



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:24 AM GMT

PDB ID : 2ABR
Title : Structure of D280A arginine deiminase with L-arginine forming a S-alkylthiouronium 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

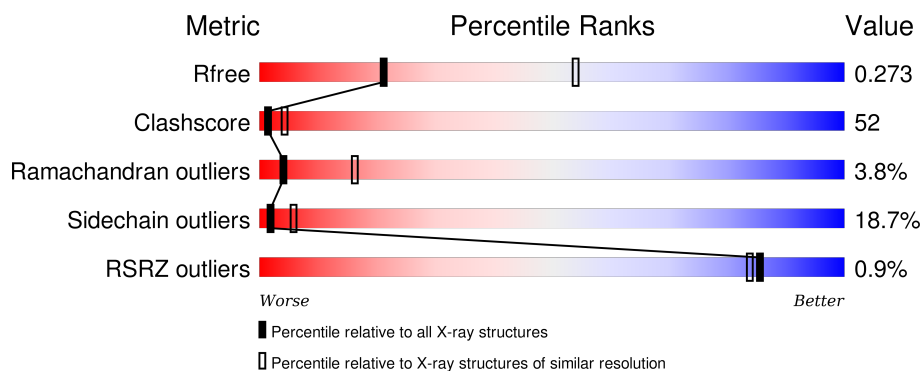
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>%</div> <div> <div></div> <div>30%</div> <div>51%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	418	<div> <div></div> <div> <div>32%</div> <div>50%</div> <div>15%</div> <div>•</div> </div> </div>
1	C	418	<div> <div>%</div> <div> <div></div> <div>31%</div> <div>50%</div> <div>14%</div> <div>• •</div> </div> </div>
1	D	418	<div> <div>%</div> <div> <div></div> <div>33%</div> <div>49%</div> <div>14%</div> <div>•</div> </div> </div>

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			

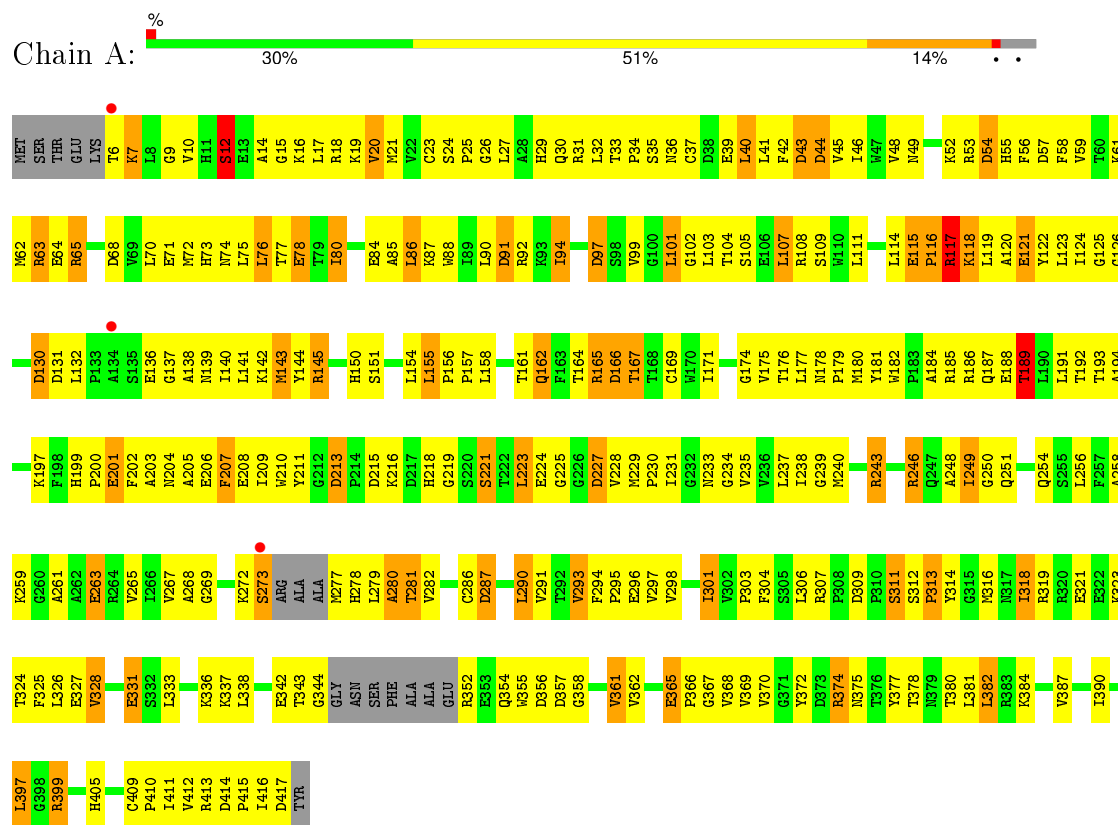
There are 8 discrepancies between the modelled and reference sequences:

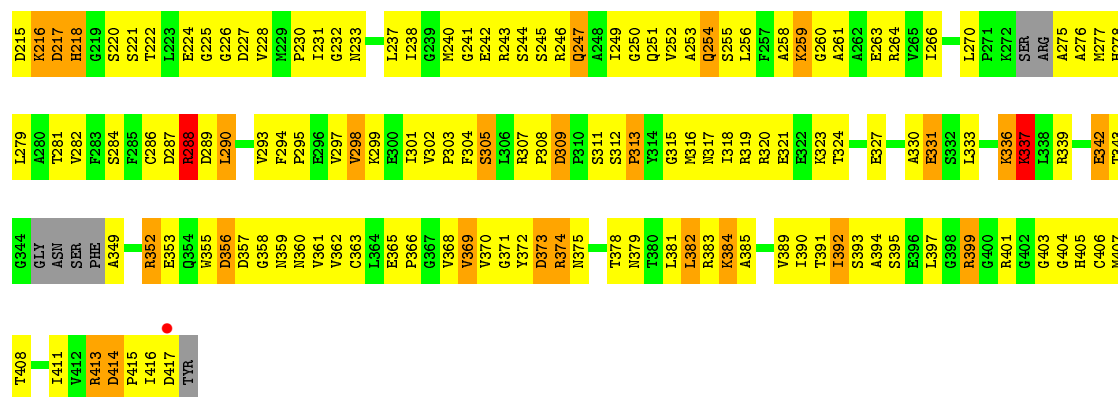
Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ALA	ASP	ENGINEERED	UNP P13981
A	406	CYR	CYS	MODIFIED RESIDUE	UNP P13981
B	280	ALA	ASP	ENGINEERED	UNP P13981
B	406	CYR	CYS	MODIFIED RESIDUE	UNP P13981
C	280	ALA	ASP	ENGINEERED	UNP P13981
C	406	CYR	CYS	MODIFIED RESIDUE	UNP P13981
D	280	ALA	ASP	ENGINEERED	UNP P13981
D	406	CYR	CYS	MODIFIED RESIDUE	UNP P13981

3 Residue-property plots

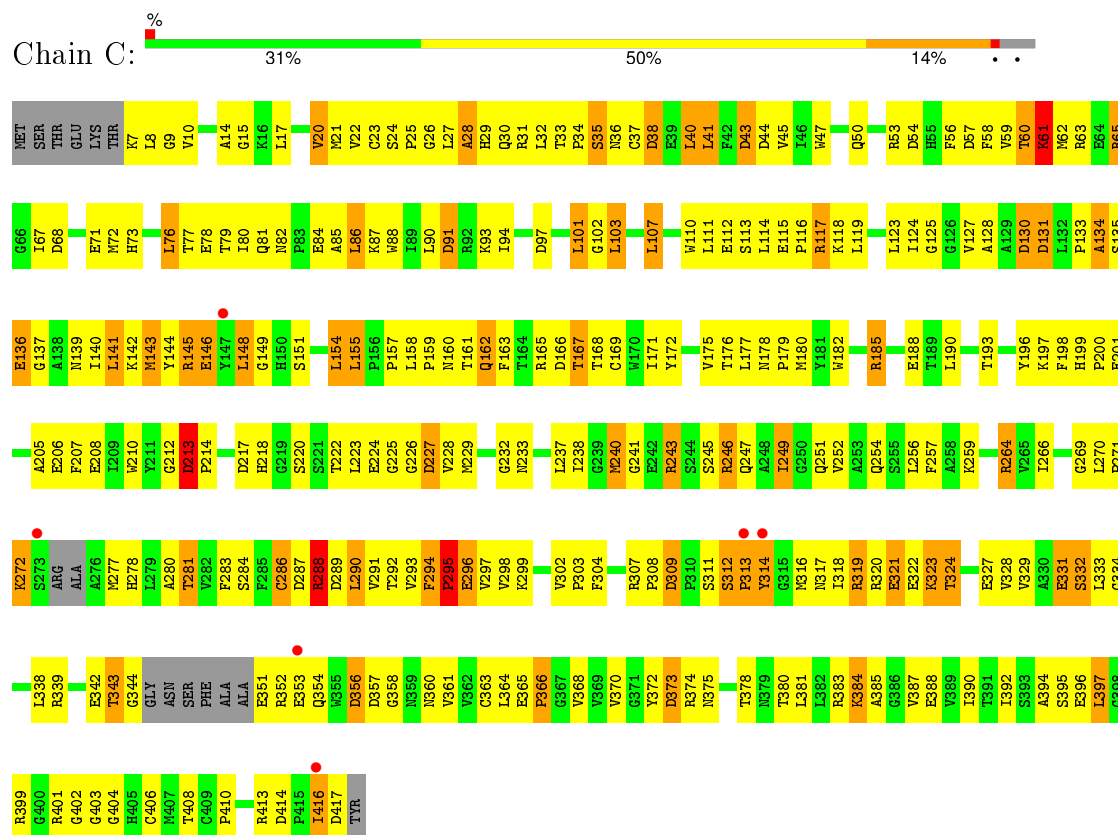
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

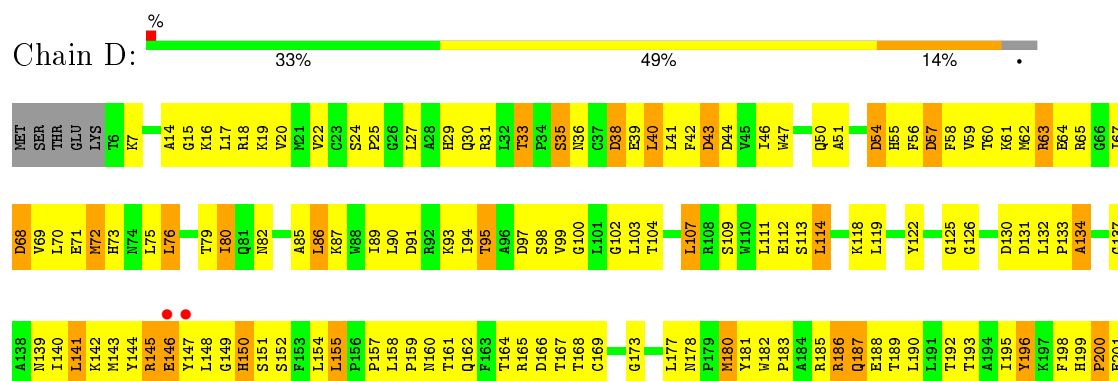




• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase



V412	R413	D414	P415	T416	ASP	TYR	ASN	SER	PHE	ALA	ALA	GLU	R352	E353	Q354	W355	D356	D357	G358	R359	N360	L364	E365	P366	G367	V368	V369	V370	D373	R374	Y377	T378	N379	T380	L381	L382	R383	K384	V387	I390	T391	I392	S393	A394	S395	E396	L397	G398	R399	G400	R401	G402	G403	G404	H405	C406	M407	T408	C409	P410	I411
F202	A203	E208	I209	W210	D213	P214	D215	K216	D217	H218	G219	S220	S221	T222	L223	F224	G225	G226	D227	P230	I231	G232	N233	V235	V236	L237	T238	G239	W240	G241	E242	R243	S244	S245	R246	Q247	A248	T249	G250	Q251	V252	L256	F257	R264	V265	I266	K272	S273	R274	ALA	ALA	N277									
H278	L279	V282	F283	S284	F285	C286	D287	R288	D289	L290	V291	T292	V293	F294	P295	E296	V297	V298	K299	F304	S305	L306	R307	P308	D309	G234	P310	S311	S312	P313	Y314	I318	R319	R320	E321	T324	E327	V328	V329	A330	E331	S332	L333	L335	K336	K337	L338	R339	V340	V341	E342	T343	G344	GLY							

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 19.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 96.0 (19.92-2.90)	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	1714 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 34924 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/3199	0.76	13/4336 (0.3%)
1	B	0.47	0/3222	0.75	11/4368 (0.3%)
1	C	0.46	0/3206	0.78	17/4345 (0.4%)
1	D	0.47	0/3202	0.77	14/4339 (0.3%)
All	All	0.47	0/12829	0.77	55/17388 (0.3%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	373	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	227	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	44	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	217	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	357	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	217	ASP	CB-CG-OD2	5.82	123.53	118.30
1	D	54	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	131	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	373	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	43	ASP	CB-CG-OD2	5.65	123.38	118.30
1	C	131	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	417	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	200	PRO	CA-N-CD	-5.62	103.64	111.50
1	D	130	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	215	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	414	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	44	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	287	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	356	ASP	CB-CG-OD2	5.54	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	68	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	213	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	130	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	356	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	38	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	166	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	68	ASP	CB-CG-OD2	5.43	123.18	118.30
1	C	356	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	97	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	97	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	38	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	213	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	309	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	44	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	166	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	91	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	44	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	357	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	43	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	38	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	68	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	417	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	97	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	414	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	131	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	57	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	43	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	309	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	227	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	357	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	43	ASP	CB-CG-OD2	5.04	122.83	118.30
1	D	357	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	91	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	414	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	54	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3151	0	3139	345	0
1	B	3174	0	3160	298	0
1	C	3158	0	3143	347	0
1	D	3154	0	3148	388	0
All	All	12637	0	12590	1319	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 52.

All (1319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D: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
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:CG	1:D:186:ARG:HH11	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:229:MET:HE3	1:A:279:LEU:HD23	1.28	1.10
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:D:186:ARG:HH11	1:D:186:ARG:HG2	1.08	1.10
1:A:180:MET:HE3	1:A:224:GLU:HG3	1.25	1.08
1:A:180:MET:CE	1:A:224:GLU:HG3	1.83	1.08
1:D:352:ARG:HH11	1:D:352:ARG:HB3	0.93	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:401:ARG:HH11	1:D:401:ARG:HG2	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:A:180:MET:HE1	1:A:224:GLU:CG	1.89	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:CB	1:D:352:ARG:NH1	2.22	1.00
1:D:274:ARG:HA	1:D:274:ARG:HE	1.27	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:B:167:THR:O	1:B:168:THR:CG2	2.09	0.99
1:A:180:MET:CE	1:A:224:GLU:CG	2.40	0.99
1:D:43:ASP:HB2	1:D:401:ARG:HH12	0.84	0.99
1:D:183:PRO:HA	1:D:186:ARG:HD2	1.42	0.98
1:B:399:ARG:HH11	1:B:399:ARG:HG2	1.28	0.97
1:D:111:LEU:O	1:D:114:LEU:HB2	1.64	0.97
1:A:272:LYS:CE	1:D:149:GLY:HA3	1.94	0.97
1:A:293:VAL:HB	1:A:298:VAL:HG21	1.43	0.97
1:D:352:ARG:CB	1:D:352:ARG:HH11	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:C:140:ILE:HA	1:C:143:MET:HE2	1.44	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: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:115:GLU:CD	1:A:115:GLU:H	1.68	0.95
1:A:101:LEU:HD13	1:A:102:GLY:H	1.32	0.95
1:C:137:GLY:HA2	1:C:140:ILE:HD12	1.47	0.94
1:C:167:THR:C	1:C:178:ASN:HD22	1.70	0.94
1:C:101:LEU:HD12	1:C:102:GLY:N	1.83	0.94
1:A:228:VAL:HG22	1:A:238:ILE:HG12	1.45	0.94
1:A:86:LEU:CD1	1:A:90:LEU:HG	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:HD12	1:D:119:LEU:HA	1.50	0.93
1:C:360:ASN:ND2	1:C:406:CYR:SG	2.40	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:C:102:GLY:C	1:C:103:LEU:HD12	1.89	0.93
1:B:101:LEU:HD11	1:C:316:MET:CE	1.99	0.93
1:B:293:VAL:CG1	1:B:298:VAL:HG21	1.99	0.92
1:A:32:LEU:HD23	1:A:40:LEU:HD23	1.49	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
1:D:413:ARG:HG3	1:D:413:ARG:NH1	1.74	0.90
1:C:240:MET:HE1	1:C:246:ARG:HB3	1.53	0.89
1:C:117:ARG:O	1:C:117:ARG:HD2	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:HD23	1:C:154:LEU:N	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:274:ARG:HA	1:D:274:ARG:NE	1.84	0.88
1:D:186:ARG:NH1	1:D:186:ARG:HG2	1.82	0.88
1:C:14:ALA:O	1:C:366:PRO:HD3	1.72	0.88
1:B:217:ASP:O	1:B:218:HIS:HB2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:292:THR:C	1:D:293:VAL:HG23	1.97	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:B:124:ILE:HG23	1:B:161:THR:HG21	1.59	0.84
1:D:413:ARG:CG	1:D:413:ARG:HH11	1.90	0.84
1:C:294:PHE:HE1	1:C:296:GLU:HG2	1.42	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
1:B:17:LEU:CD1	1:B:413:ARG:NH1	2.41	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:D:237:LEU:HD23	1:D:237:LEU:N	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: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:313:PRO:HB2	1:C:314:TYR:CE1	2.15	0.81
1:C:229:MET:HB2	1:C:237:LEU:HB2	1.62	0.81
1:B:295:PRO:HG3	1:B:342:GLU:HB3	1.59	0.81
1:D:292:THR:C	1:D:293:VAL:CG2	2.49	0.81
1:A:240:MET:HB2	1:A:249:ILE:HD12	1.62	0.81
1:C:137:GLY:O	1:C:141:LEU:HD23	1.80	0.81
1:B:336:LYS:O	1:B:337:LYS:HB3	1.79	0.81
1:C:312:SER:CB	1:C:316:MET:O	2.29	0.80
1:A:180:MET:HE1	1:A:224:GLU:HG2	1.62	0.80
1:C:101:LEU:C	1:C:101:LEU:CD1	2.50	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:D:186:ARG:CG	1:D:186:ARG:NH1	2.33	0.79
1:A:103:LEU:HD13	1:A:154:LEU:HD11	1.65	0.79
1:A:269:GLY:HA3	1:D:148:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:107:LEU:HD22	1:D:107:LEU:O	1.82	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:B:245:SER:O	1:B:249:ILE:HG13	1.83	0.78
1:D:80:ILE:HG22	1:D:86:LEU:HG	1.64	0.78
1:A:80:ILE:HD11	1:A:120:ALA:HB2	1.64	0.78
1:B:142:LYS:CD	1:B:145:ARG:NH2	2.47	0.78
1:A:213:ASP:OD1	1:A:215:ASP:HB2	1.84	0.78
1:D:43:ASP:CA	1:D:401:ARG:HH22	1.97	0.78
1:A:272:LYS:HG2	1:D:149:GLY:O	1.83	0.78
1:B:101:LEU:HD11	1:C:316:MET:HE3	1.65	0.78
1:A:381:LEU:HA	1:A:384:LYS:HG3	1.65	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:D:273:SER:OG	1:D:274:ARG:N	2.15	0.78
1:A:65:ARG:HB3	1:A:65:ARG:NH1	1.97	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:D:293:VAL:HG12	1:D:298:VAL:HG21	1.66	0.77
1:B:169:CYS:O	1:B:175:VAL:HG23	1.83	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:C:199:HIS:CG	1:C:200:PRO:CD	2.67	0.77
1:B:365:GLU:HG2	1:B:368:VAL:HB	1.66	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:D:286:CYS:HB2	1:D:290:LEU:HD13	1.66	0.76
1:C:288:ARG:NH1	1:C:416:ILE:HG22	1.98	0.76
1:B:242:GLU:HB2	1:B:275:ALA:C	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:THR:HG21	1:D:214:PRO:HG2	1.65	0.76
1:D:286:CYS:HB2	1:D:290:LEU:CD1	2.16	0.76
1:A:356:ASP:OD1	1:A:356:ASP:O	2.03	0.76
1:A:231:ILE:HD12	1:A:333:LEU:HD13	1.68	0.76
1:C:286:CYS:SG	1:C:292:THR:HG23	2.26	0.76
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:356:ASP:HB2	1:C:375:ASN:OD1	1.86	0.75
1:C:353:GLU:HA	1:C:353:GLU:OE2	1.87	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:D:72:MET:CE	1:D:192:THR:OG1	2.36	0.74
1:A:24:SER:HA	1:A:55:HIS:CE1	2.21	0.74
1:D:94:ILE:CD1	1:D:107:LEU:HD13	2.18	0.74
1:C:8:LEU:HD12	1:C:205:ALA:HB1	1.68	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:C:117:ARG:C	1:C:117:ARG:HD2	2.06	0.73
1:B:167:THR:C	1:B:168:THR:HG23	2.09	0.73
1:D:16:LYS:HD2	1:D:18:ARG:HH12	1.53	0.73
1:A:71:GLU:HG3	1:A:73:HIS:H	1.53	0.73
1:A:229:MET:HE1	1:A:279:LEU:CD2	2.19	0.73
1:D:178:ASN:HB3	1:D:223:LEU:O	1.88	0.73
1:A:202:PHE:O	1:A:204:ASN:N	2.22	0.73
1:A:343:THR:HG21	1:A:378:THR:OG1	1.88	0.72
1:D:157:PRO:O	1:D:159:PRO:HD2	1.89	0.72
1:B:97:ASP:HB3	1:C:218:HIS:O	1.89	0.72
1:C:321:GLU:OE1	1:C:321:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:CD1	1:B:413:ARG:HH12	2.02	0.72
1:A:101:LEU:CD1	1:A:101:LEU:N	2.52	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:365:GLU:HB2	1:A:366:PRO:CD	2.19	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:D:273:SER:O	1:D:274:ARG:CB	2.37	0.71
1:D:27:LEU:HD21	1:D:31:ARG:HH21	1.55	0.71
1:B:41:LEU:HD23	1:B:184:ALA:CB	2.19	0.71
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:D:257:PHE:CD2	1:D:308:PRO:HD3	2.25	0.71
1:D:55:HIS:O	1:D:58:PHE:HB3	1.90	0.71
1:B:302:VAL:HB	1:C:148:LEU:HD21	1.73	0.71
1:B:64:GLU:OE2	1:B:64:GLU:CA	2.29	0.71
1:C:167:THR:C	1:C:178:ASN:ND2	2.44	0.71
1:A:27:LEU:O	1:A:27:LEU:HD12	1.89	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:139:ASN:O	1:D:143:MET:N	2.24	0.70
1:C:178:ASN:HB2	1:C:180:MET:HE3	1.72	0.70
1:D:54:ASP:HB3	1:D:397:LEU:HD22	1.73	0.70
1:B:318:ILE:O	1:B:318:ILE:HG23	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: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:OE1	1:B:247:GLN:N	2.25	0.70
1:C:199:HIS:HD2	1:C:201:GLU:H	1.38	0.70
1:B:282:VAL:HB	1:B:294:PHE:HB3	1.73	0.70
1:A:248:ALA:O	1:A:250:GLY:N	2.24	0.69
1:A:223:LEU:HD22	1:A:224:GLU:N	2.06	0.69
1:C:290:LEU:HD22	1:C:291:VAL:N	2.08	0.69
1:A:97:ASP:HB3	1:D:218:HIS:O	1.90	0.69
1:C:31:ARG:HD2	1:C:157:PRO:HG3	1.73	0.69
1:A:94:ILE:HD13	1:A:107:LEU:HD13	1.74	0.69
1:C:320:ARG:HH11	1:C:320:ARG:HG2	1.57	0.69
1:C:199:HIS:NE2	1:C:200:PRO:HD2	2.08	0.69
1:C:178:ASN:OD1	1:C:223:LEU:HD12	1.91	0.69
1:D:277:MET:O	1:D:277:MET:CG	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:C	1:C:101:LEU:HD12	2.09	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:D:139:ASN:O	1:D:143:MET:HB2	1.92	0.69
1:B:94:ILE:HG21	1:B:107:LEU:HD12	1.75	0.69
1:A:314:TYR:HE1	1:A:316:MET:O	1.76	0.69
1:C:295:PRO:CG	1:C:342:GLU:HB2	2.22	0.69
1:D:318:ILE:O	1:D:319:ARG:HD3	1.91	0.69
1:D:24:SER:HB3	1:D:55:HIS:ND1	2.08	0.69
1:B:72:MET:CE	1:B:164:THR:HG22	2.23	0.69
1:A:25:PRO:HA	1:A:29:HIS:HE1	1.56	0.68
1:C:343:THR:OG1	1:C:344:GLY:N	2.23	0.68
1:D:186:ARG:HG3	1:D:186:ARG:HH11	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: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:A:101:LEU:N	1:A:101:LEU:HD12	2.07	0.68
1:B:79:THR:O	1:B:81:GLN:N	2.26	0.68
1:D:365:GLU:CD	1:D:368:VAL:HG21	2.14	0.68
1:B:80:ILE:O	1:B:80:ILE:HG22	1.94	0.68
1:D:43:ASP:HB2	1:D:401:ARG:CZ	2.24	0.67
1:C:85:ALA:O	1:C:88:TRP:HB3	1.94	0.67
1:B:73:HIS:CD2	1:B:124:ILE:HD12	2.29	0.67
1:C:240:MET:HB2	1:C:249:ILE:HD12	1.75	0.67
1:B:33:THR:HG23	1:B:36:ASN:ND2	2.09	0.67
1:C:21:MET:O	1:C:22:VAL:CG1	2.43	0.67
1:B:370:VAL:HG22	1:B:390:ILE:HB	1.75	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:B:182:TRP:C	1:B:184:ALA:H	1.98	0.67
1:B:182:TRP:O	1:B:184:ALA:N	2.27	0.67
1:A:178:ASN:HB3	1:A:223:LEU:O	1.94	0.67
1:B:399:ARG:NH1	1:B:399:ARG:HG2	2.06	0.67
1:C:141:LEU:N	1:C:141:LEU:HD22	2.10	0.67
1:C:154:LEU:N	1:C:154:LEU:CD2	2.57	0.67
1:D:394:ALA:O	1:D:396:GLU:N	2.27	0.67
1:A:74:ASN:O	1:A:77:THR:HB	1.95	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:C:163:PHE:CE2	1:C:406:CYR:HC2	2.29	0.66
1:B:360:ASN:ND2	1:B:405:HIS:HB3	2.10	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:D:401:ARG:NH1	1:D:401:ARG:CG	2.46	0.66
1:B:246:ARG:HG2	1:B:247:GLN:OE1	1.95	0.66
1:D:227:ASP:O	1:D:238:ILE:HA	1.95	0.66
1:B:323:LYS:HB3	1:B:327:GLU:OE1	1.95	0.66
1:A:54:ASP:HB2	1:A:397:LEU:HD22	1.77	0.66
1:C:331:GLU:O	1:C:334:GLY:N	2.26	0.66
1:A:54:ASP:HB2	1:A:397:LEU:CD2	2.26	0.66
1:C:141:LEU:CD2	1:C:141:LEU:N	2.59	0.66
1:C:290:LEU:HD23	1:C:291:VAL:N	2.08	0.66
1:A:107:LEU:O	1:A:107:LEU:HD22	1.96	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:314:TYR:CD2	1:D:102:GLY:HA2	2.32	0.65
1:D:365:GLU:CD	1:D:368:VAL:CG2	2.65	0.65
1:D:18:ARG:CG	1:D:18:ARG:HH11	2.08	0.65
1:A:88:TRP:HZ3	1:A:194:ALA:HB2	1.60	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:HG2	1:C:162:GLN:O	1.96	0.65
1:A:303:PRO:HG3	1:A:328:VAL:HG21	1.78	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:D:94:ILE:CD1	1:D:107:LEU:CD1	2.75	0.65
1:D:240:MET:HB2	1:D:249:ILE:CD1	2.26	0.65
1:C:9:GLY:HA2	1:C:172:TYR:O	1.97	0.65
1:B:282:VAL:O	1:B:293:VAL:HA	1.97	0.65
1:A:229:MET:CE	1:A:279:LEU:HG	2.27	0.65
1:D:306:LEU:HD12	1:D:318:ILE:CB	2.27	0.65
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:293:VAL:HG23	1:A:294:PHE:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:C	1:B:107:LEU:HD13	2.17	0.64
1:D:331:GLU:O	1:D:331:GLU:HG2	1.97	0.64
1:A:31:ARG:HG2	1:A:31:ARG:NH1	2.12	0.64
1:A:59:VAL:HG12	1:A:63:ARG:NH1	2.11	0.64
1:A:33:THR:HG22	1:A:36:ASN:CG	2.18	0.64
1:B:142:LYS:HD3	1:B:145:ARG:HH22	1.62	0.64
1:C:168:THR:CA	1:C:178:ASN:ND2	2.61	0.64
1:B:231:ILE:HD12	1:B:333:LEU:HD21	1.79	0.64
1:C:399:ARG:NH2	1:D:396:GLU:OE1	2.29	0.64
1:C:182:TRP:HE1	1:C:243:ARG:HH11	1.46	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: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:365:GLU:OE1	1:D:368:VAL:HG21	1.98	0.64
1:B:290:LEU:HD23	1:B:339:ARG:O	1.98	0.64
1:D:80:ILE:CG2	1:D:86:LEU:HG	2.27	0.64
1:C:101:LEU:CD1	1:C:102:GLY:N	2.61	0.64
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:169:CYS:O	1:A:175:VAL:CG2	2.46	0.63
1:A:88:TRP:CZ3	1:A:194:ALA:HB2	2.33	0.63
1:C:314:TYR:CD1	1:C:314:TYR:N	2.65	0.63
1:C:27:LEU:O	1:C:30:GLN:N	2.29	0.63
1:B:238:ILE:HG22	1:B:249:ILE:HD13	1.80	0.63
1:A:72:MET:CE	1:A:192:THR:OG1	2.46	0.63
1:A:356:ASP:HB2	1:A:375:ASN:OD1	1.98	0.63
1:B:349:ALA:N	1:B:352:ARG:NH2	2.47	0.63
1:C:272:LYS:HD2	1:C:272:LYS:C	2.17	0.63
1:C:380:THR:O	1:C:384:LYS:HB2	1.99	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:A:248:ALA:O	1:A:249:ILE:C	2.36	0.63
1:C:399:ARG:HH21	1:D:396:GLU:CD	2.02	0.63
1:C:17:LEU:HD21	1:C:20:VAL:HG11	1.80	0.63
1:C:140:ILE:HA	1:C:143:MET:CE	2.25	0.63
1:C:90:LEU:HD22	1:C:94:ILE:HD11	1.81	0.63
1:B:80:ILE:O	1:B:80:ILE:CG2	2.47	0.63
1:D:72:MET:HE1	1:D:192:THR:OG1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:PHE:O	1:D:57:ASP:C	2.35	0.62
1:A:362:VAL:C	1:A:369:VAL:HG23	2.19	0.62
1:B:166:ASP:HA	1:B:225:GLY:HA3	1.80	0.62
1:C:399:ARG:NH2	1:D:396:GLU:CD	2.52	0.62
1:D:82:ASN:C	1:D:82:ASN:OD1	2.37	0.62
1:A:180:MET:HA	1:A:180:MET:HE3	1.81	0.62
1:A:102:GLY:HA2	1:D:314:TYR:CE2	2.33	0.62
1:A:101:LEU:H	1:A:101:LEU:HD12	1.64	0.62
1:B:211:TYR:CB	1:B:252:VAL:HG22	2.30	0.62
1:B:9:GLY:HA2	1:B:172:TYR:O	1.98	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:399:ARG:CG	1:B:399:ARG:HE	2.11	0.62
1:A:124:ILE:HG23	1:A:161:THR:HG21	1.82	0.62
1:A:304:PHE:CE1	1:D:144:TYR:CE1	2.87	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: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:D:187:GLN:OE1	1:D:187:GLN:HA	2.00	0.61
1:D:352:ARG:HB2	1:D:352:ARG:NH1	2.12	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: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: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:D:20:VAL:HG12	1:D:410:PRO:HA	1.81	0.61
1:A:180:MET:HA	1:A:180:MET:CE	2.30	0.61
1:C:293:VAL:HG13	1:C:298:VAL:HG21	1.83	0.61
1:A:229:MET:CE	1:A:279:LEU:CG	2.78	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:A:279:LEU:C	1:A:281:THR:H	2.02	0.61
1:C:178:ASN:HB3	1:C:223:LEU:O	2.01	0.61
1:A:231:ILE:HD11	1:A:235:VAL:HG11	1.83	0.61
1:D:352:ARG:CZ	1:D:352:ARG:CB	2.78	0.60
1:A:304:PHE:CZ	1:D:144:TYR:CE1	2.89	0.60
1:A:72:MET:HE2	1:A:192:THR:OG1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:HG2	1:B:146:GLU:N	2.14	0.60
1:C:245:SER:O	1:C:249:ILE:CG1	2.49	0.60
1:D:25:PRO:HA	1:D:29:HIS:CE1	2.36	0.60
1:D:19:LYS:HD3	1:D:70:LEU:HD11	1.84	0.60
1:D:304:PHE:CE1	1:D:320:ARG:HG3	2.36	0.60
1:A:356:ASP:OD1	1:A:356:ASP:C	2.39	0.60
1:B:98:SER:OG	1:B:99:VAL:HG23	2.02	0.60
1:D:141:LEU:HD23	1:D:154:LEU:HD21	1.83	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:27:LEU:HA	1:D:30:GLN:NE2	2.17	0.60
1:D:223:LEU:C	1:D:223:LEU:HD23	2.22	0.60
1:A:362:VAL:O	1:A:369:VAL:HG23	2.00	0.60
1:A:91:ASP:OD1	1:A:108:ARG:NH1	2.34	0.60
1:A:40:LEU:O	1:A:41:LEU:HB2	2.00	0.60
1:B:73:HIS:NE2	1:B:124:ILE:HD12	2.17	0.60
1:B:231:ILE:HG21	1:B:237:LEU:CD1	2.30	0.60
1:B:99:VAL:HG12	1:B:103:LEU:HB2	1.84	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: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:C:33:THR:O	1:C:36:ASN:N	2.35	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:D:63:ARG:C	1:D:65:ARG:H	2.06	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:C:319:ARG:HH11	1:C:319:ARG:HG2	0.67	0.59
1:D:103:LEU:CD1	1:D:141:LEU:CD2	2.81	0.59
1:A:41:LEU:HD11	1:A:182:TRP:CG	2.38	0.59
1:D:158:LEU:O	1:D:160:ASN:N	2.35	0.59
1:D:17:LEU:HD21	1:D:20:VAL:CG1	2.31	0.59
1:C:312:SER:O	1:C:314:TYR:N	2.36	0.59
1:C:303:PRO:HB2	1:C:321:GLU:HB2	1.85	0.59
1:B:304:PHE:CE1	1:B:320:ARG:HG3	2.37	0.59
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:137:GLY:O	1:A:140:ILE:HG12	2.03	0.59
1:B:17:LEU:HB2	1:B:413:ARG:HH12	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD22	1:A:224:GLU:H	1.68	0.59
1:A:75:LEU:HA	1:A:78:GLU:HG3	1.84	0.59
1:A:280:ALA:HB1	1:A:405:HIS:ND1	2.17	0.59
1:C:54:ASP:O	1:C:57:ASP:HB3	2.02	0.59
1:B:312:SER:OG	1:B:313:PRO:HD2	2.02	0.59
1:D:287:ASP:HB2	1:D:290:LEU:CB	2.33	0.59
1:D:199:HIS:ND1	1:D:201:GLU:HB2	2.17	0.59
1:A:36:ASN:C	1:A:36:ASN:OD1	2.39	0.59
1:A:240:MET:HE1	1:A:246:ARG:HB2	1.85	0.58
1:B:33:THR:HG23	1:B:36:ASN:HD21	1.66	0.58
1:C:128:ALA:HB3	1:C:131:ASP:OD2	2.03	0.58
1:D:243:ARG:NH2	1:D:406:CYR:O1	2.36	0.58
1:D:43:ASP:OD1	1:D:43:ASP:C	2.40	0.58
1:A:304:PHE:CE1	1:D:144:TYR:HE1	2.21	0.58
1:D:103:LEU:CD1	1:D:141:LEU:HD22	2.32	0.58
1:B:72:MET:HE3	1:B:164:THR:HG22	1.84	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: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:B:15:GLY:HA3	1:B:414:ASP:O	2.03	0.58
1:C:331:GLU:HG3	1:C:332:SER:N	2.18	0.58
1:A:25:PRO:CA	1:A:29:HIS:CE1	2.83	0.58
1:D:401:ARG:CB	1:D:406:CYR:H32	2.30	0.58
1:B:399:ARG:HH11	1:B:399:ARG:CG	2.07	0.58
1:B:238:ILE:CG2	1:B:249:ILE:HD13	2.34	0.58
1:A:70:LEU:HD13	1:A:75:LEU:HD11	1.85	0.58
1:C:77:THR:CG2	1:C:116:PRO:O	2.49	0.58
1:B:217:ASP:O	1:B:218:HIS:CB	2.45	0.58
1:C:158:LEU:N	1:C:159:PRO:CD	2.67	0.58
1:D:76:LEU:CD2	1:D:80:ILE:CD1	2.67	0.58
1:B:23:CYS:HB2	1:B:72:MET:HE3	1.85	0.58
1:B:29:HIS:NE2	1:B:159:PRO:O	2.37	0.58
1:A:246:ARG:HA	1:A:249:ILE:HB	1.86	0.58
1:D:284:SER:O	1:D:291:VAL:HG12	2.04	0.58
1:B:216:LYS:HD3	1:B:218:HIS:CD2	2.39	0.58
1:A:84:GLU:O	1:A:88:TRP:HB2	2.04	0.58
1:D:95:THR:HG23	1:D:98:SER:OG	2.04	0.58
1:B:210:TRP:CH2	1:B:261:ALA:HB2	2.39	0.58
1:D:22:VAL:CA	1:D:164:THR:HG21	2.33	0.57
1:D:43:ASP:CA	1:D:401:ARG:NH2	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:HIS:CG	1:C:200:PRO:HD2	2.29	0.57
1:D:294:PHE:CD2	1:D:297:VAL:CG2	2.87	0.57
1:C:372:TYR:CG	1:C:394:ALA:HB2	2.39	0.57
1:D:160:ASN:HB3	1:D:185:ARG:NE	2.18	0.57
1:D:336:LYS:C	1:D:336:LYS:HD2	2.22	0.57
1:C:199:HIS:CD2	1:C:201:GLU:H	2.21	0.57
1:C:154:LEU:HD23	1:C:154:LEU:H	1.70	0.57
1:A:86:LEU:C	1:A:86:LEU:HD12	2.24	0.57
1:C:331:GLU:CG	1:C:332:SER:N	2.67	0.57
1:B:171:ILE:HG23	1:B:230:PRO:HG3	1.86	0.57
1:A:248:ALA:O	1:A:251:GLN:N	2.38	0.57
1:C:27:LEU:HB3	1:C:125:GLY:HA3	1.86	0.57
1:A:358:GLY:HA3	1:A:378:THR:HG21	1.87	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:290:LEU:C	1:A:290:LEU:HD22	2.25	0.57
1:D:16:LYS:CD	1:D:18:ARG:HH12	2.17	0.57
1:C:111:LEU:C	1:C:113:SER:N	2.58	0.57
1:B:221:SER:OG	1:B:247:GLN:HB2	2.05	0.57
1:B:77:THR:HG23	1:B:117:ARG:HA	1.87	0.57
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.15	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:330:ALA:C	1:D:332:SER:H	2.07	0.56
1:D:167:THR:C	1:D:168:THR:HG23	2.25	0.56
1:D:293:VAL:O	1:D:295:PRO:CD	2.50	0.56
1:C:323:LYS:HB3	1:C:327:GLU:HB3	1.86	0.56
1:C:27:LEU:HD21	1:C:31:ARG:NH2	2.20	0.56
1:A:355:TRP:CH2	1:B:34:PRO:HG2	2.41	0.56
1:D:63:ARG:HG2	1:D:63:ARG:NH1	2.20	0.56
1:B:88:TRP:NE1	1:B:92:ARG:NH2	2.53	0.56
1:C:43:ASP:HB2	1:C:401:ARG:HH21	1.68	0.56
1:B:171:ILE:HA	1:B:230:PRO:HG3	1.87	0.56
1:A:237:LEU:O	1:A:238:ILE:HG13	2.05	0.56
1:A:25:PRO:HG3	1:A:162:GLN:OE1	2.04	0.56
1:C:240:MET:HB2	1:C:249:ILE:CD1	2.36	0.56
1:B:33:THR:O	1:B:37:CYS:HB3	2.05	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:D:137:GLY:O	1:D:140:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PHE:C	1:A:204:ASN:H	2.09	0.56
1:B:241:GLY:HA3	1:B:270:LEU:HD12	1.88	0.56
1:C:329:VAL:HG12	1:C:338:LEU:HD11	1.88	0.56
1:D:158:LEU:O	1:D:161:THR:HG23	2.07	0.56
1:A:331:GLU:O	1:A:331:GLU:HG2	2.06	0.56
1:B:298:VAL:O	1:B:301:ILE:HG13	2.06	0.55
1:A:267:VAL:HB	1:A:304:PHE:HB2	1.88	0.55
1:B:358:GLY:HA3	1:B:378:THR:HG21	1.86	0.55
1:D:366:PRO:CG	1:D:416:ILE:HD11	2.35	0.55
1:B:318:ILE:HG21	1:C:140:ILE:HD13	1.88	0.55
1:D:287:ASP:HB2	1:D:290:LEU:HB2	1.88	0.55
1:D:252:VAL:O	1:D:256:LEU:HG	2.07	0.55
1:A:297:VAL:O	1:A:301:ILE:HG22	2.06	0.55
1:C:145:ARG:O	1:C:145:ARG:HG2	2.04	0.55
1:D:94:ILE:HD12	1:D:107:LEU:HD13	1.88	0.55
1:D:286:CYS:SG	1:D:292:THR:HG23	2.46	0.55
1:D:160:ASN:HB2	1:D:188:GLU:OE2	2.06	0.55
1:B:36:ASN:O	1:B:40:LEU:HB2	2.07	0.55
1:C:111:LEU:C	1:C:113:SER:H	2.08	0.55
1:B:94:ILE:HD13	1:B:107:LEU:CD1	2.37	0.55
1:C:103:LEU:N	1:C:103:LEU:HD12	2.20	0.55
1:C:302:VAL:HG12	1:C:304:PHE:HE2	1.71	0.55
1:C:320:ARG:NH1	1:C:320:ARG:HG2	2.18	0.55
1:A:75:LEU:HD22	1:A:199:HIS:CD2	2.42	0.55
1:B:110:TRP:O	1:B:111:LEU:C	2.45	0.55
1:C:140:ILE:HG22	1:C:144:TYR:CZ	2.41	0.55
1:A:18:ARG:HB2	1:A:412:VAL:O	2.07	0.55
1:A:59:VAL:CG1	1:A:63:ARG:NH1	2.70	0.55
1:C:395:SER:HB3	1:D:395:SER:HB3	1.89	0.55
1:D:140:ILE:HA	1:D:143:MET:CB	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: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:A:269:GLY:CA	1:D:148:LEU:HD13	2.36	0.55
1:D:277:MET:O	1:D:277:MET:HG2	2.07	0.55
1:B:12:SER:HA	1:B:230:PRO:O	2.07	0.55
1:D:57:ASP:OD1	1:D:61:LYS:CE	2.54	0.55
1:B:79:THR:C	1:B:81:GLN:H	2.10	0.55
1:C:110:TRP:O	1:C:113:SER:OG	2.20	0.55
1:B:358:GLY:O	1:B:361:VAL:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MET:O	1:A:64:GLU:N	2.40	0.55
1:D:330:ALA:C	1:D:332:SER:N	2.58	0.54
1:A:116:PRO:O	1:A:117:ARG:C	2.46	0.54
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:D:240:MET:HG3	1:D:241:GLY:N	2.22	0.54
1:B:231:ILE:HG21	1:B:237:LEU:HD12	1.89	0.54
1:B:148:LEU:HD11	1:C:269:GLY:HA3	1.88	0.54
1:D:17:LEU:HD11	1:D:20:VAL:HG12	1.86	0.54
1:B:70:LEU:CB	1:B:75:LEU:HD11	2.29	0.54
1:B:167:THR:C	1:B:168:THR:CG2	2.62	0.54
1:C:127:VAL:O	1:C:127:VAL:HG12	2.06	0.54
1:A:86:LEU:HD11	1:A:90:LEU:CG	2.37	0.54
1:C:396:GLU:OE2	1:D:399:ARG:NH2	2.41	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:33:THR:N	1:C:36:ASN:OD1	2.40	0.54
1:C:33:THR:O	1:C:34:PRO:C	2.45	0.54
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.72	0.54
1:B:293:VAL:HG13	1:B:298:VAL:CB	2.36	0.54
1:A:246:ARG:NE	1:D:141:LEU:HD11	2.22	0.54
1:A:192:THR:O	1:A:193:THR:C	2.46	0.54
1:D:168:THR:HG21	1:D:192:THR:HG21	1.88	0.54
1:B:356:ASP:O	1:B:356:ASP:OD1	2.24	0.54
1:A:370:VAL:HA	1:A:390:ILE:O	2.07	0.54
1:C:383:ARG:HG2	1:C:387:VAL:O	2.07	0.54
1:D:43:ASP:OD1	1:D:43:ASP:O	2.26	0.54
1:B:70:LEU:HB3	1:B:75:LEU:CD1	2.29	0.54
1:B:352:ARG:HD2	1:B:355:TRP:HA	1.89	0.54
1:B:72:MET:HE1	1:B:164:THR:HG22	1.90	0.54
1:B:101:LEU:CD1	1:C:316:MET:HE3	2.36	0.54
1:C:404:GLY:O	1:C:408:THR:HG23	2.07	0.54
1:C:111:LEU:HA	1:C:114:LEU:HD12	1.89	0.54
1:C:78:GLU:CD	1:C:199:HIS:HE1	2.11	0.54
1:A:240:MET:CE	1:A:246:ARG:HB2	2.38	0.54
1:D:225:GLY:C	1:D:227:ASP:H	2.12	0.54
1:C:158:LEU:CB	1:C:161:THR:HG23	2.39	0.54
1:A:361:VAL:HB	1:A:369:VAL:HG21	1.90	0.54
1:D:133:PRO:O	1:D:134:ALA:C	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:CZ	1:C:141:LEU:HD11	2.38	0.53
1:D:140:ILE:HA	1:D:143:MET:HB2	1.91	0.53
1:C:257:PHE:CE2	1:C:308:PRO:HD3	2.43	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:A:306:LEU:CD1	1:A:318:ILE:HG23	2.15	0.53
1:D:141:LEU:C	1:D:143:MET:N	2.60	0.53
1:C:294:PHE:O	1:C:294:PHE:HD1	1.91	0.53
1:C:85:ALA:HA	1:C:198:PHE:CE1	2.43	0.53
1:A:21:MET:HB3	1:A:409:CYS:HB3	1.89	0.53
1:C:287:ASP:O	1:C:288:ARG:C	2.46	0.53
1:B:182:TRP:C	1:B:184:ALA:N	2.59	0.53
1:D:397:LEU:HG	1:D:407:MET:SD	2.48	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:401:ARG:HB2	1:D:406:CYR:C3	2.34	0.53
1:D:312:SER:OG	1:D:313:PRO:HD2	2.08	0.53
1:A:268:ALA:HB1	1:A:301:ILE:HD11	1.91	0.53
1:D:33:THR:O	1:D:35:SER:N	2.41	0.53
1:A:138:ALA:O	1:A:141:LEU:HB2	2.09	0.53
1:C:28:ALA:CB	1:C:125:GLY:HA2	2.39	0.53
1:C:93:LYS:HE3	1:C:155:LEU:HG	1.91	0.53
1:C:101:LEU:HD13	1:C:101:LEU:C	2.27	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:C:160:ASN:HB3	1:C:185:ARG:CZ	2.38	0.53
1:A:122:TYR:O	1:A:126:GLY:N	2.39	0.53
1:A:279:LEU:O	1:A:281:THR:N	2.42	0.53
1:A:269:GLY:HA3	1:D:148:LEU:HD13	1.88	0.53
1:A:188:GLU:O	1:A:191:LEU:N	2.42	0.53
1:B:251:GLN:C	1:B:253:ALA:N	2.60	0.53
1:A:61:LYS:HA	1:A:64:GLU:OE2	2.08	0.53
1:C:213:ASP:C	1:C:213:ASP:OD1	2.47	0.53
1:C:180:MET:CE	1:C:224:GLU:HG2	2.39	0.53
1:A:229:MET:HE2	1:A:279:LEU:HG	1.90	0.52
1:A:61:LYS:O	1:A:64:GLU:HG2	2.09	0.52
1:B:343:THR:OG1	1:B:359:ASN:ND2	2.39	0.52
1:B:58:PHE:HB2	1:B:392:ILE:HG21	1.91	0.52
1:D:287:ASP:CB	1:D:290:LEU:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:CYS:HB2	1:D:290:LEU:HD12	1.91	0.52
1:B:158:LEU:O	1:B:161:THR:HG23	2.09	0.52
1:D:257:PHE:CE1	1:D:308:PRO:HD3	2.43	0.52
1:A:213:ASP:OD1	1:A:215:ASP:CB	2.56	0.52
1:C:399:ARG:NH2	1:D:396:GLU:OE2	2.42	0.52
1:C:169:CYS:O	1:C:175:VAL:HA	2.09	0.52
1:C:90:LEU:HD22	1:C:94:ILE:CD1	2.39	0.52
1:C:71:GLU:HG3	1:C:73:HIS:H	1.75	0.52
1:A:295:PRO:HG3	1:A:342:GLU:CD	2.29	0.52
1:C:107:LEU:CD2	1:C:127:VAL:HG11	2.30	0.52
1:B:17:LEU:CD1	1:B:413:ARG:HH11	2.22	0.52
1:D:114:LEU:CD1	1:D:118:LYS:HG2	2.38	0.52
1:A:10:VAL:O	1:A:10:VAL:HG12	2.09	0.52
1:B:237:LEU:HD23	1:B:266:ILE:HB	1.91	0.52
1:C:264:ARG:HD3	1:C:307:ARG:CZ	2.40	0.52
1:B:254:GLN:HB3	1:B:316:MET:HE1	1.92	0.52
1:B:371:GLY:O	1:B:391:THR:HA	2.10	0.52
1:C:85:ALA:CB	1:C:198:PHE:CG	2.90	0.52
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:177:LEU:CD1	1:C:193:THR:HG23	2.40	0.52
1:B:279:LEU:C	1:B:281:THR:H	2.11	0.52
1:B:101:LEU:HD11	1:C:316:MET:HE1	1.85	0.52
1:A:17:LEU:HD21	1:A:20:VAL:HG11	1.92	0.52
1:A:202:PHE:C	1:A:204:ASN:N	2.62	0.52
1:C:199:HIS:CG	1:C:200:PRO:HD3	2.45	0.52
1:B:242:GLU:CA	1:B:275:ALA:HA	2.40	0.52
1:A:87:LYS:HG2	1:A:91:ASP:OD2	2.09	0.52
1:A:36:ASN:OD1	1:A:37:CYS:N	2.43	0.52
1:C:238:ILE:HG21	1:C:249:ILE:HG23	1.92	0.51
1:B:166:ASP:CG	1:B:278:HIS:HE1	2.13	0.51
1:C:57:ASP:OD1	1:C:61:LYS:HE3	2.10	0.51
1:D:377:TYR:O	1:D:380:THR:HB	2.09	0.51
1:C:167:THR:O	1:C:178:ASN:ND2	2.44	0.51
1:C:27:LEU:O	1:C:28:ALA:C	2.48	0.51
1:C:264:ARG:CZ	1:C:266:ILE:HD11	2.41	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: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:C:47:TRP:CZ3	1:D:373:ASP:OD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:218:HIS:O	1:A:219:GLY:C	2.48	0.51
1:A:19:LYS:HD2	1:A:411:ILE:HG21	1.92	0.51
1:D:72:MET:O	1:D:73:HIS:C	2.48	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:C:313:PRO:C	1:C:314:TYR:CD1	2.84	0.51
1:A:56:PHE:O	1:A:57:ASP:C	2.49	0.51
1:C:133:PRO:O	1:C:134:ALA:O	2.28	0.51
1:A:352:ARG:N	1:A:377:TYR:CD1	2.79	0.51
1:A:180:MET:HE1	1:A:224:GLU:CD	2.31	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: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:B:50:GLN:NE2	1:B:54:ASP:OD1	2.43	0.51
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:D:366:PRO:HG2	1:D:416:ILE:HD11	1.92	0.50
1:C:168:THR:N	1:C:178:ASN:ND2	2.59	0.50
1:D:199:HIS:HE1	1:D:201:GLU:HB2	1.71	0.50
1:C:10:VAL:HG21	1:C:410:PRO:HB2	1.93	0.50
1:A:304:PHE:CZ	1:D:144:TYR:HE1	2.28	0.50
1:B:356:ASP:C	1:B:356:ASP:OD1	2.49	0.50
1:D:233:ASN:O	1:D:233:ASN:CG	2.50	0.50
1:A:279:LEU:C	1:A:281:THR:N	2.65	0.50
1:B:360:ASN:CG	1:B:406:CYR:SG	2.88	0.50
1:A:17:LEU:HD12	1:A:18:ARG:H	1.77	0.50
1:D:140:ILE:O	1:D:144:TYR:N	2.38	0.50
1:A:29:HIS:CD2	1:A:46:ILE:HD11	2.46	0.50
1:D:321:GLU:HA	1:D:321:GLU:OE2	2.12	0.50
1:D:257:PHE:HB3	1:D:308:PRO:HG3	1.92	0.50
1:D:72:MET:HE2	1:D:192:THR:OG1	2.08	0.50
1:A:158:LEU:O	1:A:161:THR:HG23	2.12	0.50
1:B:404:GLY:O	1:B:408:THR:HG23	2.12	0.50
1:D:141:LEU:O	1:D:142:LYS:C	2.49	0.50
1:D:290:LEU:HD23	1:D:339:ARG:HB2	1.93	0.50
1:C:26:GLY:O	1:C:27:LEU:C	2.50	0.50
1:C:290:LEU:CD2	1:C:291:VAL:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:THR:CG2	1:D:188:GLU:OE1	2.60	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:D:343:THR:HG22	1:D:356:ASP:O	2.11	0.50
1:D:158:LEU:HB3	1:D:161:THR:HG23	1.94	0.50
1:A:49:ASN:HB3	1:A:53:ARG:HH12	1.77	0.50
1:B:167:THR:HG22	1:B:167:THR:O	2.12	0.50
1:D:85:ALA:HB2	1:D:198:PHE:CG	2.47	0.50
1:A:72:MET:O	1:A:76:LEU:HB2	2.11	0.50
1:D:19:LYS:HE2	1:D:68:ASP:OD2	2.12	0.50
1:A:6:THR:O	1:A:205:ALA:HB1	2.12	0.50
1:B:85:ALA:O	1:B:89:ILE:HG13	2.11	0.50
1:D:165:ARG:HB2	1:D:408:THR:O	2.11	0.49
1:D:57:ASP:CG	1:D:61:LYS:HE3	2.32	0.49
1:C:212:GLY:O	1:C:213:ASP:HB2	2.12	0.49
1:A:234:GLY:HA3	1:A:263:GLU:HG3	1.93	0.49
1:D:140:ILE:O	1:D:143:MET:HB3	2.11	0.49
1:C:185:ARG:NH2	1:C:188:GLU:OE1	2.41	0.49
1:A:256:LEU:HD22	1:A:261:ALA:CB	2.41	0.49
1:A:176:THR:HA	1:A:211:TYR:O	2.13	0.49
1:D:213:ASP:OD1	1:D:215:ASP:HB2	2.13	0.49
1:D:225:GLY:O	1:D:227:ASP:N	2.45	0.49
1:B:144:TYR:HE1	1:C:304:PHE:CE1	2.31	0.49
1:C:145:ARG:O	1:C:149:GLY:HA2	2.12	0.49
1:C:56:PHE:HA	1:C:59:VAL:HB	1.94	0.49
1:B:161:THR:C	1:B:163:PHE:N	2.66	0.49
1:D:279:LEU:O	1:D:282:VAL:HG23	2.12	0.49
1:C:71:GLU:HG3	1:C:73:HIS:HB2	1.95	0.49
1:A:231:ILE:HD11	1:A:235:VAL:CG1	2.43	0.49
1:C:161:THR:HG22	1:C:188:GLU:HG2	1.95	0.49
1:B:19:LYS:HE3	1:B:201:GLU:OE2	2.12	0.49
1:C:163:PHE:CE1	1:C:402:GLY:HA3	2.48	0.49
1:D:321:GLU:HB3	1:D:328:VAL:HG21	1.93	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:A:34:PRO:HG2	1:B:355:TRP:CZ2	2.48	0.49
1:C:133:PRO:O	1:C:134:ALA:C	2.51	0.49
1:D:352:ARG:HB2	1:D:352:ARG:CZ	2.43	0.49
1:D:167:THR:C	1:D:168:THR:CG2	2.81	0.49
1:C:33:THR:HB	1:C:36:ASN:CG	2.32	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:C:312:SER:C	1:C:314:TYR:H	2.17	0.49
1:B:211:TYR:CD2	1:B:252:VAL:HG23	2.47	0.49
1:B:24:SER:HB2	1:B:55:HIS:ND1	2.28	0.49
1:B:309:ASP:OD2	1:B:311:SER:CB	2.61	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:D:401:ARG:CB	1:D:406:CYR:C3	2.91	0.48
1:D:14:ALA:C	1:D:366:PRO:HD3	2.24	0.48
1:B:318:ILE:HG21	1:C:140:ILE:CD1	2.43	0.48
1:B:141:LEU:CD1	1:B:154:LEU:HD21	2.42	0.48
1:A:286:CYS:HB2	1:A:290:LEU:HD12	1.95	0.48
1:A:76:LEU:O	1:A:80:ILE:HG12	2.12	0.48
1:B:81:GLN:O	1:B:83:PRO:HD3	2.13	0.48
1:A:294:PHE:HE1	1:A:344:GLY:C	2.16	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:D:318:ILE:HG12	1:D:319:ARG:N	2.28	0.48
1:C:257:PHE:CE1	1:C:308:PRO:HD3	2.48	0.48
1:A:415:PRO:O	1:A:416:ILE:HG13	2.13	0.48
1:C:353:GLU:CA	1:C:353:GLU:OE2	2.58	0.48
1:D:240:MET:CB	1:D:249:ILE:HD12	2.40	0.48
1:C:373:ASP:N	1:C:392:ILE:O	2.45	0.48
1:A:92:ARG:HH11	1:A:92:ARG:HG3	1.78	0.48
1:A:238:ILE:HG21	1:A:249:ILE:HG12	1.94	0.48
1:B:220:SER:HB2	1:B:247:GLN:HE21	1.78	0.48
1:D:266:ILE:HD13	1:D:328:VAL:HG12	1.94	0.48
1:B:161:THR:O	1:B:162:GLN:C	2.51	0.48
1:B:163:PHE:HE2	1:B:406:CYR:HN22	1.60	0.48
1:C:287:ASP:O	1:C:289:ASP:N	2.47	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: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:A:352:ARG:N	1:A:377:TYR:CE1	2.82	0.48
1:A:103:LEU:O	1:A:104:THR:C	2.51	0.48
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.69	0.48
1:B:41:LEU:HD23	1:B:184:ALA:HB3	1.93	0.48
1:D:195:ILE:HG22	1:D:196:TYR:N	2.28	0.48
1:D:173:GLY:O	1:D:210:TRP:CZ2	2.67	0.48
1:B:303:PRO:HG2	1:B:321:GLU:HB2	1.95	0.48
1:D:401:ARG:NH1	1:D:401:ARG:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LYS:HG3	1:D:122:TYR:HE2	1.78	0.48
1:B:13:GLU:C	1:B:413:ARG:HE	2.16	0.48
1:C:85:ALA:O	1:C:88:TRP:CB	2.60	0.48
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.79	0.48
1:D:125:GLY:O	1:D:157:PRO:HB3	2.14	0.48
1:A:343:THR:CG2	1:A:378:THR:OG1	2.59	0.48
1:A:188:GLU:O	1:A:189:THR:C	2.51	0.48
1:C:280:ALA:HA	1:C:283:PHE:O	2.14	0.48
1:D:309:ASP:O	1:D:310:PRO:C	2.49	0.48
1:C:288:ARG:CZ	1:C:416:ILE:HG22	2.44	0.48
1:A:372:TYR:HB2	1:A:375:ASN:HD22	1.78	0.48
1:C:286:CYS:O	1:C:363:CYS:SG	2.72	0.48
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.48	0.48
1:A:70:LEU:HB3	1:A:75:LEU:HD11	1.95	0.48
1:C:358:GLY:HA3	1:C:378:THR:HG21	1.96	0.48
1:B:129:ALA:O	1:B:130:ASP:C	2.52	0.48
1:C:406:CYR:C4	1:C:406:CYR:O1	2.61	0.48
1:C:28:ALA:HA	1:C:125:GLY:CA	2.37	0.48
1:D:199:HIS:O	1:D:203:ALA:CB	2.61	0.48
1:B:120:ALA:HA	1:B:123:LEU:HB2	1.95	0.48
1:B:111:LEU:HD22	1:B:119:LEU:CD2	2.44	0.48
1:B:150:HIS:NE2	1:C:241:GLY:HA2	2.29	0.48
1:D:257:PHE:CB	1:D:308:PRO:HG3	2.43	0.48
1:C:158:LEU:O	1:C:160:ASN:N	2.46	0.48
1:B:148:LEU:CD2	1:C:271:PRO:HD3	2.44	0.48
1:A:269:GLY:CA	1:D:148:LEU:CD1	2.84	0.48
1:A:17:LEU:HB2	1:A:413:ARG:HH21	1.79	0.48
1:B:373:ASP:OD1	1:B:393:SER:HA	2.14	0.48
1:D:20:VAL:HG21	1:D:62:MET:HE1	1.96	0.47
1:D:306:LEU:HD11	1:D:318:ILE:HB	1.96	0.47
1:A:120:ALA:O	1:A:123:LEU:N	2.47	0.47
1:D:167:THR:HG21	1:D:188:GLU:HB3	1.96	0.47
1:D:65:ARG:NH1	1:D:390:ILE:CD1	2.78	0.47
1:B:356:ASP:HB2	1:B:375:ASN:OD1	2.13	0.47
1:D:122:TYR:O	1:D:126:GLY:N	2.43	0.47
1:D:225:GLY:C	1:D:227:ASP:N	2.67	0.47
1:C:312:SER:OG	1:C:316:MET:O	2.29	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:B:108:ARG:O	1:B:112:GLU:HG3	2.13	0.47
1:C:294:PHE:CD1	1:C:294:PHE:C	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:H	1:A:36:ASN:CG	2.17	0.47
1:D:394:ALA:O	1:D:395:SER:C	2.51	0.47
1:A:74:ASN:O	1:A:78:GLU:HG2	2.14	0.47
1:C:142:LYS:O	1:C:146:GLU:HB3	2.14	0.47
1:B:135:SER:O	1:B:136:GLU:C	2.49	0.47
1:A:75:LEU:CD2	1:A:199:HIS:CD2	2.97	0.47
1:B:99:VAL:CG1	1:B:103:LEU:HB2	2.44	0.47
1:B:232:GLY:O	1:B:233:ASN:CB	2.61	0.47
1:B:192:THR:O	1:B:195:ILE:N	2.47	0.47
1:D:198:PHE:O	1:D:199:HIS:C	2.53	0.47
1:C:252:VAL:HG12	1:C:256:LEU:CD1	2.44	0.47
1:D:340:VAL:O	1:D:340:VAL:HG23	2.13	0.47
1:C:141:LEU:CD2	1:C:141:LEU:H	2.27	0.47
1:B:414:ASP:HB3	1:B:415:PRO:HD2	1.96	0.47
1:D:186:ARG:HG3	1:D:186:ARG:NH1	2.22	0.47
1:D:290:LEU:HG	1:D:339:ARG:NH2	2.29	0.47
1:C:71:GLU:O	1:C:72:MET:C	2.53	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:A:118:LYS:O	1:A:121:GLU:HB3	2.15	0.47
1:C:339:ARG:NH1	1:C:385:ALA:HB1	2.30	0.47
1:A:33:THR:HG22	1:A:36:ASN:CB	2.45	0.47
1:A:150:HIS:NE2	1:D:241:GLY:HA3	2.29	0.47
1:D:223:LEU:C	1:D:223:LEU:CD2	2.83	0.47
1:D:56:PHE:O	1:D:59:VAL:HB	2.15	0.47
1:C:324:THR:O	1:C:328:VAL:HG23	2.15	0.47
1:A:180:MET:CE	1:A:224:GLU:OE2	2.63	0.47
1:C:303:PRO:C	1:C:304:PHE:CD2	2.88	0.47
1:D:61:LYS:NZ	1:D:391:THR:O	2.46	0.47
1:B:88:TRP:O	1:B:92:ARG:NH1	2.42	0.47
1:B:72:MET:HE3	1:B:164:THR:CG2	2.44	0.47
1:B:213:ASP:C	1:B:215:ASP:H	2.18	0.47
1:A:144:TYR:CZ	1:D:240:MET:CE	2.98	0.47
1:D:39:GLU:C	1:D:40:LEU:HD13	2.35	0.47
1:C:288:ARG:CZ	1:C:416:ILE:CG2	2.93	0.46
1:B:79:THR:C	1:B:81:GLN:N	2.68	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:A:367:GLY:O	1:A:387:VAL:HG13	2.15	0.46
1:D:343:THR:HG21	1:D:357:ASP:HA	1.94	0.46
1:A:171:ILE:CG2	1:A:230:PRO:HB3	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:144:TYR:CZ	1:D:240:MET:HE1	2.49	0.46
1:A:115:GLU:N	1:A:115:GLU:CD	2.46	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:B:251:GLN:C	1:B:253:ALA:H	2.18	0.46
1:B:301:ILE:HG22	1:B:302:VAL:N	2.30	0.46
1:D:112:GLU:C	1:D:114:LEU:H	2.19	0.46
1:A:278:HIS:H	1:A:281:THR:HB	1.80	0.46
1:A:213:ASP:OD1	1:A:215:ASP:N	2.42	0.46
1:C:331:GLU:O	1:C:332:SER:C	2.54	0.46
1:C:21:MET:C	1:C:22:VAL:HG13	2.36	0.46
1:A:362:VAL:O	1:A:369:VAL:CG2	2.63	0.46
1:C:58:PHE:HB2	1:C:392:ILE:HG21	1.96	0.46
1:D:257:PHE:CG	1:D:308:PRO:HD3	2.50	0.46
1:A:10:VAL:HG21	1:A:410:PRO:HB2	1.97	0.46
1:C:331:GLU:C	1:C:333:LEU:N	2.68	0.46
1:B:287:ASP:O	1:B:288:ARG:C	2.54	0.46
1:A:111:LEU:HA	1:A:114:LEU:HG	1.97	0.46
1:C:60:THR:C	1:C:62:MET:N	2.68	0.46
1:C:60:THR:O	1:C:62:MET:N	2.49	0.46
1:D:20:VAL:HG21	1:D:62:MET:CE	2.46	0.46
1:C:25:PRO:HA	1:C:29:HIS:CE1	2.51	0.46
1:B:50:GLN:HE21	1:B:54:ASP:CG	2.19	0.46
1:B:307:ARG:HB3	1:B:308:PRO:CD	2.46	0.46
1:B:11:HIS:HA	1:B:172:TYR:CD2	2.50	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: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:A:142:LYS:HG2	1:A:145:ARG:HH22	1.81	0.46
1:B:191:LEU:O	1:B:194:ALA:HB3	2.16	0.46
1:A:325:PHE:O	1:A:326:LEU:C	2.54	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
1:C:319:ARG:NH1	1:C:319:ARG:CG	2.34	0.46
1:A:246:ARG:HE	1:D:141:LEU:HD11	1.81	0.46
1:C:155:LEU:HA	1:C:155:LEU:HD12	1.84	0.46
1:C:290:LEU:C	1:C:290:LEU:CD2	2.84	0.46
1:D:56:PHE:O	1:D:59:VAL:N	2.50	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:C:182:TRP:HE1	1:C:243:ARG:NH1	2.12	0.46
1:B:330:ALA:O	1:B:331:GLU:C	2.53	0.46
1:D:248:ALA:O	1:D:251:GLN:N	2.47	0.46
1:B:111:LEU:HA	1:B:114:LEU:HD12	1.99	0.45
1:B:10:VAL:HB	1:B:170:TRP:O	2.15	0.45
1:D:95:THR:OG1	1:D:97:ASP:N	2.45	0.45
1:D:90:LEU:O	1:D:94:ILE:HB	2.16	0.45
1:B:413:ARG:NH1	1:B:413:ARG:HG3	2.31	0.45
1:C:102:GLY:CA	1:C:103:LEU:HD12	2.47	0.45
1:A:158:LEU:HD21	1:A:187:GLN:CB	2.45	0.45
1:B:399:ARG:CG	1:B:399:ARG:NH1	2.71	0.45
1:B:154:LEU:HD23	1:B:154:LEU:N	2.32	0.45
1:C:158:LEU:HB3	1:C:161:THR:CG2	2.46	0.45
1:D:160:ASN:HB3	1:D:185:ARG:CZ	2.46	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:D:324:THR:OG1	1:D:327:GLU:HB2	2.17	0.45
1:D:43:ASP:N	1:D:401:ARG:NH2	2.64	0.45
1:B:116:PRO:O	1:B:117:ARG:C	2.55	0.45
1:B:360:ASN:CG	1:B:405:HIS:HB3	2.36	0.45
1:D:355:TRP:CZ2	1:D:357:ASP:HB2	2.52	0.45
1:C:197:LYS:HG2	1:C:198:PHE:CE2	2.51	0.45
1:A:72:MET:HE1	1:A:192:THR:OG1	2.16	0.45
1:D:168:THR:HG21	1:D:192:THR:CG2	2.46	0.45
1:A:33:THR:HG22	1:A:36:ASN:HB3	1.97	0.45
1:D:249:ILE:O	1:D:250:GLY:C	2.55	0.45
1:C:278:HIS:H	1:C:281:THR:CG2	2.30	0.45
1:C:245:SER:O	1:C:249:ILE:HG12	2.15	0.45
1:A:286:CYS:O	1:A:287:ASP:HB2	2.17	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:A:311:SER:OG	1:A:311:SER:O	2.28	0.45
1:D:403:GLY:O	1:D:404:GLY:C	2.53	0.45
1:A:48:VAL:O	1:A:49:ASN:C	2.55	0.45
1:D:213:ASP:C	1:D:213:ASP:OD1	2.55	0.45
1:B:379:ASN:O	1:B:383:ARG:HG3	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:A:58:PHE:O	1:A:59:VAL:C	2.53	0.45
1:A:218:HIS:O	1:A:221:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:PRO:HG3	1:D:416:ILE:HD11	1.99	0.45
1:A:229:MET:HE1	1:A:279:LEU:HD21	1.98	0.45
1:D:158:LEU:C	1:D:160:ASN:H	2.20	0.45
1:D:70:LEU:CB	1:D:75:LEU:HD11	2.46	0.45
1:C:137:GLY:C	1:C:139:ASN:N	2.68	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:294:PHE:CD1	1:A:344:GLY:HA3	2.52	0.45
1:C:254:GLN:HB2	1:C:316:MET:HE2	1.99	0.45
1:A:14:ALA:HB3	1:A:416:ILE:CD1	2.47	0.45
1:B:166:ASP:CG	1:B:278:HIS:CE1	2.90	0.44
1:C:338:LEU:HA	1:C:338:LEU:HD23	1.89	0.44
1:D:230:PRO:C	1:D:232:GLY:H	2.21	0.44
1:B:90:LEU:HD13	1:B:108:ARG:HG3	2.00	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:C:102:GLY:C	1:C:103:LEU:CD1	2.75	0.44
1:D:399:ARG:O	1:D:400:GLY:C	2.53	0.44
1:A:142:LYS:CB	1:A:145:ARG:HH21	2.30	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:A:272:LYS:O	1:A:273:SER:CB	2.38	0.44
1:C:294:PHE:CD1	1:C:294:PHE:O	2.70	0.44
1:A:21:MET:HE3	1:A:192:THR:HG23	1.99	0.44
1:D:29:HIS:CD2	1:D:46:ILE:HD11	2.53	0.44
1:C:323:LYS:HB3	1:C:327:GLU:HB2	1.98	0.44
1:B:287:ASP:O	1:B:289:ASP:N	2.50	0.44
1:B:394:ALA:O	1:B:395:SER:C	2.56	0.44
1:B:295:PRO:CG	1:B:342:GLU:HB3	2.39	0.44
1:D:86:LEU:HD22	1:D:90:LEU:HG	1.98	0.44
1:C:206:GLU:O	1:C:207:PHE:HB3	2.17	0.44
1:D:118:LYS:HG3	1:D:122:TYR:CE2	2.53	0.44
1:D:79:THR:OG1	1:D:199:HIS:HB2	2.18	0.44
1:A:117:ARG:HB2	1:A:117:ARG:HE	1.56	0.44
1:D:282:VAL:HG11	1:D:297:VAL:HG11	1.99	0.44
1:A:415:PRO:C	1:A:416:ILE:HG13	2.38	0.44
1:C:158:LEU:C	1:C:160:ASN:N	2.71	0.44
1:B:213:ASP:HA	1:B:214:PRO:HD2	1.90	0.44
1:D:93:LYS:HE3	1:D:155:LEU:HG	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HB2	1:B:413:ARG:NH1	2.30	0.44
1:A:18:ARG:NH2	1:A:414:ASP:OD1	2.51	0.44
1:B:25:PRO:HA	1:B:29:HIS:CE1	2.53	0.44
1:A:233:ASN:OD1	1:A:233:ASN:N	2.50	0.44
1:B:413:ARG:CG	1:B:413:ARG:HH11	2.31	0.44
1:D:282:VAL:HG12	1:D:294:PHE:HB3	2.00	0.44
1:A:71:GLU:HG3	1:A:73:HIS:N	2.26	0.44
1:B:263:GLU:O	1:B:308:PRO:HD3	2.18	0.44
1:D:277:MET:O	1:D:277:MET:HG3	2.16	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:C:352:ARG:HD3	1:C:354:GLN:O	2.18	0.44
1:A:265:VAL:HB	1:A:306:LEU:HB3	2.00	0.44
1:D:141:LEU:CD2	1:D:154:LEU:HD21	2.45	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:158:LEU:C	1:D:160:ASN:N	2.70	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:B:178:ASN:HA	1:B:179:PRO:HD3	1.82	0.44
1:D:166:ASP:HB3	1:D:180:MET:HE1	2.00	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:C:127:VAL:HG12	1:C:154:LEU:HB2	2.00	0.44
1:A:91:ASP:OD1	1:A:108:ARG:NH2	2.48	0.44
1:C:238:ILE:HD12	1:C:249:ILE:HG23	1.98	0.44
1:A:326:LEU:HD22	1:A:338:LEU:HD12	2.00	0.44
1:A:164:THR:O	1:A:165:ARG:C	2.54	0.44
1:B:105:SER:O	1:B:106:GLU:C	2.56	0.44
1:D:15:GLY:HA2	1:D:416:ILE:HD13	2.00	0.43
1:A:286:CYS:HB2	1:A:290:LEU:HD13	1.98	0.43
1:C:416:ILE:O	1:C:417:ASP:C	2.57	0.43
1:D:167:THR:O	1:D:168:THR:CG2	2.66	0.43
1:B:362:VAL:O	1:B:369:VAL:HG22	2.18	0.43
1:D:333:LEU:HB2	1:D:335:LEU:HD13	1.98	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:C:312:SER:C	1:C:314:TYR:N	2.71	0.43
1:D:16:LYS:HD2	1:D:18:ARG:NH1	2.28	0.43
1:C:21:MET:C	1:C:22:VAL:CG1	2.85	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:D:82:ASN:OD1	1:D:82:ASN:O	2.37	0.43
1:A:181:TYR:O	1:A:186:ARG:NH2	2.51	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:378:THR:HG22	1:A:382:LEU:HD22	2.00	0.43
1:A:280:ALA:CB	1:A:405:HIS:CE1	3.01	0.43
1:B:374:ARG:HG2	1:B:394:ALA:CB	2.49	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:C:135:SER:O	1:C:136:GLU:C	2.56	0.43
1:B:175:VAL:HG22	1:B:176:THR:N	2.34	0.43
1:A:15:GLY:HA3	1:A:414:ASP:O	2.17	0.43
1:D:160:ASN:CB	1:D:188:GLU:OE2	2.67	0.43
1:D:19:LYS:HG3	1:D:68:ASP:HB3	2.00	0.43
1:A:361:VAL:HB	1:A:369:VAL:CG2	2.48	0.43
1:C:177:LEU:HD13	1:C:193:THR:HG23	1.99	0.43
1:C:78:GLU:OE1	1:C:199:HIS:HE1	2.02	0.43
1:D:114:LEU:HB3	1:D:119:LEU:HB2	2.00	0.43
1:A:294:PHE:CE1	1:A:344:GLY:C	2.92	0.43
1:D:103:LEU:HD13	1:D:141:LEU:CD2	2.48	0.43
1:C:197:LYS:HG2	1:C:198:PHE:CD2	2.54	0.43
1:B:228:VAL:HG22	1:B:238:ILE:HG12	2.01	0.43
1:C:289:ASP:N	1:C:289:ASP:OD2	2.51	0.43
1:A:227:ASP:OD2	1:A:278:HIS:HA	2.18	0.43
1:C:143:MET:HB2	1:C:143:MET:HE2	1.73	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:B:14:ALA:O	1:B:15:GLY:O	2.36	0.43
1:B:33:THR:C	1:B:35:SER:H	2.21	0.43
1:D:63:ARG:CG	1:D:63:ARG:HH11	2.32	0.43
1:A:237:LEU:C	1:A:238:ILE:HG13	2.39	0.43
1:D:287:ASP:HB2	1:D:290:LEU:HB3	2.00	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:C:225:GLY:O	1:C:226:GLY:C	2.57	0.43
1:B:171:ILE:HA	1:B:230:PRO:CG	2.49	0.43
1:D:196:TYR:CD1	1:D:202:PHE:CD1	3.07	0.43
1:D:47:TRP:CD2	1:D:50:GLN:HB2	2.54	0.43
1:B:282:VAL:HG11	1:B:297:VAL:HG11	2.01	0.43
1:C:127:VAL:HB	1:C:155:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:HIS:O	1:C:77:THR:OG1	2.33	0.43
1:B:231:ILE:HG21	1:B:237:LEU:HD11	2.00	0.43
1:D:43:ASP:HA	1:D:401:ARG:NH2	2.22	0.43
1:B:107:LEU:HD11	1:B:111:LEU:HD12	2.00	0.43
1:A:31:ARG:HD3	1:A:157:PRO:HG3	2.01	0.43
1:C:21:MET:O	1:C:22:VAL:HG13	2.18	0.43
1:D:100:GLY:O	1:D:104:THR:HG23	2.18	0.43
1:B:317:ASN:OD1	1:B:318:ILE:N	2.52	0.42
1:C:87:LYS:HD3	1:C:91:ASP:OD2	2.19	0.42
1:C:294:PHE:CD1	1:C:297:VAL:HB	2.54	0.42
1:C:88:TRP:NE1	1:C:197:LYS:HE2	2.34	0.42
1:A:120:ALA:O	1:A:121:GLU:C	2.57	0.42
1:C:93:LYS:C	1:C:94:ILE:HG13	2.40	0.42
1:D:330:ALA:O	1:D:331:GLU:C	2.58	0.42
1:B:309:ASP:OD2	1:B:311:SER:HB3	2.18	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:D:63:ARG:C	1:D:65:ARG:N	2.69	0.42
1:D:87:LYS:HG2	1:D:91:ASP:OD2	2.18	0.42
1:B:297:VAL:O	1:B:298:VAL:C	2.55	0.42
1:A:282:VAL:HB	1:A:294:PHE:HB3	2.01	0.42
1:A:26:GLY:N	1:A:29:HIS:ND1	2.67	0.42
1:B:240:MET:HE1	1:C:144:TYR:CE1	2.54	0.42
1:C:71:GLU:O	1:C:73:HIS:N	2.52	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:164:THR:C	1:A:166:ASP:N	2.72	0.42
1:A:43:ASP:O	1:A:44:ASP:HB2	2.18	0.42
1:D:146:GLU:HG3	1:D:147:TYR:N	2.34	0.42
1:D:94:ILE:HD11	1:D:107:LEU:CD1	2.50	0.42
1:D:80:ILE:HG12	1:D:80:ILE:H	1.36	0.42
1:D:165:ARG:NH1	1:D:405:HIS:O	2.48	0.42
1:B:216:LYS:HG2	1:B:217:ASP:N	2.33	0.42
1:D:312:SER:OG	1:D:313:PRO:CD	2.67	0.42
1:B:18:ARG:NH1	1:B:414:ASP:OD2	2.50	0.42
1:D:25:PRO:HG2	1:D:51:ALA:HB1	2.01	0.42
1:A:303:PRO:HG2	1:A:321:GLU:HB2	2.00	0.42
1:B:73:HIS:HB3	1:B:117:ARG:NH2	2.35	0.42
1:A:31:ARG:NH1	1:A:31:ARG:CG	2.75	0.42
1:A:169:CYS:O	1:A:175:VAL:HA	2.20	0.42
1:A:54:ASP:CB	1:A:397:LEU:CD2	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ASP:OD2	1:B:401:ARG:HB2	2.20	0.42
1:D:257:PHE:CZ	1:D:265:VAL:HG23	2.54	0.42
1:C:28:ALA:N	1:C:125:GLY:HA2	2.34	0.42
1:A:80:ILE:CD1	1:A:120:ALA:HB2	2.42	0.42
1:D:223:LEU:CD1	1:D:252:VAL:HG21	2.48	0.42
1:A:27:LEU:O	1:A:30:GLN:HB2	2.20	0.42
1:D:39:GLU:HG3	1:D:40:LEU:HD13	2.01	0.42
1:C:397:LEU:HD12	1:C:397:LEU:HA	1.81	0.42
1:D:36:ASN:C	1:D:38:ASP:N	2.72	0.42
1:C:190:LEU:HD12	1:C:214:PRO:HB2	2.01	0.42
1:D:243:ARG:HH11	1:D:274:ARG:HH12	1.68	0.42
1:A:224:GLU:CD	1:A:243:ARG:HD3	2.38	0.42
1:A:144:TYR:CE1	1:D:240:MET:HE1	2.54	0.42
1:D:56:PHE:O	1:D:57:ASP:O	2.37	0.42
1:A:140:ILE:HA	1:A:143:MET:HB2	2.01	0.42
1:C:60:THR:C	1:C:62:MET:H	2.22	0.42
1:A:296:GLU:N	1:A:296:GLU:OE2	2.47	0.42
1:C:78:GLU:O	1:C:81:GLN:HB2	2.20	0.42
1:A:86:LEU:O	1:A:87:LYS:C	2.58	0.42
1:D:365:GLU:CD	1:D:368:VAL:HG23	2.37	0.42
1:A:180:MET:CE	1:A:224:GLU:CD	2.88	0.42
1:C:286:CYS:SG	1:C:292:THR:CG2	3.05	0.42
1:C:160:ASN:HB3	1:C:185:ARG:NH1	2.35	0.42
1:D:158:LEU:O	1:D:159:PRO:C	2.58	0.42
1:A:24:SER:HB2	1:A:55:HIS:ND1	2.35	0.42
1:A:343:THR:HG21	1:A:378:THR:CG2	2.50	0.42
1:A:256:LEU:HD22	1:A:261:ALA:HB3	2.02	0.42
1:A:272:LYS:HE2	1:D:149:GLY:CA	2.34	0.42
1:C:223:LEU:HD13	1:C:223:LEU:C	2.41	0.42
1:A:326:LEU:HA	1:A:326:LEU:HD23	1.84	0.42
1:D:67:ILE:HG22	1:D:69:VAL:HG22	2.02	0.42
1:C:247:GLN:O	1:C:251:GLN:HG3	2.20	0.42
1:D:189:THR:O	1:D:190:LEU:C	2.58	0.42
1:C:50:GLN:HA	1:C:53:ARG:HG3	2.02	0.42
1:C:178:ASN:OD1	1:C:223:LEU:CD1	2.64	0.41
1:C:77:THR:HG23	1:C:117:ARG:HA	2.02	0.41
1:A:18:ARG:CG	1:A:18:ARG:HH11	2.33	0.41
1:D:160:ASN:C	1:D:162:GLN:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:HD11	1:C:193:THR:HG23	2.02	0.41
1:D:94:ILE:HG22	1:D:94:ILE:O	2.19	0.41
1:D:399:ARG:C	1:D:400:GLY:O	2.58	0.41
1:B:227:ASP:O	1:B:238:ILE:HA	2.20	0.41
1:A:33:THR:O	1:A:36:ASN:OD1	2.37	0.41
1:D:59:VAL:O	1:D:60:THR:C	2.59	0.41
1:A:85:ALA:O	1:A:88:TRP:HB3	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:B:379:ASN:CG	1:B:389:VAL:HG11	2.40	0.41
1:B:259:LYS:O	1:B:260:GLY:C	2.57	0.41
1:A:80:ILE:H	1:A:80:ILE:HG12	1.62	0.41
1:A:33:THR:HG22	1:A:36:ASN:ND2	2.35	0.41
1:D:22:VAL:HA	1:D:164:THR:CG2	2.49	0.41
1:B:88:TRP:CE2	1:B:92:ARG:CZ	3.04	0.41
1:B:254:GLN:HB3	1:B:316:MET:CE	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:141:LEU:HD21	1:C:246:ARG:CD	2.50	0.41
1:B:216:LYS:HD2	1:B:218:HIS:NE2	2.35	0.41
1:A:199:HIS:ND1	1:A:200:PRO:N	2.68	0.41
1:A:19:LYS:CD	1:A:411:ILE:HG21	2.50	0.41
1:A:158:LEU:HB3	1:A:161:THR:HG23	2.03	0.41
1:A:199:HIS:C	1:A:199:HIS:ND1	2.73	0.41
1:A:199:HIS:CE1	1:A:201:GLU:H	2.38	0.41
1:A:142:LYS:CB	1:A:145:ARG:NH2	2.84	0.41
1:B:312:SER:O	1:B:313:PRO:C	2.59	0.41
1:C:383:ARG:HA	1:C:387:VAL:O	2.20	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:B:381:LEU:O	1:B:382:LEU:C	2.56	0.41
1:C:63:ARG:C	1:C:65:ARG:H	2.23	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: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:C:9:GLY:CA	1:C:172:TYR:O	2.66	0.41
1:B:372:TYR:HB2	1:B:375:ASN:HD22	1.85	0.41
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.91	0.41
1:C:56:PHE:CD1	1:C:56:PHE:C	2.94	0.41
1:A:197:LYS:HG2	1:A:197:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ILE:CG2	1:B:161:THR:HG21	2.39	0.41
1:A:56:PHE:O	1:A:59:VAL:N	2.53	0.41
1:A:34:PRO:HG2	1:B:355:TRP:CH2	2.56	0.41
1:A:70:LEU:CD1	1:A:75:LEU:HD11	2.50	0.41
1:B:193:THR:O	1:B:194:ALA:C	2.59	0.41
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.83	0.41
1:A:318:ILE:H	1:A:318:ILE:HG12	1.58	0.41
1:D:141:LEU:HA	1:D:141:LEU:HD12	1.65	0.41
1:C:86:LEU:O	1:C:87:LYS:C	2.58	0.41
1:A:41:LEU:HD12	1:A:184:ALA:HB3	2.03	0.41
1:A:10:VAL:HG12	1:A:230:PRO:HG2	2.01	0.41
1:A:187:GLN:OE1	1:A:187:GLN:HA	2.20	0.41
1:A:282:VAL:O	1:A:293:VAL:HA	2.20	0.41
1:A:40:LEU:HA	1:A:40:LEU:HD12	1.58	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:B:83:PRO:O	1:B:87:LYS:HB2	2.20	0.41
1:D:365:GLU:CG	1:D:368:VAL:HG23	2.51	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:324:THR:OG1	1:A:327:GLU:HG3	2.20	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:A:254:GLN:HG2	1:A:254:GLN:O	2.21	0.41
1:C:82:ASN:OD1	1:C:82:ASN:C	2.60	0.41
1:B:165:ARG:HH11	1:B:165:ARG:HD2	1.77	0.41
1:A:7:LYS:HE3	1:A:7:LYS:HB2	1.50	0.41
1:B:107:LEU:C	1:B:107:LEU:CD1	2.89	0.41
1:C:137:GLY:C	1:C:139:ASN:H	2.23	0.41
1:C:71:GLU:CG	1:C:73:HIS:HB2	2.51	0.41
1:A:15:GLY:N	1:A:416:ILE:HD11	2.36	0.41
1:B:182:TRP:HA	1:B:183:PRO:HD3	1.86	0.41
1:B:36:ASN:C	1:B:36:ASN:OD1	2.59	0.41
1:D:145:ARG:HG2	1:D:145:ARG:O	2.19	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:B:31:ARG:HH11	1:B:31:ARG:HG2	1.86	0.41
1:A:229:MET:HE1	1:A:279:LEU:HG	2.00	0.40
1:C:86:LEU:HD22	1:C:90:LEU:HG	2.03	0.40
1:D:165:ARG:O	1:D:225:GLY:HA3	2.21	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:373:ASP:OD1	1:D:393:SER:HA	2.21	0.40
1:D:329:VAL:O	1:D:330:ALA:C	2.58	0.40
1:C:73:HIS:CD2	1:C:124:ILE:HD12	2.57	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:279:LEU:C	1:B:281:THR:N	2.75	0.40
1:B:382:LEU:HA	1:B:382:LEU:HD12	1.78	0.40
1:B:8:LEU:HD22	1:B:411:ILE:HG22	2.02	0.40
1:C:360:ASN:OD1	1:C:403:GLY:HA3	2.21	0.40
1:B:161:THR:C	1:B:163:PHE:H	2.25	0.40
1:D:380:THR:O	1:D:381:LEU:C	2.58	0.40
1:D:43:ASP:HB2	1:D:401:ARG:NH2	2.36	0.40
1:B:294:PHE:HA	1:B:295:PRO:HD3	1.81	0.40
1:C:360:ASN:OD1	1:C:403:GLY:CA	2.69	0.40
1:C:158:LEU:CB	1:C:161:THR:CG2	2.99	0.40
1:D:397:LEU:HD12	1:D:397:LEU:HA	1.86	0.40
1:C:41:LEU:HD11	1:C:182:TRP:CG	2.57	0.40
1:D:299:LYS:O	1:D:299:LYS:HG3	2.21	0.40
1:D:111:LEU:HA	1:D:111:LEU:HD23	1.96	0.40
1:D:193:THR:CG2	1:D:214:PRO:HG2	2.44	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:C:397:LEU:CD1	1:C:397:LEU:N	2.84	0.40
1:B:31:ARG:HD3	1:B:153:PHE:CE1	2.57	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%)	3 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	399/418 (96%)	332 (83%)	50 (12%)	17 (4%)	3	13
1	C	396/418 (95%)	323 (82%)	61 (15%)	12 (3%)	5	22
1	D	395/418 (94%)	327 (83%)	54 (14%)	14 (4%)	4	18
All	All	1585/1672 (95%)	1295 (82%)	230 (14%)	60 (4%)	4	16

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%)	278 (81%)	64 (19%)	2	6
1	B	342/353 (97%)	279 (82%)	63 (18%)	2	6
1	C	342/353 (97%)	276 (81%)	66 (19%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	342/353 (97%)	279 (82%)	63 (18%)	2	6
All	All	1368/1412 (97%)	1112 (81%)	256 (19%)	2	6

All (256) 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	23	CYS
1	A	35	SER
1	A	39	GLU
1	A	40	LEU
1	A	42	PHE
1	A	52	LYS
1	A	65	ARG
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	105	SER
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	143	MET
1	A	145	ARG
1	A	151	SER
1	A	155	LEU
1	A	165	ARG
1	A	167	THR
1	A	177	LEU
1	A	189	THR
1	A	201	GLU
1	A	208	GLU

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Mol	Chain	Res	Type
1	A	209	ILE
1	A	216	LYS
1	A	223	LEU
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	290	LEU
1	A	293	VAL
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	336	LYS
1	A	337	LYS
1	A	354	GLN
1	A	361	VAL
1	A	365	GLU
1	A	374	ARG
1	A	382	LEU
1	A	397	LEU
1	A	399	ARG
1	B	6	THR
1	B	19	LYS
1	B	20	VAL
1	B	37	CYS
1	B	39	GLU
1	B	40	LEU
1	B	41	LEU
1	B	42	PHE
1	B	60	THR
1	B	64	GLU
1	B	65	ARG
1	B	76	LEU
1	B	86	LEU
1	B	92	ARG

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Mol	Chain	Res	Type
1	B	94	ILE
1	B	98	SER
1	B	101	LEU
1	B	105	SER
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	150	HIS
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	216	LYS
1	B	243	ARG
1	B	247	GLN
1	B	254	GLN
1	B	259	LYS
1	B	277	MET
1	B	284	SER
1	B	288	ARG
1	B	290	LEU
1	B	299	LYS
1	B	305	SER
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

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Mol	Chain	Res	Type
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	20	VAL
1	C	24	SER
1	C	35	SER
1	C	37	CYS
1	C	40	LEU
1	C	41	LEU
1	C	60	THR
1	C	61	LYS
1	C	65	ARG
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	119	LEU
1	C	130	ASP
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	208	GLU
1	C	220	SER
1	C	240	MET
1	C	243	ARG
1	C	246	ARG
1	C	249	ILE

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Mol	Chain	Res	Type
1	C	259	LYS
1	C	264	ARG
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
1	C	331	GLU
1	C	343	THR
1	C	351	GLU
1	C	361	VAL
1	C	374	ARG
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	42	PHE
1	D	63	ARG
1	D	72	MET
1	D	76	LEU
1	D	80	ILE
1	D	86	LEU
1	D	95	THR

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Mol	Chain	Res	Type
1	D	107	LEU
1	D	109	SER
1	D	113	SER
1	D	114	LEU
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	177	LEU
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	272	LYS
1	D	273	SER
1	D	274	ARG
1	D	277	MET
1	D	282	VAL
1	D	283	PHE
1	D	284	SER
1	D	287	ASP
1	D	288	ARG
1	D	290	LEU
1	D	299	LYS
1	D	306	LEU
1	D	311	SER
1	D	314	TYR
1	D	318	ILE
1	D	331	GLU
1	D	332	SER
1	D	333	LEU

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Mol	Chain	Res	Type
1	D	336	LYS
1	D	337	LYS
1	D	352	ARG
1	D	374	ARG
1	D	384	LYS
1	D	397	LEU
1	D	401	ARG
1	D	411	ILE
1	D	413	ARG
1	D	416	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	HIS
1	C	74	ASN
1	C	162	GLN
1	C	178	ASN
1	C	199	HIS
1	C	218	HIS
1	C	354	GLN
1	D	30	GLN

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	A	406	1	11,16,17	2.31	3 (27%)	6,19,21	1.67	1 (16%)
1	CYR	B	406	1	11,16,17	2.35	3 (27%)	6,19,21	2.17	2 (33%)
1	CYR	C	406	1	11,16,17	2.26	3 (27%)	6,19,21	2.07	3 (50%)
1	CYR	D	406	1	11,16,17	2.43	3 (27%)	6,19,21	1.87	2 (33%)

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	A	406	1	-	0/10/18/20	0/0/0/0
1	CYR	B	406	1	-	0/10/18/20	0/0/0/0
1	CYR	C	406	1	-	1/10/18/20	0/0/0/0
1	CYR	D	406	1	-	0/10/18/20	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	406	CYR	CB-SG	-4.56	1.75	1.81
1	B	406	CYR	CB-SG	-4.45	1.75	1.81
1	C	406	CYR	CB-SG	-3.60	1.77	1.81
1	A	406	CYR	CB-SG	-3.50	1.77	1.81
1	B	406	CYR	C7-N6	4.25	1.45	1.36
1	C	406	CYR	C7-N6	4.30	1.45	1.36
1	D	406	CYR	C7-N6	4.47	1.45	1.36
1	B	406	CYR	C7-N7	4.56	1.45	1.28
1	A	406	CYR	C7-N7	4.61	1.45	1.28
1	D	406	CYR	C7-N7	4.75	1.46	1.28
1	C	406	CYR	C7-N7	4.82	1.46	1.28
1	A	406	CYR	C7-N6	4.84	1.46	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	CYR	N6-C7-N7	-4.37	109.51	120.88
1	C	406	CYR	N6-C7-N7	-3.89	110.76	120.88
1	D	406	CYR	N6-C7-N7	-3.43	111.96	120.88
1	A	406	CYR	N6-C7-N7	-3.38	112.09	120.88
1	C	406	CYR	O-C-CA	-2.37	119.32	125.49
1	D	406	CYR	C5-N6-C7	-2.23	118.90	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	CYR	O-C-CA	-2.21	119.75	125.49
1	C	406	CYR	C5-N6-C7	-2.13	119.09	123.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	406	CYR	SG-C7-N6-C5

There are no ring outliers.

3 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/418 (95%)	-0.49	3 (0%) 89 88	12, 40, 72, 99	0
1	B	405/418 (96%)	-0.54	1 (0%) 95 95	13, 37, 73, 99	0
1	C	402/418 (96%)	-0.43	6 (1%) 76 74	14, 45, 79, 98	0
1	D	401/418 (95%)	-0.42	5 (1%) 81 78	17, 43, 79, 98	0
All	All	1609/1672 (96%)	-0.47	15 (0%) 85 84	12, 41, 77, 99	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	SER	4.4
1	D	147	TYR	3.5
1	A	134	ALA	3.4
1	D	353	GLU	3.2
1	C	313	PRO	2.9
1	A	6	THR	2.7
1	D	310	PRO	2.4
1	B	417	ASP	2.4
1	C	416	ILE	2.4
1	D	312	SER	2.4
1	A	273	SER	2.3
1	C	353	GLU	2.2
1	D	146	GLU	2.2
1	C	314	TYR	2.2
1	C	147	TYR	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CYR	D	406	17/18	0.97	0.10	-	15,40,60,62	0
1	CYR	B	406	17/18	0.93	0.15	-	22,42,60,63	0
1	CYR	C	406	17/18	0.95	0.12	-	21,34,46,50	0
1	CYR	A	406	17/18	0.96	0.13	-	14,45,58,60	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.