	0.53
1:A:269:GLY:HA3	1:D:148:LEU:HD13	1.88	0.53
1:A:279:LEU:O	1:A:281:THR:N	2.42	0.53
1:A:61:LYS:HA	1:A:64:GLU:OE2	2.08	0.53
1:B:129:ALA:O	1:B:130:ASP:C	2.52	0.53
1:C:110:TRP:O	1:C:113:SER:OG	2.20	0.53
1:C:180:MET:CE	1:C:224:GLU:HG2	2.39	0.53
1:A:61:LYS:O	1:A:64:GLU:HG2	2.09	0.52
1:A:277:MET:HE1	1:A:297:VAL:HG21	1.90	0.52
1:B:58:PHE:HB2	1:B:392:ILE:HG21	1.91	0.52
1:B:343:THR:OG1	1:B:359:ASN:ND2	2.39	0.52
1:A:213:ASP:OD1	1:A:215:ASP:CB	2.56	0.52
1:B:158:LEU:O	1:B:161:THR:HG23	2.09	0.52
1:C:169:CYS:O	1:C:175:VAL:HA	2.09	0.52
1:C:399:ARG:NH2	1:D:396:GLU:OE2	2.42	0.52
1:D:225:GLY:C	1:D:227:ASP:N	2.67	0.52
1:D:257:PHE:CE1	1:D:308:PRO:HD3	2.43	0.52
1:D:286:CYS:HB2	1:D:290:LEU:HD12	1.91	0.52
1:D:287:ASP:CB	1:D:290:LEU:HB2	2.39	0.52
1:C:71:GLU:HG3	1:C:73:HIS:H	1.75	0.52
1:C:90:LEU:HD22	1:C:94:ILE:CD1	2.39	0.52
1:C:294:PHE:C	1:C:294:PHE:CD1	2.87	0.52
1:C:107:LEU:CD2	1:C:127:VAL:HG11	2.30	0.52
1:A:33:THR:H	1:A:36:ASN:CG	2.17	0.52
1:B:17:LEU:CD1	1:B:413:ARG:HH11	2.22	0.52
1:B:135:SER:O	1:B:136:GLU:C	2.49	0.52
1:D:394:ALA:O	1:D:395:SER:C	2.51	0.52
1:A:10:VAL:HG12	1:A:10:VAL:O	2.09	0.52
1:A:188:GLU:O	1:A:189:THR:C	2.51	0.52
1:B:237:LEU:HD23	1:B:266:ILE:HB	1.91	0.52
1:B:371:GLY:O	1:B:391:THR:HA	2.10	0.52
1:C:264:ARG:HD3	1:C:307:ARG:CZ	2.40	0.52
1:D:114:LEU:CD1	1:D:118:LYS:HG2	2.38	0.52
1:C:85:ALA:CB	1:C:198:PHE:CG	2.90	0.52
1:D:198:PHE:O	1:D:199:HIS:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:HG2	1:A:375:ASN:N	2.24	0.52
1:B:324:THR:O	1:B:327:GLU:HB2	2.10	0.52
1:C:71:GLU:O	1:C:72:MET:C	2.53	0.52
1:C:177:LEU:CD1	1:C:193:THR:HG23	2.40	0.52
1:A:17:LEU:HD21	1:A:20:VAL:HG11	1.92	0.52
1:B:72:MET:HE3	1:B:164:THR:HG22	1.92	0.52
1:D:309:ASP:O	1:D:310:PRO:C	2.49	0.52
1:A:36:ASN:OD1	1:A:37:CYS:N	2.43	0.52
1:A:87:LYS:HG2	1:A:91:ASP:OD2	2.09	0.52
1:B:242:GLU:CA	1:B:275:ALA:HA	2.40	0.52
1:C:199:HIS:CG	1:C:200:PRO:HD3	2.45	0.52
1:C:303:PRO:C	1:C:304:PHE:CD2	2.88	0.52
1:C:57:ASP:OD1	1:C:61:LYS:HE3	2.10	0.51
1:C:238:ILE:HG21	1:C:249:ILE:HG23	1.92	0.51
1:D:377:TYR:O	1:D:380:THR:HB	2.09	0.51
1:B:213:ASP:C	1:B:215:ASP:H	2.18	0.51
1:C:167:THR:O	1:C:178:ASN:ND2	2.44	0.51
1:C:264:ARG:CZ	1:C:266:ILE:HD11	2.41	0.51
1:D:223:LEU:C	1:D:223:LEU:CD2	2.83	0.51
1:A:312:SER:OG	1:A:313:PRO:CD	2.57	0.51
1:B:148:LEU:HD22	1:C:271:PRO:HD3	1.93	0.51
1:B:166:ASP:HA	1:B:225:GLY:CA	2.41	0.51
1:B:231:ILE:HD13	1:B:237:LEU:HD11	1.92	0.51
1:C:47:TRP:CZ3	1:D:373:ASP:OD2	2.63	0.51
1:C:60:THR:C	1:C:62:MET:N	2.68	0.51
1:A:144:TYR:CE1	1:D:240:MET:HE1	2.45	0.51
1:A:304:PHE:CZ	1:D:144:TYR:CD1	2.98	0.51
1:D:199:HIS:O	1:D:203:ALA:HB2	2.11	0.51
1:A:19:LYS:HD2	1:A:411:ILE:HG21	1.92	0.51
1:A:144:TYR:CE2	1:D:240:MET:HE1	2.44	0.51
1:A:180:MET:CE	1:A:180:MET:HA	2.30	0.51
1:B:143:MET:O	1:B:147:TYR:HB2	2.11	0.51
1:B:17:LEU:HD13	1:B:413:ARG:HH11	1.68	0.51
1:B:86:LEU:HD22	1:B:90:LEU:HG	1.93	0.51
1:B:251:GLN:C	1:B:253:ALA:H	2.18	0.51
1:C:21:MET:C	1:C:22:VAL:HG13	2.36	0.51
1:C:102:GLY:C	1:C:103:LEU:CD1	2.75	0.51
1:C:331:GLU:O	1:C:332:SER:C	2.54	0.51
1:A:352:ARG:N	1:A:377:TYR:CD1	2.79	0.51
1:B:50:GLN:HE21	1:B:54:ASP:CG	2.19	0.51
1:B:287:ASP:O	1:B:288:ARG:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:PRO:O	1:C:134:ALA:O	2.28	0.51
1:C:331:GLU:C	1:C:333:LEU:N	2.68	0.51
1:A:372:TYR:HB2	1:A:375:ASN:ND2	2.26	0.51
1:B:140:ILE:HD11	1:C:318:ILE:CG2	2.40	0.51
1:D:39:GLU:C	1:D:40:LEU:HD13	2.35	0.51
1:A:325:PHE:O	1:A:326:LEU:C	2.54	0.51
1:B:50:GLN:NE2	1:B:54:ASP:OD1	2.43	0.51
1:C:79:THR:HG23	1:C:198:PHE:HB2	1.93	0.51
1:D:181:TYR:HA	1:D:222:THR:CG2	2.41	0.51
1:A:240:MET:CE	1:A:246:ARG:HB2	2.38	0.50
1:C:10:VAL:HG13	1:C:413:ARG:HB3	1.93	0.50
1:C:370:VAL:HG22	1:C:390:ILE:HB	1.93	0.50
1:C:10:VAL:HG21	1:C:410:PRO:HB2	1.93	0.50
1:C:290:LEU:CD2	1:C:290:LEU:C	2.84	0.50
1:D:199:HIS:HE1	1:D:201:GLU:HB2	1.71	0.50
1:D:366:PRO:HG2	1:D:416:ILE:HD11	1.92	0.50
1:A:304:PHE:CZ	1:D:144:TYR:HE1	2.28	0.50
1:B:330:ALA:O	1:B:331:GLU:C	2.53	0.50
1:C:168:THR:N	1:C:178:ASN:ND2	2.59	0.50
1:A:17:LEU:HD12	1:A:18:ARG:H	1.77	0.50
1:A:29:HIS:CD2	1:A:46:ILE:HD11	2.46	0.50
1:A:158:LEU:O	1:A:161:THR:HG23	2.12	0.50
1:B:101:LEU:CD1	1:C:316:MET:HE3	2.36	0.50
1:B:404:GLY:O	1:B:408:THR:HG23	2.12	0.50
1:D:140:ILE:O	1:D:144:TYR:N	2.38	0.50
1:D:257:PHE:HB3	1:D:308:PRO:HG3	1.92	0.50
1:D:321:GLU:HA	1:D:321:GLU:OE2	2.12	0.50
1:B:116:PRO:O	1:B:117:ARG:C	2.55	0.50
1:B:140:ILE:CD1	1:C:318:ILE:HG21	2.42	0.50
1:B:148:LEU:CD1	1:C:269:GLY:HA3	2.42	0.50
1:B:360:ASN:CG	1:B:405:HIS:HB3	2.36	0.50
1:C:290:LEU:CD2	1:C:291:VAL:H	2.15	0.50
1:D:112:GLU:C	1:D:114:LEU:H	2.19	0.50
1:D:167:THR:CG2	1:D:188:GLU:OE1	2.60	0.50
1:D:249:ILE:O	1:D:250:GLY:C	2.55	0.50
1:D:290:LEU:HD23	1:D:339:ARG:HB2	1.93	0.50
1:A:48:VAL:O	1:A:49:ASN:C	2.55	0.50
1:A:49:ASN:HB3	1:A:53:ARG:HH12	1.77	0.50
1:D:158:LEU:HB3	1:D:161:THR:HG23	1.94	0.50
1:D:213:ASP:C	1:D:213:ASP:OD1	2.55	0.50
1:D:343:THR:HG22	1:D:356:ASP:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:GLY:O	1:D:404:GLY:C	2.53	0.50
1:A:6:THR:O	1:A:205:ALA:HB1	2.12	0.50
1:A:72:MET:O	1:A:76:LEU:HB2	2.11	0.50
1:B:85:ALA:O	1:B:89:ILE:HG13	2.11	0.50
1:B:167:THR:O	1:B:167:THR:HG22	2.12	0.50
1:D:19:LYS:HE2	1:D:68:ASP:OD2	2.12	0.50
1:D:85:ALA:HB2	1:D:198:PHE:CG	2.47	0.50
1:A:58:PHE:O	1:A:59:VAL:C	2.53	0.49
1:A:234:GLY:HA3	1:A:263:GLU:HG3	1.93	0.49
1:C:21:MET:C	1:C:22:VAL:CG1	2.85	0.49
1:C:212:GLY:O	1:C:213:ASP:HB2	2.12	0.49
1:D:165:ARG:HB2	1:D:408:THR:O	2.11	0.49
1:C:185:ARG:NH2	1:C:188:GLU:OE1	2.41	0.49
1:D:140:ILE:O	1:D:143:MET:HB3	2.11	0.49
1:D:158:LEU:C	1:D:160:ASN:H	2.20	0.49
1:A:176:THR:HA	1:A:211:TYR:O	2.13	0.49
1:A:256:LEU:HD22	1:A:261:ALA:CB	2.41	0.49
1:D:213:ASP:OD1	1:D:215:ASP:HB2	2.13	0.49
1:B:144:TYR:HE1	1:C:304:PHE:CE1	2.31	0.49
1:C:56:PHE:HA	1:C:59:VAL:HB	1.94	0.49
1:C:137:GLY:C	1:C:139:ASN:N	2.68	0.49
1:C:145:ARG:O	1:C:149:GLY:HA2	2.12	0.49
1:D:225:GLY:O	1:D:227:ASP:N	2.45	0.49
1:B:166:ASP:CG	1:B:278:HIS:CE1	2.90	0.49
1:D:279:LEU:O	1:D:282:VAL:HG23	2.12	0.49
1:A:231:ILE:HD11	1:A:235:VAL:CG1	2.43	0.49
1:A:415:PRO:C	1:A:416:ILE:HG13	2.38	0.49
1:B:19:LYS:HE3	1:B:201:GLU:OE2	2.12	0.49
1:B:101:LEU:CD1	1:C:316:MET:CE	2.84	0.49
1:C:71:GLU:HG3	1:C:73:HIS:HB2	1.95	0.49
1:C:161:THR:HG22	1:C:188:GLU:HG2	1.95	0.49
1:C:250:GLY:O	1:C:316:MET:HE1	2.12	0.49
1:D:399:ARG:O	1:D:400:GLY:C	2.53	0.49
1:A:34:PRO:HG2	1:B:355:TRP:CZ2	2.48	0.49
1:B:394:ALA:O	1:B:395:SER:C	2.56	0.49
1:C:163:PHE:CE1	1:C:402:GLY:HA3	2.48	0.49
1:D:41:LEU:CD1	1:D:182:TRP:CD1	2.92	0.49
1:D:71:GLU:OE1	1:D:73:HIS:HB2	2.12	0.49
1:D:230:PRO:C	1:D:232:GLY:H	2.21	0.49
1:D:321:GLU:HB3	1:D:328:VAL:HG21	1.93	0.49
1:C:232:GLY:O	1:C:233:ASN:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ARG:HB2	1:D:352:ARG:CZ	2.43	0.49
1:B:24:SER:HB2	1:B:55:HIS:ND1	2.28	0.49
1:B:211:TYR:CD2	1:B:252:VAL:HG23	2.47	0.49
1:B:41:LEU:HD23	1:B:184:ALA:HB2	1.92	0.49
1:B:231:ILE:HG13	1:B:333:LEU:HD21	1.94	0.49
1:B:309:ASP:OD2	1:B:311:SER:CB	2.61	0.49
1:A:76:LEU:O	1:A:80:ILE:HG12	2.12	0.48
1:A:286:CYS:HB2	1:A:290:LEU:HD12	1.95	0.48
1:B:81:GLN:O	1:B:83:PRO:HD3	2.13	0.48
1:B:141:LEU:CD1	1:B:154:LEU:HD21	2.42	0.48
1:B:254:GLN:CB	1:B:316:MET:HE2	2.43	0.48
1:B:318:ILE:HG21	1:C:140:ILE:CD1	2.43	0.48
1:D:401:ARG:CB	1:D:406:CYR:C3	2.91	0.48
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.78	0.48
1:A:415:PRO:O	1:A:416:ILE:HG13	2.13	0.48
1:B:107:LEU:CD1	1:B:111:LEU:HD12	2.44	0.48
1:C:76:LEU:HD11	1:C:123:LEU:HD12	1.94	0.48
1:C:257:PHE:CE1	1:C:308:PRO:HD3	2.48	0.48
1:C:353:GLU:OE2	1:C:353:GLU:CA	2.58	0.48
1:C:373:ASP:N	1:C:392:ILE:O	2.45	0.48
1:D:240:MET:CB	1:D:249:ILE:HD12	2.40	0.48
1:D:318:ILE:HG12	1:D:319:ARG:N	2.28	0.48
1:A:164:THR:O	1:A:165:ARG:C	2.54	0.48
1:A:238:ILE:HG21	1:A:249:ILE:HG12	1.94	0.48
1:B:105:SER:O	1:B:106:GLU:C	2.56	0.48
1:B:163:PHE:HE2	1:B:406:CYR:HN22	1.60	0.48
1:B:220:SER:HB2	1:B:247:GLN:HE21	1.78	0.48
1:B:231:ILE:CG1	1:B:333:LEU:HD21	2.42	0.48
1:C:38:ASP:O	1:C:41:LEU:HD23	2.12	0.48
1:C:287:ASP:O	1:C:289:ASP:N	2.47	0.48
1:D:266:ILE:HD13	1:D:328:VAL:HG12	1.94	0.48
1:A:352:ARG:N	1:A:377:TYR:CE1	2.82	0.48
1:B:107:LEU:HD13	1:B:108:ARG:N	2.27	0.48
1:B:238:ILE:HG22	1:B:249:ILE:CD1	2.41	0.48
1:C:416:ILE:O	1:C:417:ASP:C	2.57	0.48
1:B:41:LEU:HD23	1:B:184:ALA:HB3	1.93	0.48
1:B:303:PRO:HG2	1:B:321:GLU:HB2	1.95	0.48
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.69	0.48
1:D:173:GLY:O	1:D:210:TRP:CZ2	2.67	0.48
1:D:195:ILE:HG22	1:D:196:TYR:N	2.28	0.48
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:THR:CG2	1:A:378:THR:OG1	2.59	0.48
1:C:85:ALA:O	1:C:88:TRP:CB	2.60	0.48
1:C:280:ALA:HA	1:C:283:PHE:O	2.14	0.48
1:D:118:LYS:HG3	1:D:122:TYR:HE2	1.78	0.48
1:D:125:GLY:O	1:D:157:PRO:HB3	2.14	0.48
1:D:401:ARG:NH1	1:D:401:ARG:HG3	2.28	0.48
1:A:70:LEU:HB3	1:A:75:LEU:HD11	1.95	0.48
1:A:372:TYR:HB2	1:A:375:ASN:HD22	1.78	0.48
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.48	0.48
1:C:135:SER:O	1:C:136:GLU:C	2.56	0.48
1:C:286:CYS:O	1:C:363:CYS:SG	2.72	0.48
1:C:288:ARG:CZ	1:C:416:ILE:HG22	2.44	0.48
1:C:358:GLY:HA3	1:C:378:THR:HG21	1.96	0.48
1:A:294:PHE:CE1	1:A:344:GLY:C	2.92	0.48
1:B:120:ALA:HA	1:B:123:LEU:HB2	1.95	0.48
1:C:28:ALA:HA	1:C:125:GLY:CA	2.37	0.48
1:C:406:CYS:O1	1:C:406:CYS:C4	2.61	0.48
1:D:199:HIS:O	1:D:203:ALA:CB	2.61	0.48
1:B:33:THR:C	1:B:35:SER:H	2.21	0.48
1:B:111:LEU:HD22	1:B:119:LEU:CD2	2.44	0.48
1:B:148:LEU:CD2	1:C:271:PRO:HD3	2.44	0.48
1:B:150:HIS:NE2	1:C:241:GLY:HA2	2.29	0.48
1:C:158:LEU:O	1:C:160:ASN:N	2.46	0.48
1:D:257:PHE:CB	1:D:308:PRO:HG3	2.43	0.48
1:A:17:LEU:HB2	1:A:413:ARG:HH21	1.79	0.48
1:A:269:GLY:CA	1:D:148:LEU:CD1	2.84	0.48
1:B:373:ASP:OD1	1:B:393:SER:HA	2.14	0.48
1:C:21:MET:HE1	1:C:192:THR:HG23	1.95	0.48
1:C:225:GLY:O	1:C:226:GLY:C	2.57	0.48
1:A:120:ALA:O	1:A:123:LEU:N	2.47	0.47
1:A:237:LEU:C	1:A:238:ILE:HG13	2.39	0.47
1:B:356:ASP:HB2	1:B:375:ASN:OD1	2.13	0.47
1:D:65:ARG:NH1	1:D:390:ILE:CD1	2.78	0.47
1:D:167:THR:HG21	1:D:188:GLU:HB3	1.96	0.47
1:D:306:LEU:HD11	1:D:318:ILE:HB	1.96	0.47
1:B:279:LEU:HD12	1:B:279:LEU:O	2.13	0.47
1:C:115:GLU:HB2	1:C:118:LYS:NZ	2.29	0.47
1:C:312:SER:OG	1:C:316:MET:O	2.29	0.47
1:D:122:TYR:O	1:D:126:GLY:N	2.43	0.47
1:A:74:ASN:O	1:A:78:GLU:HG2	2.14	0.47
1:B:108:ARG:O	1:B:112:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LYS:O	1:C:146:GLU:HB3	2.14	0.47
1:D:158:LEU:C	1:D:160:ASN:N	2.70	0.47
1:A:75:LEU:CD2	1:A:199:HIS:CD2	2.97	0.47
1:A:120:ALA:O	1:A:121:GLU:C	2.57	0.47
1:B:99:VAL:CG1	1:B:103:LEU:HB2	2.44	0.47
1:B:192:THR:O	1:B:195:ILE:N	2.47	0.47
1:B:232:GLY:O	1:B:233:ASN:CB	2.61	0.47
1:C:93:LYS:C	1:C:94:ILE:HG13	2.40	0.47
1:C:252:VAL:HG12	1:C:256:LEU:CD1	2.44	0.47
1:D:330:ALA:O	1:D:331:GLU:C	2.58	0.47
1:D:340:VAL:HG23	1:D:340:VAL:O	2.13	0.47
1:A:164:THR:C	1:A:166:ASP:N	2.72	0.47
1:B:297:VAL:O	1:B:298:VAL:C	2.55	0.47
1:B:414:ASP:HB3	1:B:415:PRO:HD2	1.96	0.47
1:C:141:LEU:CD2	1:C:141:LEU:H	2.27	0.47
1:A:33:THR:HG22	1:A:36:ASN:CB	2.45	0.47
1:A:118:LYS:O	1:A:121:GLU:HB3	2.15	0.47
1:A:150:HIS:NE2	1:D:241:GLY:HA3	2.29	0.47
1:C:28:ALA:HB2	1:C:125:GLY:HA2	1.97	0.47
1:C:84:GLU:HG2	1:C:198:PHE:HE1	1.80	0.47
1:C:324:THR:O	1:C:328:VAL:HG23	2.15	0.47
1:C:339:ARG:NH1	1:C:385:ALA:HB1	2.30	0.47
1:D:56:PHE:O	1:D:59:VAL:HB	2.15	0.47
1:D:63:ARG:C	1:D:65:ARG:N	2.69	0.47
1:D:186:ARG:NH1	1:D:186:ARG:HG3	2.22	0.47
1:D:290:LEU:HG	1:D:339:ARG:NH2	2.29	0.47
1:A:180:MET:CE	1:A:224:GLU:OE2	2.63	0.47
1:A:224:GLU:CD	1:A:243:ARG:HD3	2.38	0.47
1:B:79:THR:C	1:B:81:GLN:N	2.68	0.47
1:B:88:TRP:O	1:B:92:ARG:NH1	2.42	0.47
1:D:61:LYS:NZ	1:D:391:THR:O	2.46	0.47
1:C:60:THR:C	1:C:62:MET:H	2.22	0.47
1:D:36:ASN:C	1:D:38:ASP:N	2.72	0.47
1:A:86:LEU:O	1:A:87:LYS:C	2.58	0.47
1:A:180:MET:CE	1:A:224:GLU:CD	2.88	0.46
1:A:367:GLY:O	1:A:387:VAL:HG13	2.15	0.46
1:B:76:LEU:O	1:B:80:ILE:HG12	2.15	0.46
1:B:250:GLY:O	1:B:253:ALA:HB3	2.15	0.46
1:C:101:LEU:CD1	1:C:102:GLY:N	2.61	0.46
1:C:158:LEU:C	1:C:160:ASN:N	2.71	0.46
1:C:288:ARG:CZ	1:C:416:ILE:CG2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LEU:O	1:D:159:PRO:C	2.58	0.46
1:A:31:ARG:HD2	1:A:125:GLY:O	2.15	0.46
1:A:107:LEU:HD11	1:A:155:LEU:CD2	2.40	0.46
1:A:171:ILE:CG2	1:A:230:PRO:HB3	2.38	0.46
1:B:379:ASN:CG	1:B:389:VAL:HG11	2.40	0.46
1:C:223:LEU:HD13	1:C:223:LEU:C	2.41	0.46
1:D:189:THR:O	1:D:190:LEU:C	2.58	0.46
1:D:343:THR:HG21	1:D:357:ASP:HA	1.94	0.46
1:A:381:LEU:O	1:A:384:LYS:HB2	2.14	0.46
1:D:65:ARG:NH1	1:D:390:ILE:HD11	2.30	0.46
1:D:160:ASN:C	1:D:162:GLN:N	2.73	0.46
1:D:365:GLU:CD	1:D:368:VAL:HG23	2.37	0.46
1:A:213:ASP:OD1	1:A:215:ASP:N	2.42	0.46
1:A:278:HIS:H	1:A:281:THR:HB	1.80	0.46
1:A:362:VAL:O	1:A:369:VAL:CG2	2.63	0.46
1:B:259:LYS:O	1:B:260:GLY:C	2.57	0.46
1:B:301:ILE:HG22	1:B:302:VAL:N	2.30	0.46
1:C:58:PHE:HB2	1:C:392:ILE:HG21	1.96	0.46
1:D:59:VAL:O	1:D:60:THR:C	2.59	0.46
1:A:10:VAL:HG21	1:A:410:PRO:HB2	1.97	0.46
1:A:111:LEU:HA	1:A:114:LEU:HG	1.97	0.46
1:B:229:MET:HE1	1:B:283:PHE:CD2	2.49	0.46
1:C:60:THR:O	1:C:62:MET:N	2.49	0.46
1:D:257:PHE:CG	1:D:308:PRO:HD3	2.50	0.46
1:B:312:SER:O	1:B:313:PRO:C	2.59	0.46
1:B:381:LEU:O	1:B:382:LEU:C	2.56	0.46
1:C:25:PRO:HA	1:C:29:HIS:CE1	2.51	0.46
1:A:199:HIS:ND1	1:A:199:HIS:C	2.73	0.46
1:B:11:HIS:HA	1:B:172:TYR:CD2	2.50	0.46
1:B:307:ARG:HB3	1:B:308:PRO:CD	2.46	0.46
1:C:62:MET:O	1:C:67:ILE:HB	2.15	0.46
1:D:364:LEU:HD11	1:D:370:VAL:HG23	1.97	0.46
1:A:142:LYS:HG2	1:A:145:ARG:HH22	1.81	0.46
1:A:281:THR:HG22	1:A:282:VAL:HG13	1.97	0.46
1:A:343:THR:HG21	1:A:378:THR:HG23	1.97	0.46
1:B:191:LEU:O	1:B:194:ALA:HB3	2.16	0.46
1:C:56:PHE:C	1:C:56:PHE:CD1	2.94	0.46
1:B:101:LEU:HD11	1:C:316:MET:HE1	1.92	0.46
1:B:193:THR:O	1:B:194:ALA:C	2.59	0.46
1:B:363:CYS:O	1:B:413:ARG:NH2	2.38	0.46
1:C:270:LEU:HA	1:C:271:PRO:HD2	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:ND1	1:A:200:PRO:HD2	2.31	0.46
1:A:246:ARG:HE	1:D:141:LEU:HD11	1.81	0.46
1:C:86:LEU:O	1:C:87:LYS:C	2.58	0.46
1:C:155:LEU:HD12	1:C:155:LEU:HA	1.84	0.46
1:C:182:TRP:HE1	1:C:243:ARG:NH1	2.12	0.46
1:C:319:ARG:NH1	1:C:319:ARG:CG	2.34	0.46
1:D:56:PHE:O	1:D:59:VAL:N	2.50	0.46
1:D:248:ALA:O	1:D:251:GLN:N	2.47	0.46
1:B:10:VAL:HB	1:B:170:TRP:O	2.15	0.45
1:B:111:LEU:HA	1:B:114:LEU:HD12	1.99	0.45
1:C:82:ASN:C	1:C:82:ASN:OD1	2.60	0.45
1:D:95:THR:OG1	1:D:97:ASP:N	2.45	0.45
1:A:158:LEU:HD21	1:A:187:GLN:CB	2.45	0.45
1:B:413:ARG:NH1	1:B:413:ARG:HG3	2.31	0.45
1:C:63:ARG:C	1:C:65:ARG:H	2.23	0.45
1:D:90:LEU:O	1:D:94:ILE:HB	2.16	0.45
1:A:229:MET:HE1	1:A:279:LEU:CD2	2.43	0.45
1:A:280:ALA:HB1	1:A:405:HIS:CE1	2.52	0.45
1:A:309:ASP:OD2	1:A:311:SER:N	2.47	0.45
1:B:36:ASN:OD1	1:B:36:ASN:C	2.59	0.45
1:B:154:LEU:HD23	1:B:154:LEU:N	2.32	0.45
1:B:254:GLN:HB2	1:B:316:MET:HE2	1.98	0.45
1:B:399:ARG:NH1	1:B:399:ARG:CG	2.71	0.45
1:C:158:LEU:HB3	1:C:161:THR:CG2	2.46	0.45
1:C:312:SER:C	1:C:314:TYR:N	2.71	0.45
1:D:160:ASN:HB3	1:D:185:ARG:CZ	2.46	0.45
1:D:324:THR:OG1	1:D:327:GLU:HB2	2.17	0.45
1:A:33:THR:HG22	1:A:36:ASN:HB3	1.97	0.45
1:C:137:GLY:C	1:C:139:ASN:H	2.23	0.45
1:C:197:LYS:HG2	1:C:198:PHE:CE2	2.51	0.45
1:C:278:HIS:H	1:C:281:THR:CG2	2.30	0.45
1:D:43:ASP:N	1:D:401:ARG:NH2	2.64	0.45
1:D:168:THR:HG21	1:D:192:THR:CG2	2.46	0.45
1:D:355:TRP:CZ2	1:D:357:ASP:HB2	2.52	0.45
1:A:286:CYS:O	1:A:287:ASP:HB2	2.17	0.45
1:A:311:SER:O	1:A:311:SER:OG	2.28	0.45
1:A:380:THR:O	1:A:384:LYS:CG	2.65	0.45
1:B:264:ARG:HD3	1:B:307:ARG:CZ	2.47	0.45
1:C:245:SER:O	1:C:249:ILE:HG12	2.15	0.45
1:D:230:PRO:C	1:D:232:GLY:N	2.74	0.45
1:D:329:VAL:O	1:D:330:ALA:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:C	1:B:163:PHE:H	2.25	0.45
1:B:279:LEU:C	1:B:281:THR:N	2.75	0.45
1:B:379:ASN:O	1:B:383:ARG:HG3	2.17	0.45
1:D:380:THR:O	1:D:381:LEU:C	2.58	0.45
1:A:218:HIS:O	1:A:221:SER:HB2	2.17	0.45
1:C:227:ASP:O	1:C:238:ILE:HA	2.16	0.45
1:D:309:ASP:HB3	1:D:312:SER:HB3	1.98	0.45
1:D:70:LEU:CB	1:D:75:LEU:HD11	2.46	0.45
1:D:366:PRO:HG3	1:D:416:ILE:HD11	1.99	0.45
1:B:224:GLU:O	1:B:227:ASP:HB2	2.17	0.45
1:C:165:ARG:O	1:C:225:GLY:HA3	2.17	0.45
1:A:14:ALA:HB3	1:A:416:ILE:CD1	2.47	0.45
1:A:294:PHE:CD1	1:A:344:GLY:HA3	2.52	0.45
1:B:192:THR:O	1:B:193:THR:C	2.60	0.45
1:A:240:MET:HE1	1:D:144:TYR:CZ	2.52	0.44
1:C:278:HIS:O	1:C:279:LEU:C	2.60	0.44
1:C:338:LEU:HD23	1:C:338:LEU:HA	1.89	0.44
1:D:248:ALA:O	1:D:249:ILE:C	2.59	0.44
1:A:142:LYS:CB	1:A:145:ARG:HH21	2.30	0.44
1:B:90:LEU:HD13	1:B:108:ARG:HG3	2.00	0.44
1:B:251:GLN:O	1:B:252:VAL:C	2.60	0.44
1:D:58:PHE:CD1	1:D:58:PHE:C	2.94	0.44
1:D:290:LEU:HD23	1:D:339:ARG:O	2.16	0.44
1:D:292:THR:HA	1:D:341:VAL:O	2.17	0.44
1:A:272:LYS:O	1:A:273:SER:CB	2.38	0.44
1:B:17:LEU:HD21	1:B:20:VAL:HG13	1.98	0.44
1:B:111:LEU:HD22	1:B:119:LEU:HD21	1.99	0.44
1:B:287:ASP:O	1:B:289:ASP:N	2.50	0.44
1:C:74:ASN:O	1:C:75:LEU:C	2.59	0.44
1:C:294:PHE:O	1:C:294:PHE:CD1	2.70	0.44
1:C:323:LYS:HB3	1:C:327:GLU:HB2	1.98	0.44
1:D:29:HIS:CD2	1:D:46:ILE:HD11	2.53	0.44
1:D:33:THR:O	1:D:34:PRO:C	2.60	0.44
1:B:295:PRO:CG	1:B:342:GLU:HB3	2.39	0.44
1:C:206:GLU:O	1:C:207:PHE:HB3	2.17	0.44
1:D:86:LEU:HD22	1:D:90:LEU:HG	1.98	0.44
1:A:117:ARG:HE	1:A:117:ARG:HB2	1.56	0.44
1:B:213:ASP:HA	1:B:214:PRO:HD2	1.90	0.44
1:D:79:THR:OG1	1:D:199:HIS:HB2	2.18	0.44
1:D:93:LYS:HE3	1:D:155:LEU:HG	1.99	0.44
1:D:118:LYS:HG3	1:D:122:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:HIS:HD1	1:D:201:GLU:HB2	1.82	0.44
1:D:282:VAL:HG11	1:D:297:VAL:HG11	1.99	0.44
1:A:18:ARG:NH2	1:A:414:ASP:OD1	2.51	0.44
1:A:129:ALA:O	1:A:130:ASP:C	2.59	0.44
1:A:233:ASN:OD1	1:A:233:ASN:N	2.50	0.44
1:B:17:LEU:HB2	1:B:413:ARG:NH1	2.30	0.44
1:B:25:PRO:HA	1:B:29:HIS:CE1	2.53	0.44
1:B:294:PHE:CD2	1:B:297:VAL:HG21	2.50	0.44
1:D:94:ILE:HD11	1:D:107:LEU:HD13	1.95	0.44
1:D:107:LEU:HD22	1:D:107:LEU:C	2.43	0.44
1:A:71:GLU:HG3	1:A:73:HIS:N	2.26	0.44
1:A:86:LEU:C	1:A:88:TRP:N	2.73	0.44
1:B:33:THR:O	1:B:35:SER:N	2.50	0.44
1:B:211:TYR:CG	1:B:252:VAL:HG23	2.53	0.44
1:B:263:GLU:O	1:B:308:PRO:HD3	2.18	0.44
1:B:413:ARG:HH11	1:B:413:ARG:CG	2.31	0.44
1:C:352:ARG:HD3	1:C:354:GLN:O	2.18	0.44
1:D:277:MET:O	1:D:277:MET:HG3	2.16	0.44
1:D:282:VAL:HG12	1:D:294:PHE:HB3	2.00	0.44
1:A:265:VAL:HB	1:A:306:LEU:HB3	2.00	0.44
1:B:178:ASN:HA	1:B:179:PRO:HD3	1.82	0.44
1:C:8:LEU:HD12	1:C:205:ALA:CB	2.42	0.44
1:C:58:PHE:CD1	1:C:370:VAL:HG11	2.53	0.44
1:C:178:ASN:HA	1:C:179:PRO:HD3	1.77	0.44
1:C:185:ARG:HE	1:C:185:ARG:HB3	1.21	0.44
1:D:141:LEU:CD2	1:D:154:LEU:HD21	2.45	0.44
1:A:91:ASP:OD1	1:A:108:ARG:NH2	2.48	0.44
1:A:326:LEU:HD22	1:A:338:LEU:HD12	2.00	0.44
1:C:127:VAL:HG12	1:C:154:LEU:HB2	2.00	0.44
1:C:238:ILE:HD12	1:C:249:ILE:HG23	1.98	0.44
1:D:290:LEU:CD2	1:D:339:ARG:O	2.66	0.44
1:D:290:LEU:HD22	1:D:291:VAL:N	2.33	0.44
1:A:286:CYS:HB2	1:A:290:LEU:HD13	1.98	0.43
1:B:362:VAL:O	1:B:369:VAL:HG22	2.18	0.43
1:C:180:MET:HE2	1:C:224:GLU:HG2	1.99	0.43
1:C:373:ASP:OD2	1:C:373:ASP:C	2.61	0.43
1:D:15:GLY:HA2	1:D:416:ILE:HD13	2.00	0.43
1:D:167:THR:O	1:D:168:THR:CG2	2.66	0.43
1:D:333:LEU:HB2	1:D:335:LEU:HD13	1.98	0.43
1:A:181:TYR:O	1:A:186:ARG:NH2	2.51	0.43
1:B:286:CYS:HB2	1:B:290:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:C	1:C:29:HIS:N	2.74	0.43
1:D:16:LYS:HD2	1:D:18:ARG:NH1	2.28	0.43
1:D:22:VAL:C	1:D:164:THR:HG21	2.43	0.43
1:D:82:ASN:OD1	1:D:82:ASN:O	2.37	0.43
1:D:86:LEU:HD23	1:D:86:LEU:HA	1.72	0.43
1:D:139:ASN:HA	1:D:142:LYS:HB2	1.99	0.43
1:A:280:ALA:CB	1:A:405:HIS:CE1	3.01	0.43
1:A:378:THR:HG22	1:A:382:LEU:HD22	2.00	0.43
1:B:374:ARG:HG2	1:B:394:ALA:CB	2.49	0.43
1:C:160:ASN:HB2	1:C:188:GLU:OE2	2.17	0.43
1:C:356:ASP:OD2	1:C:375:ASN:HB3	2.18	0.43
1:A:15:GLY:HA3	1:A:414:ASP:O	2.17	0.43
1:A:65:ARG:NH2	1:A:368:VAL:HG11	2.33	0.43
1:A:178:ASN:HA	1:A:179:PRO:HD3	1.92	0.43
1:A:361:VAL:HB	1:A:369:VAL:CG2	2.48	0.43
1:B:175:VAL:HG22	1:B:176:THR:N	2.34	0.43
1:C:177:LEU:HD13	1:C:193:THR:HG23	1.99	0.43
1:D:19:LYS:HG3	1:D:68:ASP:HB3	2.00	0.43
1:D:160:ASN:CB	1:D:188:GLU:OE2	2.67	0.43
1:B:228:VAL:HG22	1:B:238:ILE:HG12	2.01	0.43
1:C:158:LEU:C	1:C:160:ASN:H	2.27	0.43
1:C:197:LYS:HG2	1:C:198:PHE:CD2	2.54	0.43
1:C:289:ASP:N	1:C:289:ASP:OD2	2.51	0.43
1:D:103:LEU:HD13	1:D:141:LEU:CD2	2.48	0.43
1:D:114:LEU:HB3	1:D:119:LEU:HB2	2.00	0.43
1:D:195:ILE:C	1:D:197:LYS:N	2.76	0.43
1:A:107:LEU:HD22	1:A:107:LEU:C	2.43	0.43
1:A:227:ASP:OD2	1:A:278:HIS:HA	2.18	0.43
1:B:170:TRP:CD2	1:B:175:VAL:HB	2.53	0.43
1:B:252:VAL:O	1:B:256:LEU:HG	2.18	0.43
1:C:175:VAL:HG21	1:C:196:TYR:HE2	1.84	0.43
1:D:264:ARG:NH1	1:D:305:SER:HG	2.16	0.43
1:A:202:PHE:O	1:A:203:ALA:C	2.62	0.43
1:B:14:ALA:O	1:B:15:GLY:O	2.36	0.43
1:B:63:ARG:C	1:B:65:ARG:H	2.27	0.43
1:B:103:LEU:O	1:B:104:THR:C	2.62	0.43
1:D:63:ARG:HH11	1:D:63:ARG:CG	2.32	0.43
1:A:156:PRO:HG2	1:A:187:GLN:HG3	1.99	0.43
1:A:199:HIS:CE1	1:A:201:GLU:HB2	2.54	0.43
1:B:61:LYS:NZ	1:B:391:THR:O	2.45	0.43
1:B:171:ILE:HA	1:B:230:PRO:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:TRP:CD2	1:D:50:GLN:HB2	2.54	0.43
1:D:196:TYR:CD1	1:D:202:PHE:CD1	3.07	0.43
1:D:287:ASP:HB2	1:D:290:LEU:HB3	2.00	0.43
1:B:231:ILE:HG21	1:B:237:LEU:HD11	2.00	0.43
1:B:282:VAL:HG11	1:B:297:VAL:HG11	2.01	0.43
1:C:73:HIS:O	1:C:77:THR:OG1	2.33	0.43
1:C:127:VAL:HB	1:C:155:LEU:HB2	2.01	0.43
1:A:31:ARG:HD3	1:A:157:PRO:HG3	2.01	0.43
1:B:107:LEU:HD11	1:B:111:LEU:HD12	2.00	0.43
1:B:160:ASN:O	1:B:161:THR:C	2.62	0.43
1:C:21:MET:O	1:C:22:VAL:HG13	2.18	0.43
1:D:43:ASP:HA	1:D:401:ARG:NH2	2.22	0.43
1:D:100:GLY:O	1:D:104:THR:HG23	2.18	0.43
1:D:399:ARG:C	1:D:400:GLY:O	2.58	0.43
1:A:128:ALA:O	1:A:129:ALA:C	2.61	0.42
1:A:248:ALA:C	1:A:250:GLY:N	2.77	0.42
1:B:72:MET:HE3	1:B:164:THR:CG2	2.49	0.42
1:B:317:ASN:OD1	1:B:318:ILE:N	2.52	0.42
1:C:36:ASN:CG	1:C:40:LEU:HD22	2.43	0.42
1:C:87:LYS:HD3	1:C:91:ASP:OD2	2.19	0.42
1:C:88:TRP:NE1	1:C:197:LYS:HE2	2.34	0.42
1:C:294:PHE:CD1	1:C:297:VAL:HB	2.54	0.42
1:D:157:PRO:C	1:D:159:PRO:CD	2.92	0.42
1:A:355:TRP:CH2	1:B:34:PRO:CG	3.02	0.42
1:B:14:ALA:O	1:B:366:PRO:CD	2.65	0.42
1:B:309:ASP:OD2	1:B:311:SER:HB3	2.18	0.42
1:D:87:LYS:HG2	1:D:91:ASP:OD2	2.18	0.42
1:A:26:GLY:N	1:A:29:HIS:ND1	2.67	0.42
1:A:43:ASP:O	1:A:44:ASP:HB2	2.18	0.42
1:A:282:VAL:HB	1:A:294:PHE:HB3	2.01	0.42
1:C:71:GLU:O	1:C:73:HIS:N	2.52	0.42
1:C:111:LEU:O	1:C:112:GLU:C	2.63	0.42
1:C:279:LEU:C	1:C:281:THR:N	2.77	0.42
1:D:146:GLU:HG3	1:D:147:TYR:N	2.34	0.42
1:D:157:PRO:O	1:D:159:PRO:CD	2.64	0.42
1:D:245:SER:O	1:D:249:ILE:HG13	2.19	0.42
1:A:303:PRO:HG2	1:A:321:GLU:HB2	2.00	0.42
1:B:18:ARG:NH1	1:B:414:ASP:OD2	2.50	0.42
1:B:213:ASP:C	1:B:215:ASP:N	2.76	0.42
1:B:216:LYS:HG2	1:B:217:ASP:N	2.33	0.42
1:B:287:ASP:C	1:B:289:ASP:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:PRO:HG2	1:D:51:ALA:HB1	2.01	0.42
1:D:80:ILE:HG12	1:D:80:ILE:H	1.36	0.42
1:D:94:ILE:HD11	1:D:107:LEU:CD1	2.50	0.42
1:D:165:ARG:NH1	1:D:405:HIS:O	2.48	0.42
1:D:312:SER:OG	1:D:313:PRO:CD	2.67	0.42
1:A:31:ARG:NH1	1:A:31:ARG:CG	2.75	0.42
1:A:54:ASP:CB	1:A:397:LEU:CD2	2.98	0.42
1:A:169:CYS:O	1:A:175:VAL:HA	2.20	0.42
1:A:375:ASN:O	1:A:376:THR:C	2.62	0.42
1:B:43:ASP:OD2	1:B:401:ARG:HB2	2.20	0.42
1:B:73:HIS:HB3	1:B:117:ARG:NH2	2.35	0.42
1:B:254:GLN:HB3	1:B:316:MET:CE	2.50	0.42
1:C:202:PHE:O	1:C:203:ALA:C	2.62	0.42
1:A:27:LEU:O	1:A:30:GLN:HB2	2.20	0.42
1:A:80:ILE:CD1	1:A:120:ALA:HB2	2.42	0.42
1:A:161:THR:C	1:A:163:PHE:N	2.77	0.42
1:C:28:ALA:N	1:C:125:GLY:HA2	2.34	0.42
1:C:190:LEU:HD12	1:C:214:PRO:HB2	2.01	0.42
1:C:249:ILE:C	1:C:251:GLN:N	2.77	0.42
1:C:397:LEU:HA	1:C:397:LEU:HD12	1.81	0.42
1:D:39:GLU:HG3	1:D:40:LEU:HD13	2.01	0.42
1:D:223:LEU:CD1	1:D:252:VAL:HG21	2.48	0.42
1:D:257:PHE:CZ	1:D:265:VAL:HG23	2.54	0.42
1:A:140:ILE:HA	1:A:143:MET:HB2	2.01	0.42
1:A:296:GLU:OE2	1:A:296:GLU:N	2.47	0.42
1:D:56:PHE:O	1:D:57:ASP:O	2.37	0.42
1:D:185:ARG:O	1:D:186:ARG:C	2.59	0.42
1:D:243:ARG:HH11	1:D:274:ARG:HH12	1.68	0.42
1:C:78:GLU:O	1:C:81:GLN:HB2	2.20	0.42
1:C:290:LEU:HD22	1:C:290:LEU:C	2.44	0.42
1:D:21:MET:C	1:D:22:VAL:HG13	2.45	0.42
1:A:24:SER:HB2	1:A:55:HIS:ND1	2.35	0.42
1:A:189:THR:O	1:A:190:LEU:C	2.60	0.42
1:A:256:LEU:HD22	1:A:261:ALA:HB3	2.02	0.42
1:A:327:GLU:O	1:A:328:VAL:C	2.63	0.42
1:A:343:THR:HG21	1:A:378:THR:CG2	2.50	0.42
1:C:160:ASN:HB3	1:C:185:ARG:NH1	2.35	0.42
1:C:286:CYS:SG	1:C:292:THR:CG2	3.05	0.42
1:A:272:LYS:HE2	1:D:149:GLY:CA	2.34	0.42
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.84	0.42
1:C:50:GLN:HA	1:C:53:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLU:OE1	1:C:199:HIS:HE1	2.02	0.42
1:C:247:GLN:O	1:C:251:GLN:HG3	2.20	0.42
1:D:67:ILE:HG22	1:D:69:VAL:HG22	2.02	0.42
1:A:18:ARG:HH11	1:A:18:ARG:CG	2.33	0.41
1:C:77:THR:HG23	1:C:117:ARG:HA	2.02	0.41
1:C:177:LEU:HD11	1:C:193:THR:HG23	2.02	0.41
1:C:178:ASN:OD1	1:C:223:LEU:CD1	2.64	0.41
1:C:302:VAL:HA	1:C:303:PRO:HD3	1.67	0.41
1:C:329:VAL:CG1	1:C:338:LEU:HD11	2.49	0.41
1:C:383:ARG:CG	1:C:387:VAL:O	2.68	0.41
1:A:33:THR:O	1:A:36:ASN:OD1	2.37	0.41
1:A:62:MET:C	1:A:64:GLU:N	2.78	0.41
1:A:85:ALA:O	1:A:88:TRP:HB3	2.20	0.41
1:B:227:ASP:O	1:B:238:ILE:HA	2.20	0.41
1:C:33:THR:HG22	1:C:35:SER:N	2.35	0.41
1:C:177:LEU:O	1:C:212:GLY:HA3	2.20	0.41
1:D:94:ILE:O	1:D:94:ILE:HG22	2.19	0.41
1:A:80:ILE:HG12	1:A:80:ILE:H	1.62	0.41
1:B:88:TRP:CE2	1:B:92:ARG:CZ	3.04	0.41
1:D:22:VAL:HA	1:D:164:THR:CG2	2.49	0.41
1:A:199:HIS:ND1	1:A:200:PRO:N	2.68	0.41
1:B:141:LEU:HD21	1:C:246:ARG:CD	2.50	0.41
1:B:142:LYS:HD2	1:B:145:ARG:HH21	1.72	0.41
1:B:154:LEU:HD22	1:B:154:LEU:HA	1.90	0.41
1:B:216:LYS:HD2	1:B:218:HIS:NE2	2.35	0.41
1:D:112:GLU:C	1:D:114:LEU:N	2.78	0.41
1:A:19:LYS:CD	1:A:411:ILE:HG21	2.50	0.41
1:A:142:LYS:CB	1:A:145:ARG:NH2	2.84	0.41
1:A:158:LEU:HB3	1:A:161:THR:HG23	2.03	0.41
1:A:199:HIS:CE1	1:A:201:GLU:H	2.38	0.41
1:B:251:GLN:O	1:B:253:ALA:N	2.53	0.41
1:C:171:ILE:HD11	1:C:228:VAL:HG11	2.02	0.41
1:C:383:ARG:HA	1:C:387:VAL:O	2.20	0.41
1:A:12:SER:OG	1:A:414:ASP:O	2.37	0.41
1:A:144:TYR:CE1	1:D:240:MET:CE	3.04	0.41
1:A:197:LYS:O	1:A:197:LYS:HG2	2.20	0.41
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.91	0.41
1:B:13:GLU:CD	1:B:229:MET:HG2	2.45	0.41
1:B:372:TYR:HB2	1:B:375:ASN:HD22	1.85	0.41
1:C:9:GLY:CA	1:C:172:TYR:O	2.66	0.41
1:C:58:PHE:CZ	1:C:62:MET:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:CA	1:C:103:LEU:HD12	2.47	0.41
1:D:94:ILE:HD13	1:D:99:VAL:HG21	2.03	0.41
1:D:140:ILE:HA	1:D:143:MET:HB3	2.03	0.41
1:A:34:PRO:HG2	1:B:355:TRP:CH2	2.56	0.41
1:A:56:PHE:O	1:A:59:VAL:N	2.53	0.41
1:A:70:LEU:CD1	1:A:75:LEU:HD11	2.50	0.41
1:B:124:ILE:CG2	1:B:161:THR:HG21	2.39	0.41
1:B:199:HIS:O	1:B:200:PRO:C	2.62	0.41
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.83	0.41
1:D:394:ALA:C	1:D:396:GLU:N	2.77	0.41
1:A:10:VAL:HG12	1:A:230:PRO:HG2	2.01	0.41
1:A:41:LEU:HD12	1:A:184:ALA:HB3	2.03	0.41
1:A:187:GLN:HA	1:A:187:GLN:OE1	2.20	0.41
1:A:318:ILE:H	1:A:318:ILE:HG12	1.58	0.41
1:C:272:LYS:O	1:C:273:SER:C	2.64	0.41
1:D:141:LEU:HD12	1:D:141:LEU:HA	1.65	0.41
1:A:7:LYS:HB2	1:A:7:LYS:HE3	1.50	0.41
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.58	0.41
1:A:54:ASP:CB	1:A:397:LEU:HD22	2.49	0.41
1:A:139:ASN:HA	1:A:142:LYS:CD	2.51	0.41
1:A:254:GLN:O	1:A:254:GLN:HG2	2.21	0.41
1:A:282:VAL:O	1:A:293:VAL:HA	2.20	0.41
1:A:324:THR:OG1	1:A:327:GLU:HG3	2.20	0.41
1:B:83:PRO:O	1:B:87:LYS:HB2	2.20	0.41
1:B:165:ARG:HH11	1:B:165:ARG:HD2	1.77	0.41
1:B:255:SER:O	1:B:259:LYS:HD3	2.21	0.41
1:C:176:THR:HG22	1:C:210:TRP:HB2	2.02	0.41
1:C:294:PHE:HE1	1:C:297:VAL:HG23	1.78	0.41
1:D:16:LYS:CD	1:D:18:ARG:NH1	2.83	0.41
1:D:24:SER:HB2	1:D:25:PRO:HD2	2.03	0.41
1:D:365:GLU:CG	1:D:368:VAL:HG23	2.51	0.41
1:A:15:GLY:N	1:A:416:ILE:HD11	2.36	0.41
1:B:31:ARG:HH11	1:B:31:ARG:HG2	1.86	0.41
1:B:182:TRP:HA	1:B:183:PRO:HD3	1.86	0.41
1:B:374:ARG:HG2	1:B:394:ALA:HB3	2.02	0.41
1:B:381:LEU:O	1:B:384:LYS:N	2.54	0.41
1:C:71:GLU:CG	1:C:73:HIS:HB2	2.51	0.41
1:D:118:LYS:O	1:D:119:LEU:C	2.63	0.41
1:D:145:ARG:O	1:D:145:ARG:HG2	2.19	0.41
1:B:225:GLY:C	1:B:227:ASP:N	2.78	0.40
1:C:86:LEU:HD22	1:C:90:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:LYS:HB3	1:D:412:VAL:HG23	2.03	0.40
1:D:57:ASP:O	1:D:58:PHE:C	2.64	0.40
1:D:165:ARG:O	1:D:225:GLY:HA3	2.21	0.40
1:D:373:ASP:OD1	1:D:393:SER:HA	2.21	0.40
1:A:33:THR:HG22	1:A:36:ASN:ND2	2.35	0.40
1:A:119:LEU:O	1:A:123:LEU:HG	2.22	0.40
1:A:239:GLY:HA2	1:A:268:ALA:O	2.21	0.40
1:B:8:LEU:HD22	1:B:411:ILE:HG22	2.02	0.40
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.78	0.40
1:C:73:HIS:CD2	1:C:124:ILE:HD12	2.57	0.40
1:C:360:ASN:OD1	1:C:403:GLY:HA3	2.21	0.40
1:B:186:ARG:C	1:B:188:GLU:N	2.78	0.40
1:B:294:PHE:HA	1:B:295:PRO:HD3	1.81	0.40
1:C:41:LEU:HD11	1:C:182:TRP:CG	2.57	0.40
1:C:158:LEU:CB	1:C:161:THR:CG2	2.99	0.40
1:C:360:ASN:OD1	1:C:403:GLY:CA	2.69	0.40
1:D:43:ASP:HB2	1:D:401:ARG:NH2	2.36	0.40
1:D:299:LYS:O	1:D:299:LYS:HG3	2.21	0.40
1:D:397:LEU:HD12	1:D:397:LEU:HA	1.86	0.40
1:A:142:LYS:HG2	1:A:145:ARG:NH2	2.37	0.40
1:A:256:LEU:HD22	1:A:261:ALA:HB1	2.02	0.40
1:B:31:ARG:HD3	1:B:153:PHE:CE1	2.57	0.40
1:C:245:SER:C	1:C:249:ILE:HG13	2.47	0.40
1:C:397:LEU:N	1:C:397:LEU:CD1	2.84	0.40
1:D:111:LEU:HD23	1:D:111:LEU:HA	1.96	0.40
1:D:193:THR:CG2	1:D:214:PRO:HG2	2.44	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	395/418 (94%)	313 (79%)	65 (16%)	17 (4%)	2	8
1	B	399/418 (96%)	332 (83%)	50 (12%)	17 (4%)	2	8
1	C	396/418 (95%)	323 (82%)	61 (15%)	12 (3%)	3	14
1	D	395/418 (94%)	327 (83%)	54 (14%)	14 (4%)	3	12
All	All	1585/1672 (95%)	1295 (82%)	230 (14%)	60 (4%)	2	10

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	117	ARG
1	A	203	ALA
1	A	221	SER
1	A	249	ILE
1	B	80	ILE
1	B	162	GLN
1	B	258	ALA
1	C	112	GLU
1	C	134	ALA
1	D	64	GLU
1	D	294	PHE
1	D	330	ALA
1	D	400	GLY
1	A	116	PRO
1	A	121	GLU
1	A	207	PHE
1	B	145	ARG
1	B	337	LYS
1	C	15	GLY
1	C	288	ARG
1	C	332	SER
1	D	196	TYR
1	D	273	SER
1	D	293	VAL
1	D	331	GLU
1	A	12	SER
1	A	162	GLN
1	B	130	ASP
1	B	218	HIS
1	C	136	GLU
1	D	180	MET
1	D	226	GLY

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Mol	Chain	Res	Type
1	D	324	THR
1	A	130	ASP
1	A	280	ALA
1	B	15	GLY
1	B	187	GLN
1	B	313	PRO
1	C	61	LYS
1	C	366	PRO
1	A	189	THR
1	A	258	ALA
1	A	313	PRO
1	C	28	ALA
1	C	295	PRO
1	D	134	ALA
1	D	308	PRO
1	A	185	ARG
1	B	27	LEU
1	B	288	ARG
1	B	385	ALA
1	D	395	SER
1	C	313	PRO
1	A	328	VAL
1	B	183	PRO
1	B	34	PRO
1	B	298	VAL
1	B	214	PRO
1	C	213	ASP

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	342/353 (97%)	269 (79%)	73 (21%)	1	4
1	B	342/353 (97%)	276 (81%)	66 (19%)	1	5
1	C	342/353 (97%)	263 (77%)	79 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	342/353 (97%)	273 (80%)	69 (20%)	1	4
All	All	1368/1412 (97%)	1081 (79%)	287 (21%)	1	4

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	SER
1	A	16	LYS
1	A	20	VAL
1	A	35	SER
1	A	39	GLU
1	A	40	LEU
1	A	52	LYS
1	A	65	ARG
1	A	72	MET
1	A	76	LEU
1	A	78	GLU
1	A	80	ILE
1	A	86	LEU
1	A	94	ILE
1	A	101	LEU
1	A	107	LEU
1	A	109	SER
1	A	115	GLU
1	A	117	ARG
1	A	118	LYS
1	A	130	ASP
1	A	132	LEU
1	A	136	GLU
1	A	140	ILE
1	A	143	MET
1	A	145	ARG
1	A	151	SER
1	A	155	LEU
1	A	162	GLN
1	A	165	ARG
1	A	167	THR
1	A	171	ILE
1	A	177	LEU
1	A	180	MET
1	A	189	THR

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Mol	Chain	Res	Type
1	A	190	LEU
1	A	201	GLU
1	A	208	GLU
1	A	209	ILE
1	A	216	LYS
1	A	223	LEU
1	A	240	MET
1	A	243	ARG
1	A	246	ARG
1	A	259	LYS
1	A	263	GLU
1	A	273	SER
1	A	277	MET
1	A	281	THR
1	A	288	ARG
1	A	290	LEU
1	A	293	VAL
1	A	299	LYS
1	A	301	ILE
1	A	307	ARG
1	A	311	SER
1	A	318	ILE
1	A	319	ARG
1	A	323	LYS
1	A	331	GLU
1	A	333	LEU
1	A	336	LYS
1	A	337	LYS
1	A	352	ARG
1	A	354	GLN
1	A	361	VAL
1	A	365	GLU
1	A	374	ARG
1	A	382	LEU
1	A	384	LYS
1	A	397	LEU
1	A	399	ARG
1	B	6	THR
1	B	20	VAL
1	B	37	CYS
1	B	39	GLU
1	B	40	LEU

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Mol	Chain	Res	Type
1	B	41	LEU
1	B	60	THR
1	B	64	GLU
1	B	65	ARG
1	B	76	LEU
1	B	86	LEU
1	B	92	ARG
1	B	94	ILE
1	B	98	SER
1	B	101	LEU
1	B	105	SER
1	B	107	LEU
1	B	117	ARG
1	B	118	LYS
1	B	119	LEU
1	B	131	ASP
1	B	135	SER
1	B	136	GLU
1	B	142	LYS
1	B	143	MET
1	B	146	GLU
1	B	151	SER
1	B	152	SER
1	B	154	LEU
1	B	165	ARG
1	B	166	ASP
1	B	169	CYS
1	B	171	ILE
1	B	197	LYS
1	B	206	GLU
1	B	216	LYS
1	B	243	ARG
1	B	247	GLN
1	B	254	GLN
1	B	259	LYS
1	B	277	MET
1	B	279	LEU
1	B	284	SER
1	B	288	ARG
1	B	290	LEU
1	B	296	GLU
1	B	299	LYS

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Mol	Chain	Res	Type
1	B	301	ILE
1	B	305	SER
1	B	318	ILE
1	B	319	ARG
1	B	331	GLU
1	B	336	LYS
1	B	337	LYS
1	B	342	GLU
1	B	352	ARG
1	B	353	GLU
1	B	369	VAL
1	B	374	ARG
1	B	382	LEU
1	B	384	LYS
1	B	392	ILE
1	B	397	LEU
1	B	399	ARG
1	B	413	ARG
1	B	416	ILE
1	C	7	LYS
1	C	16	LYS
1	C	20	VAL
1	C	33	THR
1	C	35	SER
1	C	37	CYS
1	C	40	LEU
1	C	41	LEU
1	C	59	VAL
1	C	60	THR
1	C	61	LYS
1	C	65	ARG
1	C	73	HIS
1	C	76	LEU
1	C	86	LEU
1	C	101	LEU
1	C	103	LEU
1	C	107	LEU
1	C	117	ARG
1	C	118	LYS
1	C	119	LEU
1	C	123	LEU
1	C	130	ASP

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Mol	Chain	Res	Type
1	C	141	LEU
1	C	143	MET
1	C	145	ARG
1	C	146	GLU
1	C	148	LEU
1	C	151	SER
1	C	154	LEU
1	C	155	LEU
1	C	162	GLN
1	C	167	THR
1	C	185	ARG
1	C	201	GLU
1	C	208	GLU
1	C	220	SER
1	C	238	ILE
1	C	240	MET
1	C	243	ARG
1	C	246	ARG
1	C	249	ILE
1	C	259	LYS
1	C	264	ARG
1	C	271	PRO
1	C	272	LYS
1	C	277	MET
1	C	281	THR
1	C	286	CYS
1	C	288	ARG
1	C	290	LEU
1	C	294	PHE
1	C	295	PRO
1	C	296	GLU
1	C	299	LYS
1	C	309	ASP
1	C	311	SER
1	C	312	SER
1	C	314	TYR
1	C	317	ASN
1	C	319	ARG
1	C	321	GLU
1	C	322	GLU
1	C	323	LYS
1	C	324	THR

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Mol	Chain	Res	Type
1	C	331	GLU
1	C	335	LEU
1	C	343	THR
1	C	351	GLU
1	C	361	VAL
1	C	363	CYS
1	C	364	LEU
1	C	369	VAL
1	C	374	ARG
1	C	381	LEU
1	C	384	LYS
1	C	388	GLU
1	C	397	LEU
1	C	416	ILE
1	D	7	LYS
1	D	33	THR
1	D	35	SER
1	D	40	LEU
1	D	53	ARG
1	D	63	ARG
1	D	72	MET
1	D	76	LEU
1	D	80	ILE
1	D	86	LEU
1	D	95	THR
1	D	107	LEU
1	D	109	SER
1	D	113	SER
1	D	114	LEU
1	D	115	GLU
1	D	121	GLU
1	D	131	ASP
1	D	132	LEU
1	D	141	LEU
1	D	145	ARG
1	D	146	GLU
1	D	150	HIS
1	D	151	SER
1	D	152	SER
1	D	155	LEU
1	D	175	VAL
1	D	177	LEU

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Mol	Chain	Res	Type
1	D	186	ARG
1	D	187	GLN
1	D	200	PRO
1	D	208	GLU
1	D	220	SER
1	D	237	LEU
1	D	240	MET
1	D	243	ARG
1	D	246	ARG
1	D	249	ILE
1	D	264	ARG
1	D	270	LEU
1	D	272	LYS
1	D	273	SER
1	D	274	ARG
1	D	277	MET
1	D	282	VAL
1	D	284	SER
1	D	287	ASP
1	D	288	ARG
1	D	290	LEU
1	D	296	GLU
1	D	299	LYS
1	D	306	LEU
1	D	308	PRO
1	D	311	SER
1	D	318	ILE
1	D	331	GLU
1	D	332	SER
1	D	333	LEU
1	D	336	LYS
1	D	337	LYS
1	D	352	ARG
1	D	369	VAL
1	D	384	LYS
1	D	387	VAL
1	D	397	LEU
1	D	401	ARG
1	D	411	ILE
1	D	413	ARG
1	D	416	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	379	ASN
1	B	74	ASN
1	B	162	GLN
1	B	359	ASN
1	C	50	GLN
1	C	73	HIS
1	C	74	ASN
1	C	160	ASN
1	C	162	GLN
1	C	178	ASN
1	C	187	GLN
1	C	199	HIS
1	C	218	HIS
1	D	30	GLN
1	D	218	HIS
1	D	375	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CYR	D	406	1	14,16,17	2.23	3 (21%)	11,19,21	1.71	4 (36%)
1	CYR	B	406	1	14,16,17	2.21	4 (28%)	11,19,21	1.67	1 (9%)
1	CYR	A	406	1	14,16,17	2.23	2 (14%)	11,19,21	1.59	2 (18%)
1	CYR	C	406	1	14,16,17	2.22	3 (21%)	11,19,21	1.92	3 (27%)

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
1	CYR	D	406	1	-	3/15/18/20	-
1	CYR	B	406	1	-	6/15/18/20	-
1	CYR	A	406	1	-	4/15/18/20	-
1	CYR	C	406	1	-	4/15/18/20	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	CYR	C7-N6	5.84	1.46	1.35
1	D	406	CYR	C7-N6	5.41	1.45	1.35
1	C	406	CYR	C7-N6	5.20	1.45	1.35
1	C	406	CYR	C7-N7	5.16	1.46	1.28
1	B	406	CYR	C7-N6	5.15	1.45	1.35
1	D	406	CYR	C7-N7	5.09	1.46	1.28
1	A	406	CYR	C7-N7	4.93	1.45	1.28
1	B	406	CYR	C7-N7	4.88	1.45	1.28
1	B	406	CYR	C7-SG	2.53	1.78	1.76
1	D	406	CYR	CB-SG	-2.48	1.75	1.81
1	B	406	CYR	CB-SG	-2.42	1.75	1.81
1	C	406	CYR	C7-SG	2.16	1.78	1.76

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	CYR	CB-SG-C7	4.16	107.38	102.56
1	B	406	CYR	N6-C7-N7	-3.79	109.51	120.61
1	C	406	CYR	N6-C7-N7	-3.36	110.76	120.61
1	A	406	CYR	CB-SG-C7	3.04	106.09	102.56
1	D	406	CYR	N6-C7-N7	-2.95	111.96	120.61
1	A	406	CYR	N6-C7-N7	-2.91	112.09	120.61
1	D	406	CYR	C5-N6-C7	-2.60	118.90	123.55
1	D	406	CYR	CB-SG-C7	2.54	105.50	102.56
1	C	406	CYR	C5-N6-C7	-2.49	119.09	123.55
1	D	406	CYR	SG-C7-N6	-2.19	110.86	117.20

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	406	CYR	SG-C7-N6-C5
1	A	406	CYR	N6-C7-SG-CB
1	A	406	CYR	N7-C7-SG-CB
1	B	406	CYR	C1-C2-C3-C4
1	B	406	CYR	N2-C2-C3-C4
1	B	406	CYR	SG-C7-N6-C5
1	B	406	CYR	N7-C7-SG-CB
1	C	406	CYR	SG-C7-N6-C5
1	C	406	CYR	N7-C7-SG-CB
1	D	406	CYR	SG-C7-N6-C5
1	D	406	CYR	N6-C7-SG-CB
1	D	406	CYR	N7-C7-SG-CB
1	A	406	CYR	C2-C3-C4-C5
1	B	406	CYR	N6-C7-SG-CB
1	C	406	CYR	N6-C7-SG-CB
1	B	406	CYR	O1-C1-C2-N2
1	C	406	CYR	C4-C5-N6-C7

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	406	CYR	5	0
1	B	406	CYR	3	0
1	C	406	CYR	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	401/418 (95%)	-0.54	0 100 100	12, 40, 72, 99	0
1	B	405/418 (96%)	-0.58	2 (0%) 87 83	12, 37, 73, 99	0
1	C	402/418 (96%)	-0.46	2 (0%) 87 83	14, 45, 79, 98	0
1	D	401/418 (95%)	-0.46	2 (0%) 87 83	17, 43, 79, 98	0
All	All	1609/1672 (96%)	-0.51	6 (0%) 88 85	12, 41, 77, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	314	TYR	2.8
1	C	273	SER	2.8
1	D	314	TYR	2.6
1	B	275	ALA	2.5
1	D	416	ILE	2.4
1	B	184	ALA	2.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CYR	B	406	17/18	0.89	0.10	22,42,60,63	0
1	CYR	C	406	17/18	0.92	0.08	21,34,46,50	0
1	CYR	A	406	17/18	0.93	0.08	14,45,58,60	0
1	CYR	D	406	17/18	0.93	0.08	15,40,60,62	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.