



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2017 – 09:52 AM EDT

PDB ID : 5XN6
Title : Heterodimer crystal structure of geranylgeranyl diphosphate synthases 1 with GGPPS Recruiting Protein(OsGRP) from Oryza sativa
Authors : Wang, C.; Zhou, F.; Lu, S.; Zhang, P.
Deposited on : 2017-05-18
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

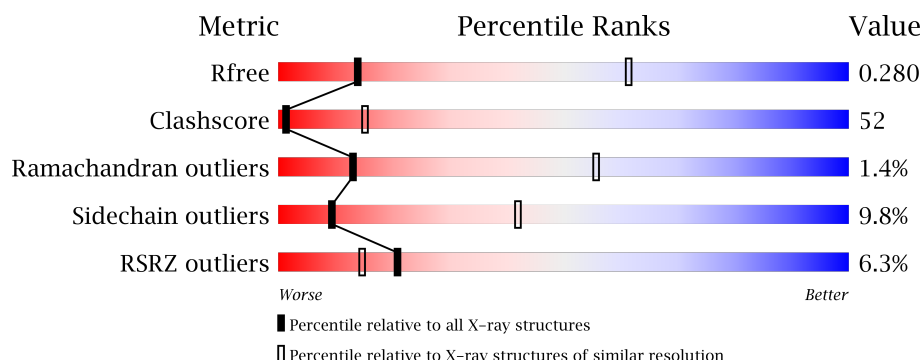
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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	305	<div> <div>6%</div> <div> <div>56%</div> <div>33%</div> <div>8%</div> </div> </div>
1	B	305	<div> <div>6%</div> <div> <div>60%</div> <div>27%</div> <div>9%</div> </div> </div>
1	E	305	<div> <div>6%</div> <div> <div>60%</div> <div>29%</div> <div>9%</div> </div> </div>
2	C	304	<div> <div>8%</div> <div> <div>35%</div> <div>39%</div> <div>12%</div> <div>14%</div> </div> </div>
2	D	304	<div> <div>6%</div> <div> <div>32%</div> <div>44%</div> <div>11%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	304	<div><div></div><div>4%</div><div>28%</div><div>45%</div><div>12%</div><div>•</div><div>13%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12244 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 Os07g0580900 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2142	1353	373	402	14			
1	B	277	Total	C	N	O	S	0	0	0
			2105	1331	368	392	14			
1	E	278	Total	C	N	O	S	0	0	0
			2117	1337	367	399	14			

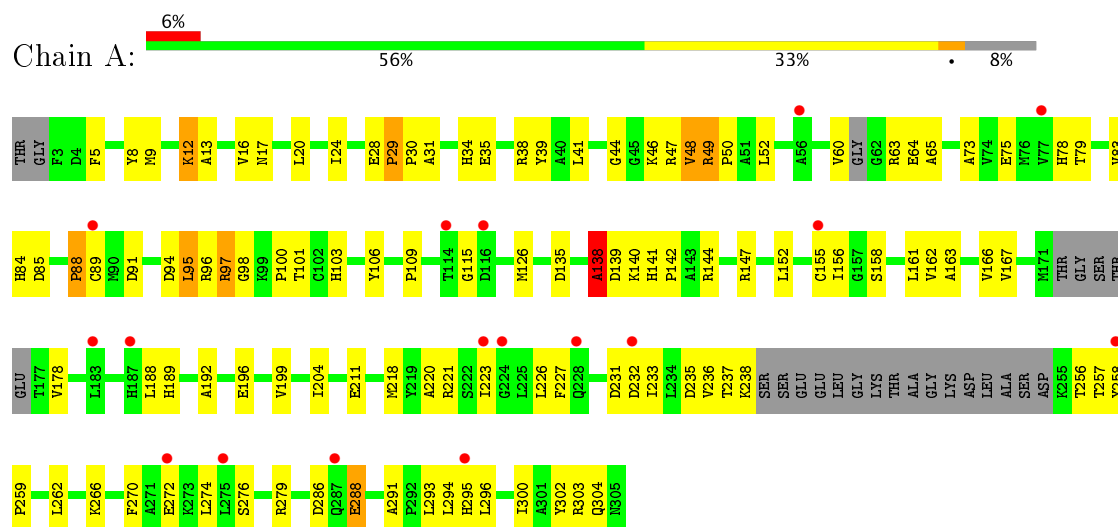
- Molecule 2 is a protein called Os02g0668100 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	262	Total	C	N	O	S	0	0	0
			1941	1232	334	359	16			
2	D	266	Total	C	N	O	S	0	0	0
			1973	1250	344	363	16			
2	F	263	Total	C	N	O	S	0	0	0
			1966	1245	344	361	16			

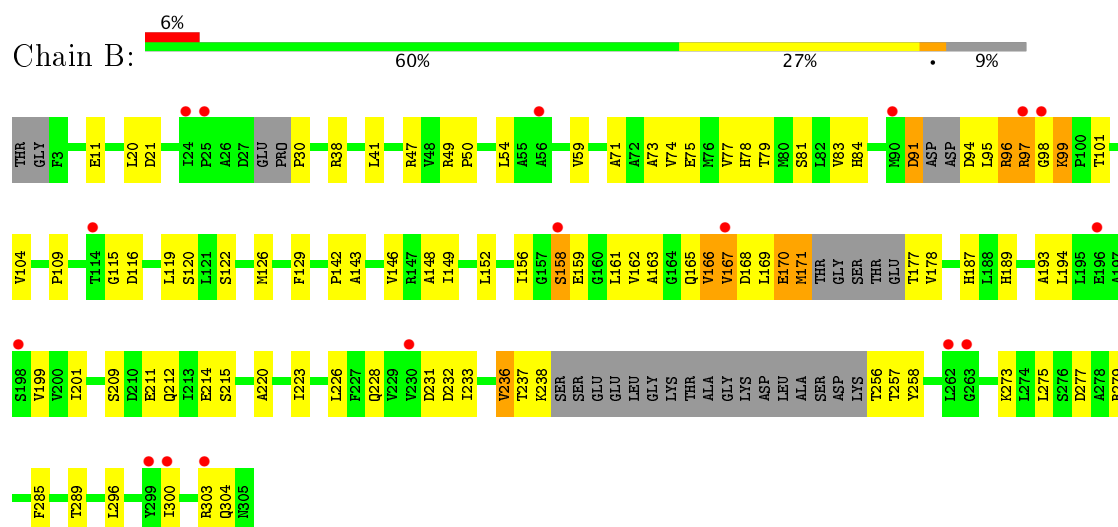
3 Residue-property plots

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

• Molecule 1: Os07g0580900 protein

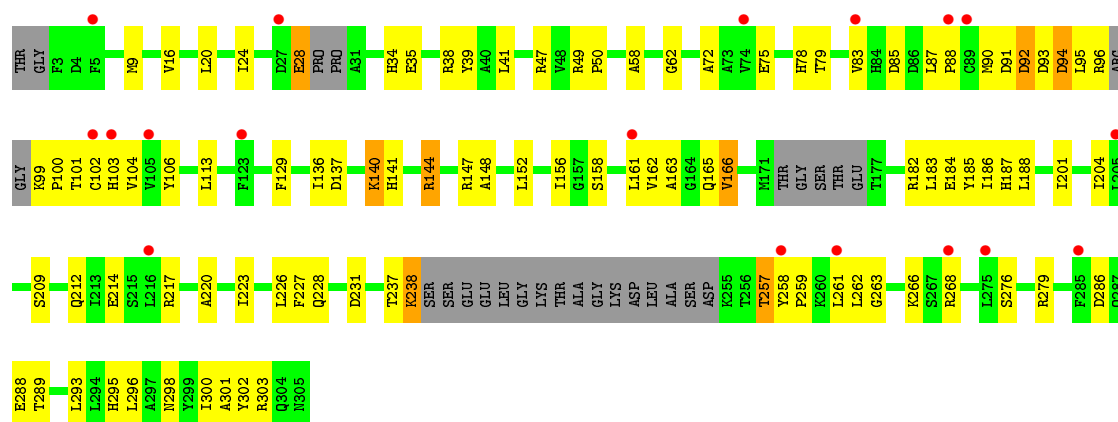


• Molecule 1: Os07g0580900 protein

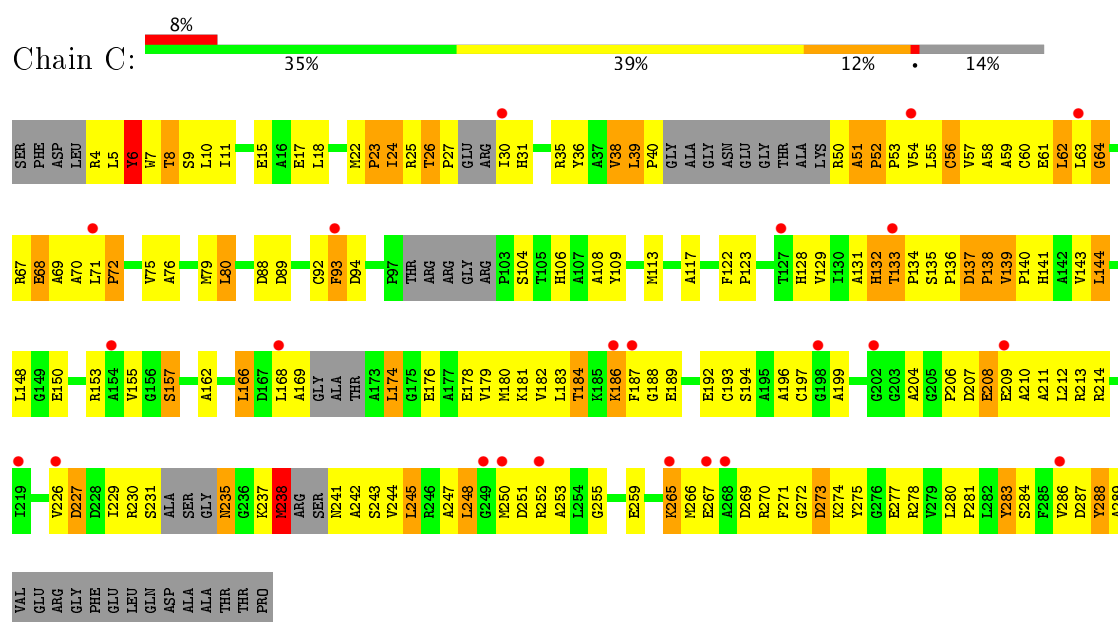


• Molecule 1: Os07g0580900 protein

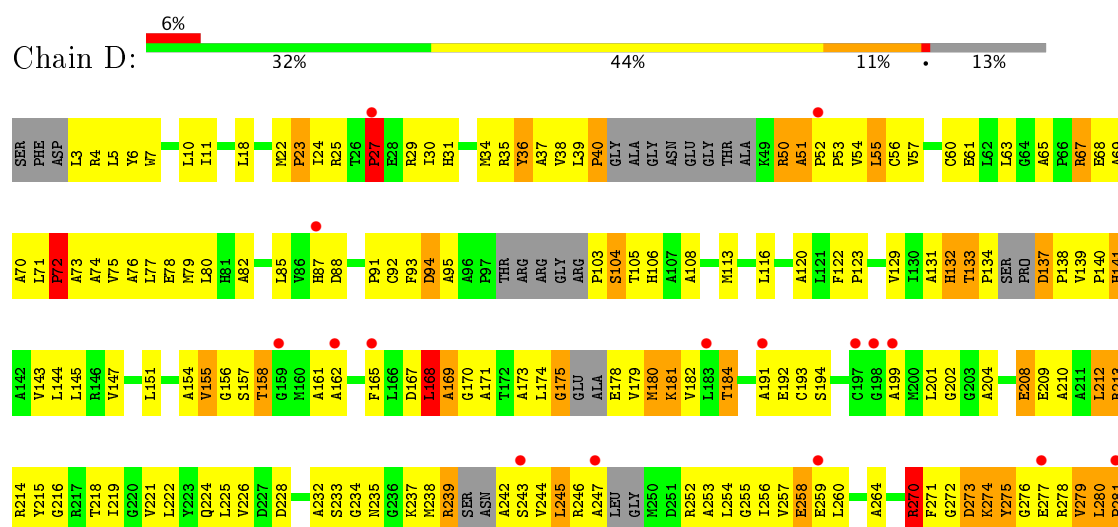


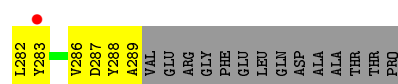


• Molecule 2: Os02g0668100 protein

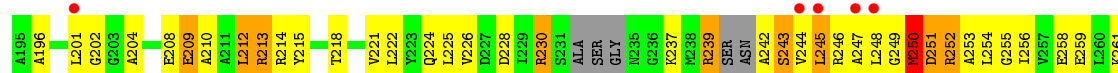
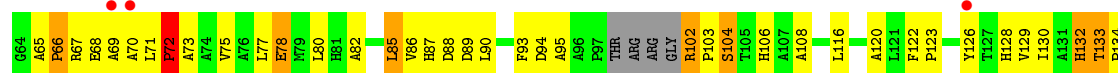


• Molecule 2: Os02g0668100 protein





• Molecule 2: Os02g0668100 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.06 Å 102.98 Å 103.49 Å 109.39° 109.59° 109.13°	Depositor
Resolution (Å)	37.76 – 3.60 37.75 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (37.76-3.60) 77.9 (37.75-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.56 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.263 0.267 , 0.280	Depositor DCC
R_{free} test set	1844 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	107.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage

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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.

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Property	Value	Source
Estimated twinning fraction	0.016 for $h+k+l,-l,-h$ 0.016 for $-l,h+k+l,-k$ 0.014 for $-k,h+k+l,-h$ 0.014 for $-l,-h,h+k+l$ 0.015 for $-k,-l,h+k+l$ 0.015 for $h+k+l,-h,-k$ 0.270 for $l,k,-h-k-l$ 0.270 for $-h-k-l,k,h$ 0.015 for $h,-h-k-l,k$ 0.015 for $h,l,-h-k-l$ 0.013 for $-h-k-l,h,l$ 0.013 for $k,-h-k-l,l$ 0.013 for l,h,k 0.013 for k,l,h 0.015 for $k,h,-h-k-l$ 0.017 for $-k,-h,-l$ 0.016 for $-h-k-l,l,k$ 0.016 for $-h,-l,-k$ 0.015 for $l,-h-k-l,h$ 0.035 for $-l,-k,-h$ 0.039 for $-h,-k,h+k+l$ 0.030 for $h+k+l,-k,-l$ 0.014 for $-h,h+k+l,-l$	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12244	wwPDB-VP
Average B, all atoms (\AA^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/2180	0.77	10/2954 (0.3%)
1	B	0.42	0/2141	0.62	1/2898 (0.0%)
1	E	0.38	0/2152	0.68	6/2913 (0.2%)
2	C	0.82	0/1975	1.05	10/2677 (0.4%)
2	D	0.80	0/2006	1.10	14/2715 (0.5%)
2	F	0.83	0/1997	1.12	24/2702 (0.9%)
All	All	0.65	0/12451	0.90	65/16859 (0.4%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	230	ARG	N-CA-C	-9.53	85.27	111.00
2	F	27	PRO	CA-N-CD	-9.49	98.21	111.50
2	D	40	PRO	N-CA-C	-9.49	87.43	112.10
2	F	250	MET	CB-CA-C	-9.45	91.51	110.40
2	F	66	PRO	CB-CA-C	-8.50	90.75	112.00
2	F	93	PHE	N-CA-C	8.37	133.60	111.00
1	E	94	ASP	CB-CA-C	8.36	127.12	110.40
1	A	138	ALA	CB-CA-C	8.28	122.52	110.10
2	D	175	GLY	N-CA-C	-8.21	92.57	113.10
1	A	60	VAL	CB-CA-C	-7.99	96.22	111.40
2	D	280	LEU	C-N-CD	7.81	144.81	128.40
2	D	158	THR	CB-CA-C	-7.66	90.93	111.60
2	D	72	PRO	CA-N-CD	-7.61	100.85	111.50
2	C	64	GLY	N-CA-C	7.39	131.57	113.10
2	F	133	THR	C-N-CD	-7.35	104.43	120.60
2	D	270	ARG	N-CA-C	7.23	130.51	111.00
2	F	251	ASP	N-CA-C	-7.14	91.71	111.00
2	F	51	ALA	N-CA-C	6.91	129.66	111.00
2	D	276	GLY	N-CA-C	-6.64	96.50	113.10
2	F	158	THR	N-CA-C	-6.61	93.16	111.00
2	C	26	THR	N-CA-C	6.51	128.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	27	PRO	C-N-CA	6.48	137.90	121.70
1	A	288	GLU	CB-CA-C	-6.45	97.49	110.40
1	A	29	PRO	N-CA-C	6.44	128.84	112.10
1	E	96	ARG	N-CA-C	-6.33	93.92	111.00
2	C	132	HIS	N-CA-C	-6.25	94.12	111.00
2	C	93	PHE	N-CA-C	6.25	127.86	111.00
2	C	238	MET	N-CA-C	6.13	127.55	111.00
1	A	139	ASP	N-CA-CB	-6.02	99.76	110.60
2	D	281	PRO	CA-N-CD	-5.96	103.16	111.50
1	E	95	LEU	N-CA-CB	-5.95	98.49	110.40
2	D	169	ALA	N-CA-C	-5.93	94.98	111.00
2	F	93	PHE	CB-CA-C	-5.92	98.56	110.40
2	D	137	ASP	N-CA-C	5.87	126.86	111.00
2	F	230	ARG	C-N-CA	5.87	136.37	121.70
2	D	137	ASP	C-N-CD	5.82	140.62	128.40
1	A	29	PRO	C-N-CD	5.81	140.60	128.40
2	F	71	LEU	C-N-CD	5.78	140.54	128.40
2	F	40	PRO	CA-N-CD	-5.76	103.44	111.50
1	E	90	MET	N-CA-C	5.73	126.48	111.00
2	C	93	PHE	CB-CA-C	-5.66	99.09	110.40
1	B	167	VAL	O-C-N	5.64	131.72	122.70
1	A	48	VAL	CB-CA-C	-5.60	100.76	111.40
1	A	139	ASP	N-CA-C	5.57	126.05	111.00
1	A	288	GLU	N-CA-C	5.57	126.05	111.00
2	C	26	THR	CB-CA-C	-5.53	96.67	111.60
2	D	274	LYS	O-C-N	5.37	131.29	122.70
2	F	250	MET	N-CA-C	5.34	125.42	111.00
2	F	137	ASP	C-N-CD	5.31	139.55	128.40
2	F	60	CYS	CA-CB-SG	-5.26	104.54	114.00
2	F	275	TYR	N-CA-C	5.21	125.08	111.00
2	C	207	ASP	CB-CG-OD2	5.21	122.99	118.30
2	F	55	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	A	97	ARG	N-CA-C	-5.19	97.00	111.00
2	C	133	THR	N-CA-C	-5.17	97.03	111.00
1	E	90	MET	CB-CA-C	-5.17	100.06	110.40
2	D	270	ARG	CB-CA-C	-5.15	100.10	110.40
2	F	270	ARG	N-CA-C	-5.15	97.11	111.00
2	C	52	PRO	C-N-CD	5.14	139.19	128.40
2	F	50	ARG	N-CA-C	5.13	124.86	111.00
1	E	92	ASP	N-CA-C	5.07	124.69	111.00
2	F	52	PRO	C-N-CD	5.06	139.03	128.40
2	F	274	LYS	N-CA-C	5.03	124.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	51	ALA	C-N-CD	5.03	138.96	128.40
2	F	72	PRO	CA-N-CD	-5.00	104.50	111.50

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	2142	0	2138	127	0
1	B	2105	0	2107	111	2
1	E	2117	0	2110	74	0
2	C	1941	0	1943	285	0
2	D	1973	0	1984	357	0
2	F	1966	0	1977	377	2
All	All	12244	0	12259	1281	2

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 (1281) 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:49:ARG:HH12	1:A:78:HIS:CD2	1.08	1.62
2:D:264:ALA:CB	2:D:283:TYR:CE1	1.81	1.59
1:A:49:ARG:NH1	1:A:78:HIS:CD2	1.74	1.51
2:D:264:ALA:HB1	2:D:283:TYR:CZ	1.45	1.51
1:A:49:ARG:NH1	1:A:78:HIS:CG	1.78	1.51
2:F:69:ALA:CB	2:F:201:LEU:HD23	1.43	1.47
1:B:94:ASP:O	1:B:101:THR:CG2	1.65	1.42
2:F:63:LEU:CD1	2:F:204:ALA:HB2	1.45	1.42
2:C:186:LYS:CE	2:C:237:LYS:HE3	1.46	1.42
2:C:186:LYS:HZ1	2:C:237:LYS:CE	1.32	1.41
2:F:69:ALA:HB1	2:F:201:LEU:CD2	1.50	1.38
2:C:18:LEU:CD2	2:C:75:VAL:HG13	1.55	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:283:TYR:O	2:F:286:VAL:CG1	1.73	1.36
2:C:265:LYS:CG	2:C:283:TYR:HE2	1.39	1.36
2:C:17:GLU:OE2	2:C:128:HIS:NE2	1.58	1.35
2:F:25:ARG:HG2	2:F:31:HIS:ND1	1.39	1.33
1:B:95:LEU:HD12	1:B:99:LYS:O	1.26	1.33
2:D:264:ALA:HB1	2:D:283:TYR:OH	1.29	1.33
2:F:60:CYS:SG	2:F:65:ALA:CB	2.17	1.32
1:A:94:ASP:O	1:A:101:THR:HG23	1.20	1.30
2:F:250:MET:O	2:F:254:LEU:CD2	1.81	1.29
1:A:49:ARG:HH12	1:A:78:HIS:CG	1.42	1.29
2:D:228:ASP:HB3	2:D:239:ARG:NH1	1.46	1.29
1:A:94:ASP:O	1:A:101:THR:CG2	1.79	1.29
2:D:264:ALA:CB	2:D:283:TYR:HE1	1.27	1.28
2:D:264:ALA:HB1	2:D:283:TYR:CE1	1.55	1.27
2:D:278:ARG:O	2:D:281:PRO:HD2	1.34	1.27
2:D:63:LEU:CD1	2:D:204:ALA:HB2	1.63	1.26
2:D:228:ASP:OD2	2:D:242:ALA:HB1	1.09	1.25
1:E:94:ASP:O	1:E:101:THR:HG23	1.11	1.25
2:D:228:ASP:OD2	2:D:242:ALA:CB	1.83	1.25
1:B:99:LYS:NZ	1:B:101:THR:HA	1.50	1.24
2:C:186:LYS:NZ	2:C:237:LYS:CE	2.01	1.23
2:D:273:ASP:HB3	2:D:275:TYR:N	1.51	1.23
1:A:44:GLY:O	1:A:47:ARG:NH1	1.71	1.22
2:D:278:ARG:O	2:D:281:PRO:CD	1.86	1.22
2:C:80:LEU:CD1	2:C:155:VAL:HG21	1.70	1.21
2:F:10:LEU:CD1	2:F:57:VAL:HG21	1.71	1.21
2:C:62:LEU:HD22	2:C:63:LEU:N	1.54	1.21
2:C:17:GLU:OE2	2:C:128:HIS:CE1	1.94	1.20
2:D:180:MET:CB	2:D:243:SER:OG	1.89	1.20
2:C:265:LYS:CG	2:C:283:TYR:CE2	2.26	1.19
2:F:25:ARG:CG	2:F:31:HIS:CE1	2.26	1.19
2:D:264:ALA:HB3	2:D:283:TYR:CE1	1.54	1.18
2:C:210:ALA:O	2:C:214:ARG:HG3	1.44	1.18
2:D:270:ARG:NH1	2:D:271:PHE:CE2	2.13	1.17
2:C:18:LEU:CD2	2:C:75:VAL:CG1	2.23	1.17
2:D:224:GLN:NE2	2:D:239:ARG:HD3	1.56	1.17
2:C:186:LYS:NZ	2:C:237:LYS:HE3	1.56	1.17
2:F:244:VAL:HG12	2:F:248:LEU:HG	1.25	1.16
2:D:270:ARG:HG3	2:D:271:PHE:N	1.56	1.15
2:F:173:ALA:CB	2:F:179:VAL:HG22	1.76	1.15
2:F:187:PHE:CD2	2:F:224:GLN:HB2	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ARG:NH1	2:D:52:PRO:HG3	1.61	1.14
2:F:63:LEU:HD13	2:F:204:ALA:HB2	1.15	1.14
2:F:228:ASP:CB	2:F:243:SER:O	1.96	1.13
1:A:49:ARG:HH12	1:A:78:HIS:CE1	1.66	1.13
2:D:180:MET:HB2	2:D:243:SER:OG	1.42	1.13
2:F:250:MET:O	2:F:254:LEU:HD23	0.97	1.13
2:C:75:VAL:HG12	2:C:79:MET:HE2	1.31	1.13
2:C:265:LYS:HG2	2:C:283:TYR:CE2	1.85	1.12
2:C:18:LEU:HD21	2:C:75:VAL:HG13	1.25	1.12
2:D:129:VAL:O	2:D:133:THR:HG23	1.46	1.12
2:F:187:PHE:CD2	2:F:224:GLN:CB	2.14	1.12
2:D:63:LEU:HD13	2:D:204:ALA:HB2	1.21	1.11
2:F:34:MET:O	2:F:37:ALA:HB3	1.46	1.11
2:F:25:ARG:HG3	2:F:31:HIS:CE1	1.84	1.11
2:F:209:GLU:HA	2:F:212:LEU:HD22	1.16	1.11
2:F:243:SER:HB3	2:F:246:ARG:HG3	1.28	1.11
2:C:4:ARG:HG3	2:C:278:ARG:HH21	1.08	1.11
2:C:277:GLU:O	2:C:281:PRO:HD3	1.50	1.10
2:F:187:PHE:HD2	2:F:224:GLN:CB	1.39	1.10
2:C:265:LYS:HG3	2:C:283:TYR:HE2	1.17	1.10
1:E:34:HIS:NE2	2:F:157:SER:OG	1.82	1.10
2:C:18:LEU:HD23	2:C:75:VAL:HG13	1.29	1.09
2:C:18:LEU:HD23	2:C:75:VAL:CG1	1.83	1.09
1:B:165:GLN:O	1:B:169:LEU:CD1	2.01	1.08
2:C:186:LYS:HZ1	2:C:237:LYS:HE2	1.00	1.08
1:E:94:ASP:O	1:E:101:THR:CG2	2.01	1.08
2:D:174:LEU:HG	2:D:175:GLY:HA2	1.31	1.08
2:F:10:LEU:HD21	2:F:54:VAL:HA	1.15	1.07
2:C:4:ARG:HG3	2:C:278:ARG:NH2	1.70	1.06
2:F:6:TYR:OH	2:F:61:GLU:OE1	1.73	1.06
2:F:173:ALA:HB1	2:F:179:VAL:HG22	1.33	1.06
2:D:215:TYR:CE1	2:D:283:TYR:OH	2.08	1.05
2:D:228:ASP:CB	2:D:239:ARG:NH1	2.20	1.05
1:A:233:ILE:O	1:A:236:VAL:HG12	1.55	1.05
1:B:95:LEU:CD1	1:B:99:LYS:O	2.04	1.05
2:D:270:ARG:HG3	2:D:271:PHE:H	0.90	1.04
2:D:10:LEU:HD23	2:D:54:VAL:HG13	1.34	1.04
2:D:264:ALA:CB	2:D:283:TYR:CZ	2.22	1.04
2:F:25:ARG:CG	2:F:31:HIS:ND1	2.19	1.04
2:D:224:GLN:HE21	2:D:239:ARG:CD	1.70	1.04
2:C:4:ARG:CG	2:C:278:ARG:HH21	1.71	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:244:VAL:CG1	2:F:248:LEU:HG	1.87	1.03
2:D:224:GLN:NE2	2:D:239:ARG:CD	2.20	1.03
2:F:60:CYS:SG	2:F:65:ALA:HB1	1.98	1.03
2:C:186:LYS:CE	2:C:237:LYS:CE	2.33	1.03
2:C:80:LEU:HD12	2:C:155:VAL:HG21	1.33	1.03
2:D:273:ASP:CB	2:D:275:TYR:N	2.21	1.03
2:F:160:MET:O	2:F:164:GLN:HG3	1.59	1.03
1:B:99:LYS:HZ2	1:B:101:THR:HA	0.97	1.02
2:F:10:LEU:HD11	2:F:57:VAL:CG2	1.90	1.02
2:D:278:ARG:C	2:D:281:PRO:HD2	1.79	1.02
2:D:233:SER:H	2:D:234:GLY:HA2	1.24	1.02
2:C:186:LYS:HE3	2:C:237:LYS:CE	1.90	1.02
2:C:62:LEU:HD21	2:C:63:LEU:HD23	1.41	1.01
2:F:157:SER:O	2:F:162:ALA:HB2	1.58	1.01
2:C:274:LYS:HB3	2:C:275:TYR:HA	1.41	1.01
2:F:10:LEU:CD2	2:F:54:VAL:HA	1.89	1.01
1:E:263:GLY:HA3	1:E:266:LYS:HD3	1.42	1.01
2:F:10:LEU:HD11	2:F:57:VAL:HG21	1.05	1.00
2:F:228:ASP:HB3	2:F:243:SER:O	1.58	1.00
2:C:24:ILE:HD12	2:C:24:ILE:H	1.21	1.00
2:F:239:ARG:H	2:F:239:ARG:HD2	1.25	1.00
2:F:63:LEU:CD1	2:F:204:ALA:CB	2.39	1.00
2:F:252:ARG:CZ	2:F:256:ILE:HD13	1.91	0.99
2:F:252:ARG:NH1	2:F:259:GLU:OE2	1.95	0.99
2:C:153:ARG:NH1	2:C:189:GLU:OE2	1.96	0.99
2:C:186:LYS:HE3	2:C:237:LYS:HE3	1.04	0.99
2:F:132:HIS:O	2:F:134:PRO:HD3	1.61	0.99
2:C:67:ARG:O	2:C:69:ALA:N	1.96	0.98
1:A:49:ARG:HH11	1:A:78:HIS:CG	1.70	0.98
2:C:80:LEU:HD12	2:C:155:VAL:CG2	1.93	0.98
2:C:278:ARG:O	2:C:281:PRO:HD2	1.62	0.98
1:A:13:ALA:O	1:A:17:ASN:ND2	1.95	0.98
2:D:224:GLN:HE21	2:D:239:ARG:HD3	0.84	0.98
2:C:5:LEU:O	2:C:8:THR:N	1.95	0.98
2:D:63:LEU:HD13	2:D:204:ALA:CB	1.93	0.98
2:D:6:TYR:OH	2:D:61:GLU:OE1	1.80	0.98
2:F:209:GLU:HA	2:F:212:LEU:CD2	1.94	0.98
2:C:5:LEU:O	2:C:8:THR:OG1	1.81	0.97
1:A:49:ARG:NH1	1:A:78:HIS:ND1	2.11	0.97
2:D:132:HIS:O	2:D:134:PRO:HD3	1.63	0.97
2:F:196:ALA:CB	2:F:213:ARG:NH2	2.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:NH1	1:A:78:HIS:CE1	2.27	0.96
2:F:154:ALA:HB2	2:F:193:CYS:SG	2.05	0.96
2:F:243:SER:H	2:F:244:VAL:HA	1.26	0.96
2:F:246:ARG:O	2:F:248:LEU:HD23	1.66	0.96
2:C:27:PRO:O	2:C:31:HIS:CD2	2.18	0.96
2:C:52:PRO:O	2:C:194:SER:OG	1.83	0.96
2:D:63:LEU:CD1	2:D:204:ALA:CB	2.43	0.96
1:B:94:ASP:O	1:B:101:THR:HG23	0.78	0.96
2:F:283:TYR:O	2:F:286:VAL:HG12	0.77	0.95
2:D:174:LEU:HD12	2:D:247:ALA:O	1.67	0.95
2:D:278:ARG:CA	2:D:281:PRO:HD2	1.96	0.95
2:C:192:GLU:OE2	2:C:213:ARG:NE	1.98	0.95
2:C:62:LEU:CD2	2:C:63:LEU:HD23	1.96	0.95
1:B:166:VAL:CG1	2:D:113:MET:SD	2.55	0.95
2:D:50:ARG:HE	2:D:53:PRO:HD3	1.32	0.94
1:A:158:SER:OG	2:C:31:HIS:NE2	2.00	0.94
2:D:215:TYR:HE1	2:D:283:TYR:CZ	1.86	0.94
2:F:50:ARG:HG2	2:F:52:PRO:CD	1.98	0.94
2:D:85:LEU:HA	2:D:237:LYS:NZ	1.82	0.94
2:F:55:LEU:HD11	2:F:194:SER:OG	1.65	0.94
2:C:10:LEU:HD21	2:C:57:VAL:HG21	1.46	0.94
2:F:184:THR:O	2:F:188:GLY:N	2.00	0.94
2:F:69:ALA:HB1	2:F:201:LEU:CG	1.97	0.93
2:D:270:ARG:CG	2:D:271:PHE:H	1.80	0.93
1:E:261:LEU:O	1:E:262:LEU:HD23	1.67	0.93
2:C:265:LYS:HG3	2:C:283:TYR:CE2	2.00	0.93
2:F:62:LEU:HD22	2:F:63:LEU:CD2	1.99	0.93
2:F:209:GLU:CA	2:F:212:LEU:HD22	1.99	0.93
2:D:215:TYR:CD1	2:D:283:TYR:OH	2.22	0.93
2:F:63:LEU:HD11	2:F:204:ALA:HB2	1.51	0.93
1:B:94:ASP:C	1:B:101:THR:HG23	1.89	0.92
2:D:270:ARG:NH1	2:D:271:PHE:CD2	2.37	0.92
2:D:174:LEU:CG	2:D:175:GLY:HA2	1.99	0.92
2:F:25:ARG:HG3	2:F:31:HIS:HE1	1.23	0.92
1:B:99:LYS:HZ2	1:B:101:THR:CA	1.82	0.91
2:F:215:TYR:CZ	2:F:279:VAL:HB	2.06	0.91
2:D:224:GLN:HE22	2:D:239:ARG:NE	1.68	0.91
2:F:68:GLU:HB3	2:F:134:PRO:HG2	1.49	0.91
2:D:278:ARG:O	2:D:281:PRO:N	2.02	0.91
2:D:25:ARG:HG2	2:D:31:HIS:ND1	1.86	0.91
2:F:55:LEU:CD1	2:F:194:SER:OG	2.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:ASP:HB3	2:D:239:ARG:HH11	1.08	0.90
2:F:62:LEU:CD2	2:F:63:LEU:HD23	2.01	0.90
2:C:52:PRO:HG2	2:C:53:PRO:HD3	1.54	0.90
2:D:140:PRO:HG2	2:D:143:VAL:CG2	2.00	0.90
2:F:25:ARG:HG2	2:F:31:HIS:CE1	1.97	0.90
1:B:166:VAL:HG11	2:D:113:MET:HE1	1.50	0.90
2:D:264:ALA:CB	2:D:283:TYR:OH	2.15	0.90
2:F:244:VAL:HG12	2:F:248:LEU:CG	2.02	0.90
2:F:60:CYS:SG	2:F:65:ALA:HB3	2.07	0.90
2:F:69:ALA:HB1	2:F:201:LEU:HD23	0.92	0.90
2:D:85:LEU:HA	2:D:237:LYS:HZ3	1.37	0.90
2:C:204:ALA:HB1	2:C:208:GLU:HG2	1.53	0.90
2:F:250:MET:CG	2:F:250:MET:O	2.18	0.90
2:D:180:MET:HB3	2:D:243:SER:OG	1.68	0.90
2:F:156:GLY:O	2:F:161:ALA:HB3	1.72	0.90
2:F:69:ALA:CA	2:F:201:LEU:HD23	2.01	0.90
2:F:85:LEU:HA	2:F:237:LYS:NZ	1.87	0.90
2:D:242:ALA:O	2:D:245:LEU:N	2.05	0.89
2:D:273:ASP:HB3	2:D:275:TYR:CA	2.01	0.89
2:D:270:ARG:HH12	2:D:271:PHE:HE2	0.96	0.89
1:E:237:THR:O	1:E:238:LYS:O	1.89	0.89
2:D:225:LEU:HD13	2:D:244:VAL:HG11	1.54	0.89
2:D:286:VAL:O	2:D:288:TYR:HA	1.73	0.89
2:F:250:MET:HG3	2:F:250:MET:O	1.72	0.89
2:C:75:VAL:HG12	2:C:79:MET:CE	2.02	0.89
2:F:243:SER:HB2	2:F:245:LEU:N	1.87	0.89
2:C:204:ALA:HB1	2:C:208:GLU:CG	2.02	0.89
2:D:273:ASP:HA	2:D:274:LYS:HB2	1.55	0.89
2:F:34:MET:O	2:F:37:ALA:CB	2.20	0.89
2:D:273:ASP:HA	2:D:274:LYS:CB	2.01	0.88
2:F:177:ALA:O	2:F:180:MET:N	2.05	0.88
2:C:283:TYR:O	2:C:286:VAL:HG12	1.73	0.88
2:F:277:GLU:O	2:F:279:VAL:N	2.06	0.88
1:A:162:VAL:O	1:A:166:VAL:HG23	1.74	0.88
2:D:224:GLN:NE2	2:D:239:ARG:NE	2.21	0.88
2:D:143:VAL:O	2:D:147:VAL:HG23	1.72	0.88
2:C:52:PRO:HG2	2:C:53:PRO:CD	2.04	0.87
2:F:243:SER:N	2:F:244:VAL:HA	1.83	0.87
2:F:55:LEU:HD12	2:F:56:CYS:N	1.90	0.87
1:B:95:LEU:HD11	1:B:99:LYS:N	1.90	0.87
2:F:247:ALA:C	2:F:248:LEU:HD22	1.94	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:264:ALA:HB2	2:D:283:TYR:HE1	1.34	0.87
2:F:68:GLU:O	2:F:72:PRO:CD	2.22	0.86
2:D:215:TYR:HE1	2:D:283:TYR:OH	1.56	0.86
1:B:170:GLU:OE2	1:B:171:MET:N	2.07	0.86
2:F:60:CYS:SG	2:F:65:ALA:HB2	2.14	0.86
1:A:34:HIS:NE2	2:C:157:SER:OG	1.94	0.86
2:D:63:LEU:HD11	2:D:204:ALA:HB2	1.56	0.86
1:A:94:ASP:OD1	1:A:95:LEU:N	2.08	0.85
2:C:206:PRO:HA	2:C:209:GLU:HB2	1.57	0.85
2:D:278:ARG:HA	2:D:281:PRO:CD	2.05	0.85
2:F:52:PRO:O	2:F:194:SER:OG	1.94	0.85
2:F:73:ALA:O	2:F:77:LEU:HD12	1.77	0.85
2:D:255:GLY:O	2:D:259:GLU:HG3	1.75	0.85
2:D:50:ARG:HE	2:D:52:PRO:HG2	1.41	0.85
2:C:277:GLU:O	2:C:281:PRO:CD	2.24	0.85
2:D:50:ARG:HH11	2:D:52:PRO:HG3	1.38	0.85
2:F:50:ARG:HG2	2:F:52:PRO:HD2	1.57	0.85
2:D:181:LYS:O	2:D:184:THR:OG1	1.95	0.85
2:F:68:GLU:O	2:F:72:PRO:HD2	1.76	0.85
2:C:283:TYR:HD1	2:C:284:SER:N	1.75	0.85
1:A:94:ASP:O	1:A:101:THR:CB	2.25	0.84
2:F:252:ARG:CZ	2:F:256:ILE:CD1	2.54	0.84
2:F:75:VAL:HG11	2:F:128:HIS:CE1	2.13	0.84
2:D:52:PRO:HG2	2:D:53:PRO:CD	2.07	0.84
2:F:196:ALA:HB2	2:F:213:ARG:HH21	1.40	0.84
2:F:277:GLU:HB2	2:F:280:LEU:HD12	1.59	0.83
2:F:242:ALA:HB2	2:F:246:ARG:NE	1.91	0.83
2:D:67:ARG:HH11	2:D:67:ARG:HG2	1.40	0.83
2:C:283:TYR:O	2:C:286:VAL:CG1	2.26	0.83
2:C:129:VAL:HG11	2:C:148:LEU:CD2	2.09	0.83
2:D:174:LEU:HD23	2:D:175:GLY:CA	2.09	0.83
2:F:184:THR:O	2:F:188:GLY:CA	2.25	0.83
2:C:186:LYS:C	2:C:186:LYS:HD3	2.00	0.83
2:F:11:ILE:O	2:F:14:VAL:HG12	1.78	0.83
2:F:243:SER:CB	2:F:246:ARG:H	1.92	0.82
2:D:174:LEU:HD23	2:D:175:GLY:N	1.94	0.82
2:D:238:MET:SD	2:D:239:ARG:NH2	2.52	0.82
2:D:179:VAL:O	2:D:182:VAL:HG23	1.79	0.82
2:F:10:LEU:CD2	2:F:54:VAL:HG13	2.09	0.82
2:C:18:LEU:HD21	2:C:75:VAL:CG1	1.96	0.82
1:E:231:ASP:OD1	1:E:303:ARG:NH2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:GLU:OE2	2:C:271:PHE:HZ	1.63	0.82
2:D:278:ARG:HA	2:D:281:PRO:HD2	1.59	0.82
2:D:52:PRO:HG2	2:D:53:PRO:HD3	1.59	0.82
2:F:187:PHE:HD2	2:F:224:GLN:HB2	1.19	0.82
1:B:95:LEU:CD1	1:B:99:LYS:C	2.48	0.81
2:D:25:ARG:HG2	2:D:31:HIS:CE1	2.14	0.81
2:F:239:ARG:CD	2:F:239:ARG:H	1.92	0.81
2:D:179:VAL:HB	2:D:180:MET:CE	2.10	0.81
2:C:181:LYS:O	2:C:184:THR:OG1	1.99	0.81
2:F:173:ALA:HB3	2:F:179:VAL:HG22	1.60	0.81
2:F:50:ARG:O	2:F:51:ALA:HB3	1.78	0.81
2:C:176:GLU:CD	2:C:179:VAL:HG21	2.00	0.81
2:D:52:PRO:O	2:D:194:SER:OG	1.98	0.81
2:F:177:ALA:O	2:F:179:VAL:N	2.14	0.81
2:F:173:ALA:HB1	2:F:179:VAL:CG2	2.11	0.80
2:F:252:ARG:O	2:F:256:ILE:HG12	1.81	0.80
2:C:25:ARG:O	2:C:31:HIS:ND1	2.13	0.80
1:A:272:GLU:HG2	2:D:24:ILE:CD1	2.12	0.80
1:B:166:VAL:HG13	2:D:113:MET:SD	2.21	0.80
2:C:129:VAL:HG11	2:C:148:LEU:HD21	1.63	0.80
2:D:68:GLU:O	2:D:72:PRO:HD2	1.80	0.80
1:A:46:LYS:HG3	1:A:48:VAL:CG2	2.11	0.80
2:F:87:HIS:O	2:F:90:LEU:HD12	1.82	0.80
2:F:69:ALA:C	2:F:201:LEU:HD23	2.02	0.80
2:C:144:LEU:O	2:C:144:LEU:HD23	1.82	0.79
2:D:140:PRO:HG2	2:D:143:VAL:HB	1.63	0.79
2:D:180:MET:HB2	2:D:243:SER:HG	1.46	0.79
2:D:288:TYR:CD1	2:D:289:ALA:N	2.49	0.79
2:D:5:LEU:HD22	2:D:5:LEU:O	1.83	0.79
2:F:141:HIS:O	2:F:144:LEU:N	2.15	0.79
2:C:72:PRO:HB2	2:C:133:THR:OG1	1.83	0.79
2:D:50:ARG:NE	2:D:52:PRO:HG2	1.98	0.79
2:F:63:LEU:HD13	2:F:204:ALA:CB	2.07	0.78
2:F:85:LEU:HA	2:F:237:LYS:HZ3	1.47	0.78
2:F:168:LEU:O	2:F:168:LEU:HD13	1.83	0.78
2:F:185:LYS:HD2	2:F:189:GLU:HG3	1.65	0.78
2:D:167:ASP:O	2:D:169:ALA:C	2.22	0.78
2:D:215:TYR:HE1	2:D:283:TYR:CE2	2.00	0.78
2:F:228:ASP:OD2	2:F:243:SER:O	2.01	0.78
2:F:177:ALA:O	2:F:178:GLU:C	2.20	0.78
1:B:99:LYS:NZ	1:B:101:THR:CA	2.41	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:ARG:CA	2:D:281:PRO:CD	2.60	0.78
2:C:265:LYS:HG2	2:C:283:TYR:CD2	2.19	0.78
2:F:62:LEU:CD2	2:F:63:LEU:CD2	2.59	0.77
2:F:7:TRP:HH2	2:F:51:ALA:HB2	1.48	0.77
1:A:50:PRO:HG3	1:A:75:GLU:HB2	1.66	0.77
2:D:228:ASP:CB	2:D:239:ARG:HH11	1.91	0.77
2:D:180:MET:CE	2:D:180:MET:H	1.96	0.77
2:F:173:ALA:CB	2:F:179:VAL:CG2	2.61	0.77
2:F:246:ARG:O	2:F:248:LEU:CD2	2.32	0.77
2:D:22:MET:O	2:D:35:ARG:HD3	1.85	0.77
2:D:273:ASP:CB	2:D:275:TYR:CA	2.62	0.77
1:B:170:GLU:OE2	1:B:171:MET:HG3	1.85	0.77
2:C:4:ARG:CB	2:C:278:ARG:HH21	1.97	0.77
2:C:59:ALA:O	2:C:62:LEU:HD12	1.85	0.77
2:D:50:ARG:NH1	2:D:52:PRO:CG	2.45	0.77
2:C:30:ILE:HG23	2:C:31:HIS:HD2	1.49	0.76
2:C:72:PRO:HG2	2:C:133:THR:N	1.99	0.76
2:D:179:VAL:HB	2:D:180:MET:HE2	1.65	0.76
2:C:67:ARG:C	2:C:69:ALA:N	2.35	0.76
2:F:222:LEU:HG	2:F:286:VAL:HG21	1.66	0.76
2:D:215:TYR:CE1	2:D:283:TYR:CZ	2.70	0.76
1:E:214:GLU:HG3	1:E:217:ARG:HE	1.50	0.76
2:F:137:ASP:OD1	2:F:138:PRO:HD2	1.85	0.76
2:D:3:LEU:CD1	2:D:278:ARG:HD2	2.15	0.76
1:A:94:ASP:O	1:A:101:THR:OG1	2.04	0.76
2:D:174:LEU:CD1	2:D:247:ALA:O	2.33	0.76
2:F:62:LEU:HD23	2:F:63:LEU:HD23	1.65	0.76
2:D:10:LEU:O	2:D:10:LEU:HD12	1.86	0.76
2:F:50:ARG:HG2	2:F:52:PRO:HD3	1.65	0.76
1:A:20:LEU:HD13	1:A:41:LEU:HD11	1.66	0.75
2:F:7:TRP:CH2	2:F:51:ALA:HB2	2.21	0.75
2:D:224:GLN:HE22	2:D:239:ARG:HE	1.31	0.75
2:D:57:VAL:HA	2:D:70:ALA:HB1	1.68	0.75
2:F:245:LEU:HD23	2:F:245:LEU:N	2.00	0.75
2:C:135:SER:HB2	2:C:141:HIS:CE1	2.21	0.75
2:D:50:ARG:HB2	2:D:50:ARG:NH2	2.01	0.75
2:D:140:PRO:HG2	2:D:143:VAL:CB	2.16	0.75
2:F:250:MET:SD	2:F:250:MET:O	2.43	0.75
2:C:10:LEU:HD21	2:C:57:VAL:CG2	2.16	0.75
2:D:63:LEU:HD11	2:D:204:ALA:CB	2.15	0.75
2:F:60:CYS:O	2:F:65:ALA:HB3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:ASP:OD2	2:C:138:PRO:HD3	1.87	0.75
2:D:3:LEU:HD12	2:D:278:ARG:HD2	1.69	0.75
2:F:129:VAL:O	2:F:133:THR:HG23	1.87	0.75
2:C:248:LEU:N	2:C:248:LEU:HD13	2.03	0.74
2:D:180:MET:H	2:D:180:MET:HE3	1.52	0.74
2:D:228:ASP:CB	2:D:239:ARG:HH12	2.00	0.74
2:F:62:LEU:HD22	2:F:63:LEU:HD21	1.69	0.74
2:C:93:PHE:CE2	2:C:168:LEU:HD21	2.22	0.74
2:F:57:VAL:HA	2:F:70:ALA:HB1	1.70	0.74
1:A:46:LYS:HG3	1:A:48:VAL:HG23	1.68	0.74
2:D:283:TYR:O	2:D:286:VAL:HG12	1.87	0.74
2:C:250:MET:O	2:C:251:ASP:C	2.26	0.74
2:C:62:LEU:HD22	2:C:63:LEU:H	1.53	0.74
1:B:99:LYS:HZ1	1:B:101:THR:HA	1.50	0.74
1:B:166:VAL:HG11	2:D:113:MET:CE	2.18	0.74
1:B:163:ALA:HB1	2:D:27:PRO:HG3	1.70	0.74
2:D:208:GLU:OE1	2:D:270:ARG:NH2	2.21	0.73
2:D:18:LEU:HD11	2:D:78:GLU:HG2	1.69	0.73
2:C:72:PRO:HG2	2:C:133:THR:H	1.53	0.73
2:C:208:GLU:OE2	2:C:271:PHE:CZ	2.41	0.73
1:E:16:VAL:HG21	1:E:50:PRO:HB3	1.68	0.73
2:F:36:TYR:OH	2:F:103:PRO:HD2	1.87	0.73
2:F:196:ALA:HB2	2:F:213:ARG:NH2	2.00	0.73
2:D:273:ASP:CB	2:D:275:TYR:H	1.99	0.73
2:D:73:ALA:O	2:D:77:LEU:HD12	1.89	0.73
2:F:26:THR:OG1	2:F:27:PRO:HD2	1.89	0.73
2:C:183:LEU:O	2:C:188:GLY:N	2.21	0.73
2:D:278:ARG:C	2:D:281:PRO:CD	2.46	0.73
2:D:50:ARG:NE	2:D:53:PRO:HD3	2.02	0.73
2:D:50:ARG:CZ	2:D:52:PRO:HG3	2.17	0.73
1:E:34:HIS:CD2	2:F:157:SER:OG	2.41	0.73
2:C:26:THR:HA	2:C:27:PRO:C	2.07	0.72
1:A:231:ASP:O	1:A:235:ASP:OD1	2.07	0.72
2:F:141:HIS:O	2:F:143:VAL:N	2.22	0.72
2:F:250:MET:HA	2:F:253:ALA:HB3	1.72	0.72
2:C:67:ARG:O	2:C:70:ALA:N	2.22	0.72
2:D:137:ASP:OD1	2:D:138:PRO:HD2	1.90	0.72
2:F:248:LEU:HB2	2:F:249:GLY:HA2	1.70	0.72
2:D:174:LEU:CD2	2:D:175:GLY:CA	2.67	0.72
2:C:129:VAL:CG1	2:C:148:LEU:HD21	2.20	0.72
2:D:129:VAL:O	2:D:133:THR:CG2	2.31	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ALA:N	2:D:52:PRO:CD	2.53	0.72
2:C:180:MET:HE3	2:C:242:ALA:O	1.89	0.72
2:D:233:SER:N	2:D:234:GLY:HA2	2.00	0.72
2:F:278:ARG:HA	2:F:281:PRO:HG2	1.71	0.72
1:B:214:GLU:HG3	1:B:215:SER:N	2.03	0.71
2:C:283:TYR:CE1	2:C:284:SER:OG	2.42	0.71
1:A:49:ARG:NH1	1:A:78:HIS:NE2	2.06	0.71
2:D:156:GLY:O	2:D:161:ALA:HB3	1.90	0.71
2:D:273:ASP:C	2:D:275:TYR:H	1.93	0.71
2:D:3:LEU:HD11	2:D:278:ARG:HH11	1.54	0.71
2:D:258:GLU:N	2:D:258:GLU:OE1	2.22	0.71
2:F:252:ARG:NH1	2:F:256:ILE:HD13	2.05	0.71
2:D:273:ASP:HB3	2:D:275:TYR:O	1.90	0.71
2:C:62:LEU:CD2	2:C:63:LEU:N	2.46	0.71
1:A:272:GLU:OE1	2:D:24:ILE:HD13	1.91	0.71
2:F:280:LEU:HB2	2:F:281:PRO:HD3	1.71	0.71
1:A:140:LYS:HG3	1:A:144:ARG:HE	1.55	0.71
2:F:228:ASP:CG	2:F:243:SER:O	2.28	0.71
1:A:286:ASP:HB3	1:A:288:GLU:HG3	1.71	0.71
1:B:167:VAL:O	1:B:170:GLU:HB3	1.90	0.70
2:F:215:TYR:OH	2:F:279:VAL:HB	1.89	0.70
2:F:24:ILE:HD12	2:F:24:ILE:O	1.90	0.70
1:A:49:ARG:HH12	1:A:78:HIS:NE2	1.26	0.70
2:C:67:ARG:C	2:C:69:ALA:H	1.93	0.70
2:D:67:ARG:HG2	2:D:67:ARG:NH1	2.05	0.70
2:F:60:CYS:O	2:F:65:ALA:CB	2.39	0.70
2:F:85:LEU:C	2:F:85:LEU:HD23	2.12	0.70
2:C:138:PRO:HG2	2:C:139:VAL:HG23	1.74	0.70
2:D:50:ARG:CZ	2:D:52:PRO:CG	2.70	0.70
2:C:56:CYS:HB2	2:C:194:SER:O	1.92	0.70
2:F:62:LEU:HD23	2:F:62:LEU:O	1.91	0.70
2:C:186:LYS:NZ	2:C:237:LYS:HE2	1.82	0.70
2:C:4:ARG:CG	2:C:278:ARG:NH2	2.44	0.70
1:B:165:GLN:O	1:B:169:LEU:HD11	1.91	0.70
2:D:277:GLU:O	2:D:280:LEU:HB2	1.92	0.70
1:E:100:PRO:HB2	1:E:104:VAL:HG21	1.72	0.70
2:F:26:THR:HG23	2:F:27:PRO:HG2	1.74	0.70
1:A:29:PRO:O	1:A:31:ALA:N	2.24	0.69
2:C:67:ARG:O	2:C:68:GLU:C	2.26	0.69
2:D:131:ALA:C	2:D:132:HIS:ND1	2.46	0.69
2:D:208:GLU:O	2:D:212:LEU:HD13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:160:MET:HG3	2:F:164:GLN:HE21	1.56	0.69
2:F:184:THR:O	2:F:188:GLY:HA3	1.91	0.69
2:C:35:ARG:O	2:C:39:LEU:HG	1.92	0.69
2:D:67:ARG:CG	2:D:67:ARG:HH11	2.05	0.69
1:A:279:ARG:NH2	2:D:108:ALA:O	2.24	0.69
2:F:62:LEU:C	2:F:62:LEU:HD23	2.13	0.69
2:F:245:LEU:HD23	2:F:245:LEU:H	1.56	0.69
2:D:174:LEU:CD2	2:D:175:GLY:HA2	2.23	0.69
2:C:186:LYS:O	2:C:186:LYS:HD3	1.92	0.69
1:B:237:THR:O	1:B:238:LYS:O	2.11	0.68
2:C:80:LEU:HD11	2:C:155:VAL:HG21	1.72	0.68
2:D:39:LEU:O	2:D:40:PRO:C	2.28	0.68
1:A:272:GLU:HG2	2:D:24:ILE:HD11	1.75	0.68
2:D:85:LEU:CA	2:D:237:LYS:NZ	2.55	0.68
2:F:68:GLU:O	2:F:72:PRO:HD3	1.94	0.68
2:D:167:ASP:O	2:D:169:ALA:N	2.27	0.68
1:E:39:TYR:HE2	1:E:102:CYS:HA	1.59	0.68
1:B:237:THR:O	1:B:238:LYS:C	2.33	0.68
2:C:39:LEU:H	2:C:40:PRO:CD	2.07	0.68
2:C:180:MET:CE	2:C:242:ALA:O	2.42	0.68
2:C:4:ARG:HB2	2:C:278:ARG:HH21	1.59	0.68
1:A:63:ARG:HH12	1:A:65:ALA:HB3	1.59	0.67
2:C:252:ARG:O	2:C:255:GLY:N	2.26	0.67
2:C:35:ARG:O	2:C:39:LEU:CG	2.42	0.67
2:F:134:PRO:HB2	2:F:138:PRO:CG	2.24	0.67
2:F:176:GLU:CD	2:F:252:ARG:HE	1.86	0.67
2:F:140:PRO:O	2:F:143:VAL:HB	1.94	0.67
2:F:10:LEU:CD1	2:F:57:VAL:CG2	2.61	0.67
2:F:242:ALA:CB	2:F:246:ARG:NE	2.56	0.67
2:D:35:ARG:C	2:D:37:ALA:H	1.98	0.67
1:A:138:ALA:O	1:A:142:PRO:CD	2.42	0.67
1:A:85:ASP:O	1:A:91:ASP:HB2	1.94	0.67
1:E:88:PRO:HA	1:E:92:ASP:HB2	1.77	0.67
2:F:243:SER:H	2:F:244:VAL:CA	2.01	0.67
2:F:85:LEU:HD23	2:F:86:VAL:N	2.09	0.67
2:D:208:GLU:O	2:D:212:LEU:HD22	1.94	0.67
2:D:50:ARG:NE	2:D:52:PRO:CG	2.58	0.67
1:B:165:GLN:O	1:B:169:LEU:HD13	1.90	0.67
1:B:99:LYS:HD2	1:B:99:LYS:C	2.15	0.67
2:F:160:MET:CG	2:F:164:GLN:HE21	2.07	0.66
2:F:62:LEU:HD22	2:F:63:LEU:HD23	1.66	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:HD2	1:B:99:LYS:O	1.95	0.66
2:C:208:GLU:O	2:C:208:GLU:HG3	1.95	0.66
2:D:167:ASP:O	2:D:169:ALA:O	2.14	0.66
2:D:233:SER:HB3	2:D:234:GLY:C	2.16	0.66
1:B:233:ILE:O	1:B:236:VAL:CG2	2.44	0.66
1:A:166:VAL:HG13	2:C:113:MET:SD	2.35	0.66
1:B:161:LEU:N	1:B:189:HIS:O	2.28	0.66
2:F:248:LEU:HD22	2:F:248:LEU:N	2.10	0.66
2:D:225:LEU:HD13	2:D:244:VAL:CG1	2.26	0.66
1:E:237:THR:O	1:E:238:LYS:C	2.31	0.66
2:F:60:CYS:HG	2:F:65:ALA:HB1	1.60	0.66
2:F:144:LEU:O	2:F:148:LEU:HG	1.94	0.66
2:F:196:ALA:HB1	2:F:213:ARG:NH2	2.11	0.66
2:D:273:ASP:HB3	2:D:274:LYS:C	2.17	0.66
2:C:227:ASP:C	2:C:229:ILE:H	2.00	0.66
2:F:173:ALA:C	2:F:179:VAL:CG2	2.63	0.66
2:C:57:VAL:O	2:C:61:GLU:HG2	1.97	0.65
2:D:173:ALA:O	2:D:243:SER:HB2	1.96	0.65
2:F:213:ARG:HH21	2:F:213:ARG:CG	2.09	0.65
1:A:257:THR:OG1	1:A:258:TYR:N	2.29	0.65
2:C:192:GLU:HG3	2:C:213:ARG:HG3	1.77	0.65
2:C:62:LEU:CD2	2:C:63:LEU:CD2	2.73	0.65
2:D:228:ASP:OD2	2:D:242:ALA:HB2	1.94	0.65
2:F:185:LYS:HD2	2:F:189:GLU:CG	2.25	0.65
2:F:277:GLU:O	2:F:281:PRO:HD2	1.96	0.65
2:D:233:SER:H	2:D:234:GLY:CA	2.06	0.65
2:D:85:LEU:CA	2:D:237:LYS:HZ1	2.09	0.65
1:E:182:ARG:HA	1:E:185:TYR:HB3	1.78	0.65
2:F:10:LEU:HD23	2:F:54:VAL:HG13	1.76	0.65
2:C:62:LEU:HD22	2:C:62:LEU:C	2.16	0.65
2:F:69:ALA:C	2:F:201:LEU:CD2	2.64	0.65
2:C:62:LEU:HD22	2:C:63:LEU:CA	2.26	0.65
2:C:241:ASN:OD1	2:C:242:ALA:N	2.30	0.65
2:C:72:PRO:CG	2:C:132:HIS:HB2	2.26	0.65
2:C:62:LEU:HD13	2:C:62:LEU:C	2.17	0.65
1:E:231:ASP:OD1	1:E:303:ARG:NH1	2.29	0.65
2:F:168:LEU:C	2:F:168:LEU:HD13	2.17	0.65
2:F:36:TYR:OH	2:F:103:PRO:HG2	1.95	0.65
2:F:69:ALA:CB	2:F:201:LEU:CD2	2.30	0.65
1:B:189:HIS:HA	1:B:193:ALA:HB2	1.77	0.65
2:F:242:ALA:HB2	2:F:246:ARG:CZ	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:HIS:HA	2:F:90:LEU:CD1	2.27	0.65
1:A:227:PHE:O	1:A:303:ARG:NH2	2.30	0.64
2:D:69:ALA:HB1	2:D:201:LEU:HD23	1.79	0.64
2:F:228:ASP:HB2	2:F:243:SER:O	1.95	0.64
1:A:49:ARG:CZ	1:A:78:HIS:CE1	2.79	0.64
2:D:50:ARG:HH11	2:D:52:PRO:CG	2.09	0.64
2:F:248:LEU:CB	2:F:249:GLY:HA2	2.27	0.64
1:B:21:ASP:OD1	1:B:38:ARG:NH2	2.31	0.64
2:D:167:ASP:O	2:D:168:LEU:C	2.34	0.64
2:F:10:LEU:HD22	2:F:54:VAL:HG13	1.78	0.64
2:F:280:LEU:HB2	2:F:281:PRO:CD	2.28	0.64
2:F:252:ARG:NE	2:F:256:ILE:HD11	2.13	0.64
1:B:94:ASP:C	1:B:101:THR:CG2	2.56	0.64
2:C:150:GLU:OE1	2:C:193:CYS:HA	1.98	0.64
2:F:80:LEU:HD11	2:F:151:LEU:HG	1.80	0.64
1:B:156:ILE:O	1:B:162:VAL:HG23	1.98	0.64
2:F:85:LEU:CA	2:F:237:LYS:NZ	2.61	0.64
2:F:243:SER:HB2	2:F:245:LEU:H	1.60	0.64
2:C:25:ARG:O	2:C:31:HIS:CE1	2.51	0.64
2:D:36:TYR:OH	2:D:103:PRO:HG2	1.97	0.64
2:F:75:VAL:CG1	2:F:128:HIS:CE1	2.81	0.63
1:B:211:GLU:O	1:B:214:GLU:HG2	1.98	0.63
2:D:25:ARG:CG	2:D:31:HIS:CE1	2.81	0.63
2:C:129:VAL:O	2:C:133:THR:HB	1.98	0.63
2:D:51:ALA:N	2:D:52:PRO:HD2	2.13	0.63
1:E:187:HIS:CD2	1:E:228:GLN:HE21	2.16	0.63
2:D:36:TYR:OH	2:D:103:PRO:HD2	1.98	0.63
2:F:134:PRO:HB2	2:F:138:PRO:HG2	1.80	0.63
1:B:126:MET:HE3	1:B:149:ILE:HG12	1.79	0.63
2:C:24:ILE:N	2:C:24:ILE:HD12	2.03	0.63
2:F:243:SER:CB	2:F:246:ARG:HG3	2.18	0.63
2:C:226:VAL:O	2:C:229:ILE:HG13	1.97	0.63
2:C:35:ARG:HB3	2:C:39:LEU:CD1	2.29	0.63
2:C:80:LEU:CD1	2:C:155:VAL:CG2	2.55	0.63
2:D:80:LEU:HD11	2:D:151:LEU:HG	1.81	0.63
2:D:279:VAL:HA	2:D:282:LEU:HD12	1.80	0.63
2:F:226:VAL:HG21	2:F:286:VAL:HG22	1.81	0.63
1:B:129:PHE:HZ	1:B:142:PRO:HG3	1.64	0.63
2:C:62:LEU:C	2:C:64:GLY:H	2.02	0.63
2:C:265:LYS:CD	2:C:283:TYR:HE2	2.09	0.62
2:F:141:HIS:O	2:F:142:ALA:C	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:252:ARG:HH12	2:F:259:GLU:CD	2.02	0.62
1:B:94:ASP:HB3	1:B:104:VAL:HG21	1.81	0.62
2:C:75:VAL:O	2:C:79:MET:HG3	1.99	0.62
2:F:242:ALA:CB	2:F:246:ARG:HE	2.13	0.62
1:B:75:GLU:O	1:B:79:THR:OG1	2.13	0.62
2:C:247:ALA:HB3	2:C:248:LEU:HD13	1.81	0.62
2:F:213:ARG:HH21	2:F:213:ARG:HG3	1.64	0.62
2:C:35:ARG:HB3	2:C:39:LEU:HD11	1.81	0.62
2:F:10:LEU:HD23	2:F:54:VAL:HG22	1.81	0.62
2:C:186:LYS:HZ1	2:C:237:LYS:CD	2.08	0.62
2:D:273:ASP:HB2	2:D:275:TYR:HA	1.82	0.62
2:C:137:ASP:HB3	2:C:138:PRO:CD	2.29	0.62
2:F:242:ALA:HB1	2:F:243:SER:CB	2.29	0.62
2:F:77:LEU:O	2:F:78:GLU:C	2.36	0.62
2:C:76:ALA:HB2	2:C:129:VAL:HG23	1.80	0.62
2:F:66:PRO:O	2:F:67:ARG:HB3	1.99	0.62
1:A:50:PRO:HD3	1:A:75:GLU:OE1	2.00	0.62
2:C:138:PRO:C	2:C:139:VAL:HG23	2.20	0.62
1:E:140:LYS:HG3	1:E:144:ARG:HH12	1.64	0.62
1:E:41:LEU:O	1:E:47:ARG:NH2	2.33	0.62
2:F:126:TYR:O	2:F:130:ILE:HG13	1.99	0.62
2:F:167:ASP:OD2	2:F:239:ARG:O	2.16	0.62
1:A:233:ILE:O	1:A:236:VAL:CG1	2.39	0.62
1:A:34:HIS:CD2	2:C:157:SER:HG	2.17	0.62
2:C:278:ARG:C	2:C:281:PRO:HD2	2.21	0.62
2:C:174:LEU:N	2:C:174:LEU:HD23	2.14	0.62
1:B:187:HIS:CD2	1:B:258:TYR:HE1	2.18	0.61
2:F:187:PHE:HD2	2:F:224:GLN:HB3	1.54	0.61
2:F:244:VAL:O	2:F:248:LEU:HB2	1.99	0.61
1:A:30:PRO:HG2	2:C:162:ALA:CB	2.29	0.61
1:B:30:PRO:HG2	2:D:162:ALA:HB1	1.81	0.61
2:F:10:LEU:CD2	2:F:54:VAL:CA	2.75	0.61
2:F:244:VAL:O	2:F:244:VAL:HG12	2.00	0.61
1:A:257:THR:OG1	1:A:259:PRO:HD2	2.01	0.61
2:F:63:LEU:HD12	2:F:204:ALA:HB2	1.71	0.61
2:F:85:LEU:CA	2:F:237:LYS:HZ1	2.13	0.61
2:F:10:LEU:HD21	2:F:54:VAL:CA	2.10	0.61
2:C:18:LEU:HD23	2:C:75:VAL:HG11	1.79	0.61
2:C:267:GLU:O	2:C:270:ARG:HG3	2.00	0.61
2:D:140:PRO:CG	2:D:143:VAL:CG2	2.76	0.61
1:A:161:LEU:HD12	1:A:161:LEU:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:HG2	2:C:162:ALA:HB2	1.83	0.61
1:E:223:ILE:HA	1:E:226:LEU:HB3	1.83	0.61
1:E:293:LEU:HA	1:E:296:LEU:HD12	1.83	0.61
1:E:47:ARG:NH1	1:E:75:GLU:OE2	2.33	0.61
1:A:50:PRO:CG	1:A:75:GLU:HB2	2.29	0.60
2:C:10:LEU:HD22	2:C:54:VAL:HG23	1.82	0.60
2:D:273:ASP:CB	2:D:275:TYR:O	2.49	0.60
2:C:30:ILE:HD11	2:C:117:ALA:HA	1.83	0.60
2:C:137:ASP:CG	2:C:138:PRO:HD3	2.21	0.60
2:C:269:ASP:O	2:C:270:ARG:C	2.37	0.60
2:C:283:TYR:CD1	2:C:284:SER:N	2.66	0.60
2:C:71:LEU:O	2:C:75:VAL:HG23	1.99	0.60
2:D:278:ARG:O	2:D:279:VAL:C	2.39	0.60
2:D:34:MET:O	2:D:37:ALA:HB3	2.01	0.60
1:E:24:ILE:O	1:E:38:ARG:NH1	2.35	0.60
2:C:247:ALA:CB	2:C:248:LEU:HD13	2.31	0.60
1:B:96:ARG:NE	1:B:96:ARG:HA	2.15	0.60
2:F:277:GLU:C	2:F:279:VAL:H	2.05	0.60
1:A:5:PHE:CE2	1:A:9:MET:CE	2.85	0.60
2:C:174:LEU:H	2:C:174:LEU:HD23	1.67	0.60
2:C:35:ARG:O	2:C:39:LEU:HD12	2.00	0.60
2:F:55:LEU:HD12	2:F:194:SER:OG	2.01	0.60
1:B:163:ALA:O	1:B:166:VAL:HG23	2.01	0.60
2:D:273:ASP:HA	2:D:274:LYS:CG	2.31	0.60
2:D:54:VAL:O	2:D:57:VAL:N	2.34	0.60
1:A:158:SER:OG	2:C:31:HIS:CD2	2.55	0.60
1:A:20:LEU:HD13	1:A:41:LEU:CD1	2.32	0.60
2:C:237:LYS:CG	2:C:238:MET:N	2.65	0.60
2:C:283:TYR:HE1	2:C:284:SER:OG	1.82	0.60
2:F:38:VAL:O	2:F:38:VAL:HG12	2.02	0.60
2:C:53:PRO:HG2	2:C:54:VAL:H	1.67	0.60
2:D:234:GLY:N	2:D:235:ASN:HA	2.17	0.60
2:D:5:LEU:HD13	2:D:5:LEU:C	2.21	0.60
1:B:273:LYS:O	1:B:277:ASP:N	2.31	0.60
2:D:140:PRO:HG2	2:D:143:VAL:HG21	1.84	0.60
2:F:226:VAL:HG21	2:F:286:VAL:CG2	2.32	0.60
2:F:249:GLY:O	2:F:250:MET:HB3	2.01	0.60
2:C:133:THR:HG22	2:C:133:THR:O	2.01	0.59
2:C:58:ALA:HA	2:C:61:GLU:HG3	1.84	0.59
2:D:38:VAL:O	2:D:38:VAL:HG12	2.01	0.59
1:A:49:ARG:NH2	1:A:78:HIS:CE1	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:SER:HB2	2:D:31:HIS:HE2	1.67	0.59
1:B:170:GLU:CD	1:B:171:MET:H	2.02	0.59
1:B:233:ILE:O	1:B:236:VAL:HG22	2.02	0.59
2:C:62:LEU:O	2:C:62:LEU:HD13	2.02	0.59
2:D:35:ARG:O	2:D:37:ALA:N	2.35	0.59
1:A:135:ASP:O	1:A:135:ASP:OD2	2.20	0.59
1:A:5:PHE:CZ	1:A:9:MET:CE	2.85	0.59
1:A:94:ASP:CG	1:A:95:LEU:HD23	2.22	0.59
2:F:208:GLU:O	2:F:212:LEU:HD13	2.02	0.59
2:F:26:THR:O	2:F:31:HIS:CE1	2.55	0.59
2:D:165:PHE:O	2:D:168:LEU:CB	2.51	0.59
2:D:273:ASP:HB3	2:D:275:TYR:C	2.22	0.59
1:E:34:HIS:CD2	2:F:157:SER:HG	2.14	0.59
2:F:212:LEU:HD13	2:F:212:LEU:N	2.16	0.59
2:F:26:THR:HG23	2:F:27:PRO:CD	2.33	0.59
2:F:277:GLU:C	2:F:279:VAL:N	2.51	0.59
1:B:165:GLN:O	1:B:169:LEU:HD12	1.95	0.59
1:E:28:GLU:HA	1:E:28:GLU:OE2	2.02	0.59
2:F:137:ASP:N	2:F:137:ASP:OD1	2.33	0.59
2:C:72:PRO:HG3	2:C:132:HIS:HB2	1.83	0.59
2:F:150:GLU:OE1	2:F:150:GLU:HA	2.03	0.59
2:F:165:PHE:HA	2:F:168:LEU:HB2	1.84	0.59
2:F:184:THR:HG22	2:F:221:VAL:HG21	1.84	0.59
1:A:24:ILE:O	1:A:38:ARG:NH1	2.35	0.58
2:D:85:LEU:HA	2:D:237:LYS:HZ1	1.66	0.58
2:D:131:ALA:O	2:D:132:HIS:ND1	2.37	0.58
1:E:231:ASP:OD1	1:E:303:ARG:CZ	2.51	0.58
1:A:223:ILE:HA	1:A:226:LEU:HB3	1.85	0.58
1:B:50:PRO:HB3	1:B:71:ALA:HB1	1.83	0.58
1:B:119:LEU:O	1:B:122:SER:OG	2.20	0.58
2:F:55:LEU:HD11	2:F:194:SER:CB	2.33	0.58
2:F:26:THR:HG23	2:F:27:PRO:CG	2.32	0.58
2:C:274:LYS:CB	2:C:275:TYR:HA	2.14	0.58
2:D:271:PHE:CD1	2:D:272:GLY:N	2.72	0.58
2:D:50:ARG:HG3	2:D:53:PRO:HD2	1.86	0.58
2:F:34:MET:O	2:F:37:ALA:N	2.37	0.58
2:F:55:LEU:HD12	2:F:56:CYS:H	1.64	0.58
1:A:161:LEU:HA	1:A:189:HIS:O	2.02	0.58
2:D:145:LEU:HD23	2:D:145:LEU:N	2.18	0.58
1:A:304:GLN:HE21	2:D:29:ARG:NH2	2.02	0.58
2:D:140:PRO:CG	2:D:143:VAL:HG21	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:ILE:HG13	2:D:113:MET:HE3	1.86	0.58
2:F:175:GLY:O	2:F:179:VAL:HB	2.04	0.58
2:D:244:VAL:O	2:D:253:ALA:HB2	2.02	0.58
2:D:226:VAL:HG21	2:D:286:VAL:CG2	2.33	0.58
2:F:63:LEU:HD23	2:F:63:LEU:N	2.18	0.57
1:A:49:ARG:HH22	1:A:78:HIS:CE1	2.21	0.57
2:C:5:LEU:O	2:C:6:TYR:C	2.42	0.57
2:D:212:LEU:HD13	2:D:212:LEU:N	2.19	0.57
2:F:35:ARG:C	2:F:37:ALA:N	2.56	0.57
2:D:65:ALA:HB2	2:D:202:GLY:HA2	1.87	0.57
2:F:243:SER:HB3	2:F:246:ARG:CG	2.18	0.57
2:F:209:GLU:OE1	2:F:210:ALA:N	2.37	0.57
2:C:150:GLU:OE1	2:C:193:CYS:CB	2.52	0.57
2:C:27:PRO:O	2:C:31:HIS:CG	2.56	0.57
2:D:3:LEU:HD11	2:D:278:ARG:NH1	2.19	0.57
1:A:140:LYS:HG3	1:A:144:ARG:NE	2.18	0.57
2:D:254:LEU:N	2:D:254:LEU:HD22	2.20	0.57
2:F:173:ALA:O	2:F:179:VAL:HG21	2.04	0.57
2:F:243:SER:CB	2:F:244:VAL:HA	2.34	0.57
2:C:57:VAL:O	2:C:60:CYS:HB3	2.05	0.57
2:D:174:LEU:CG	2:D:175:GLY:CA	2.80	0.57
2:F:50:ARG:O	2:F:51:ALA:CB	2.49	0.57
2:F:10:LEU:HD13	2:F:57:VAL:HG21	1.80	0.57
2:D:25:ARG:O	2:D:31:HIS:ND1	2.38	0.57
2:F:196:ALA:HB2	2:F:213:ARG:HG3	1.85	0.57
2:F:208:GLU:O	2:F:212:LEU:HD22	2.05	0.57
2:F:252:ARG:O	2:F:252:ARG:HD2	2.04	0.57
1:B:49:ARG:CZ	1:B:78:HIS:CD2	2.87	0.56
1:A:39:TYR:OH	1:A:100:PRO:O	2.17	0.56
1:E:257:THR:HG23	1:E:259:PRO:HD2	1.87	0.56
1:B:161:LEU:HA	1:B:189:HIS:O	2.05	0.56
1:B:209:SER:OG	1:B:212:GLN:HG3	2.05	0.56
2:C:132:HIS:O	2:C:133:THR:HB	2.03	0.56
2:D:277:GLU:O	2:D:281:PRO:HD3	2.04	0.56
1:E:220:ALA:HA	1:E:223:ILE:HG12	1.87	0.56
2:C:283:TYR:CD1	2:C:284:SER:OG	2.57	0.56
2:D:133:THR:HG21	2:D:144:LEU:HD21	1.86	0.56
2:C:168:LEU:O	2:C:169:ALA:HB3	2.06	0.56
1:A:262:LEU:O	1:A:266:LYS:NZ	2.32	0.56
1:A:28:GLU:CD	1:A:29:PRO:HD2	2.26	0.56
2:C:5:LEU:O	2:C:7:TRP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASP:C	1:A:101:THR:HG23	2.14	0.56
2:C:204:ALA:CB	2:C:208:GLU:OE1	2.54	0.56
1:B:95:LEU:HD21	1:B:98:GLY:HA2	1.88	0.56
1:E:302:TYR:CD1	1:E:302:TYR:N	2.72	0.56
2:C:247:ALA:C	2:C:248:LEU:HD13	2.26	0.56
2:D:225:LEU:HD11	2:D:244:VAL:HB	1.88	0.56
2:D:94:ASP:O	2:D:95:ALA:HB3	2.05	0.56
1:E:93:ASP:O	1:E:94:ASP:C	2.43	0.56
2:F:243:SER:OG	2:F:246:ARG:N	2.39	0.56
2:C:137:ASP:CB	2:C:138:PRO:CD	2.84	0.55
2:D:165:PHE:O	2:D:168:LEU:HB2	2.06	0.55
1:B:91:ASP:N	1:B:91:ASP:OD1	2.38	0.55
2:C:58:ALA:HA	2:C:61:GLU:CG	2.36	0.55
2:D:233:SER:HB3	2:D:234:GLY:O	2.05	0.55
1:A:304:GLN:NE2	2:D:29:ARG:NH2	2.55	0.55
2:D:60:CYS:SG	2:D:65:ALA:HB3	2.46	0.55
1:E:88:PRO:HD3	1:E:103:HIS:CE1	2.41	0.55
2:F:242:ALA:HB1	2:F:246:ARG:HB2	1.88	0.55
1:A:49:ARG:CZ	1:A:78:HIS:NE2	2.69	0.55
1:B:159:GLU:HA	1:B:159:GLU:OE1	2.06	0.55
2:C:62:LEU:C	2:C:64:GLY:N	2.57	0.55
2:F:69:ALA:HB3	2:F:201:LEU:HB3	1.88	0.55
2:F:68:GLU:CB	2:F:134:PRO:HG2	2.29	0.55
2:C:192:GLU:OE2	2:C:213:ARG:CD	2.54	0.55
2:D:225:LEU:CD1	2:D:244:VAL:HB	2.35	0.55
2:C:186:LYS:HD2	2:C:187:PHE:CE1	2.40	0.55
2:F:141:HIS:C	2:F:143:VAL:N	2.58	0.55
2:C:137:ASP:HB3	2:C:138:PRO:HD2	1.88	0.55
2:C:35:ARG:O	2:C:39:LEU:CD1	2.54	0.55
2:D:273:ASP:HB2	2:D:275:TYR:CA	2.37	0.55
1:E:182:ARG:O	1:E:186:ILE:HD13	2.07	0.55
2:F:280:LEU:CB	2:F:281:PRO:HD3	2.37	0.55
2:C:238:MET:O	2:C:238:MET:HG2	2.07	0.54
2:F:67:ARG:O	2:F:67:ARG:HD3	2.07	0.54
2:F:69:ALA:HB1	2:F:201:LEU:HG	1.84	0.54
1:A:138:ALA:O	1:A:142:PRO:HD3	2.06	0.54
2:D:245:LEU:HD12	2:D:246:ARG:N	2.23	0.54
2:F:243:SER:CB	2:F:244:VAL:CA	2.85	0.54
2:F:62:LEU:C	2:F:63:LEU:HD23	2.26	0.54
2:C:4:ARG:HB2	2:C:278:ARG:NH2	2.21	0.54
2:D:209:GLU:HA	2:D:212:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:150:GLU:OE1	2:F:153:ARG:HD3	2.08	0.54
2:F:267:GLU:OE1	2:F:267:GLU:HA	2.07	0.54
2:F:52:PRO:O	2:F:55:LEU:HD12	2.08	0.54
2:D:170:GLY:O	2:D:171:ALA:HB3	2.07	0.54
2:D:85:LEU:N	2:D:237:LYS:HZ1	2.05	0.54
2:F:156:GLY:O	2:F:161:ALA:CB	2.52	0.54
2:F:183:LEU:HD21	2:F:224:GLN:HG2	1.89	0.54
1:A:16:VAL:O	1:A:20:LEU:HG	2.07	0.54
2:D:54:VAL:O	2:D:56:CYS:N	2.40	0.54
2:D:286:VAL:HG13	2:D:287:ASP:N	2.22	0.54
2:D:38:VAL:O	2:D:39:LEU:HD23	2.07	0.54
1:E:136:ILE:HD12	1:E:141:HIS:CD2	2.42	0.54
1:E:147:ARG:HG2	1:E:204:ILE:HD13	1.90	0.54
1:E:237:THR:C	1:E:238:LYS:O	2.45	0.54
1:A:5:PHE:CD2	1:A:295:HIS:HB3	2.43	0.54
2:C:53:PRO:HG2	2:C:54:VAL:N	2.22	0.54
1:A:141:HIS:HA	1:A:144:ARG:HD2	1.89	0.54
2:D:288:TYR:CG	2:D:289:ALA:N	2.76	0.54
2:F:165:PHE:O	2:F:168:LEU:CB	2.56	0.54
2:F:184:THR:HA	2:F:221:VAL:HG22	1.90	0.54
1:B:96:ARG:C	1:B:97:ARG:HG3	2.29	0.54
2:C:273:ASP:OD1	2:C:273:ASP:N	2.41	0.54
2:D:157:SER:O	2:D:162:ALA:HB2	2.08	0.54
2:D:271:PHE:HD1	2:D:272:GLY:H	1.54	0.54
2:F:137:ASP:CG	2:F:138:PRO:HD2	2.28	0.54
2:D:173:ALA:O	2:D:243:SER:CB	2.56	0.54
1:E:227:PHE:O	1:E:303:ARG:NH2	2.41	0.54
2:F:252:ARG:CZ	2:F:256:ILE:HD11	2.38	0.54
1:A:220:ALA:HA	1:A:223:ILE:HG12	1.91	0.53
1:A:94:ASP:OD1	1:A:95:LEU:HG	2.07	0.53
2:C:227:ASP:C	2:C:229:ILE:N	2.62	0.53
2:D:273:ASP:CG	2:D:275:TYR:O	2.47	0.53
1:E:137:ASP:HB3	1:E:140:LYS:HD3	1.90	0.53
2:F:277:GLU:O	2:F:278:ARG:C	2.46	0.53
2:F:5:LEU:HG	2:F:6:TYR:N	2.24	0.53
1:A:178:VAL:CG2	1:A:256:THR:HG21	2.39	0.53
2:D:273:ASP:CA	2:D:274:LYS:CB	2.84	0.53
2:F:36:TYR:OH	2:F:103:PRO:CD	2.55	0.53
1:A:5:PHE:CE2	1:A:9:MET:HE1	2.43	0.53
1:E:184:GLU:O	1:E:188:LEU:HB2	2.07	0.53
2:D:167:ASP:C	2:D:169:ALA:N	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:ARG:O	2:D:280:LEU:N	2.42	0.53
2:D:35:ARG:C	2:D:37:ALA:N	2.57	0.53
1:B:233:ILE:O	1:B:236:VAL:HG23	2.07	0.53
2:C:132:HIS:O	2:C:133:THR:C	2.46	0.53
2:D:55:LEU:HD22	2:D:219:ILE:HD13	1.89	0.53
2:D:215:TYR:HD1	2:D:283:TYR:OH	1.84	0.53
1:B:95:LEU:HD11	1:B:98:GLY:C	2.29	0.53
2:C:252:ARG:O	2:C:253:ALA:C	2.45	0.53
2:F:14:VAL:HG13	2:F:15:GLU:N	2.23	0.53
2:F:280:LEU:CB	2:F:281:PRO:CD	2.86	0.53
1:B:170:GLU:CG	1:B:171:MET:N	2.72	0.53
2:F:248:LEU:CD2	2:F:248:LEU:N	2.71	0.53
1:B:161:LEU:CA	1:B:189:HIS:O	2.56	0.53
1:B:49:ARG:NH1	1:B:78:HIS:CD2	2.77	0.53
2:D:215:TYR:CE1	2:D:283:TYR:CE2	2.91	0.53
2:C:208:GLU:HA	2:C:211:ALA:HB3	1.91	0.53
1:E:113:LEU:HD22	2:F:164:GLN:OE1	2.09	0.53
2:D:132:HIS:O	2:D:134:PRO:CD	2.49	0.52
2:D:273:ASP:C	2:D:274:LYS:HG2	2.30	0.52
2:F:122:PHE:HB2	2:F:123:PRO:HD3	1.91	0.52
2:D:156:GLY:O	2:D:161:ALA:CB	2.57	0.52
2:F:134:PRO:O	2:F:138:PRO:HG2	2.09	0.52
2:C:265:LYS:CD	2:C:283:TYR:CE2	2.89	0.52
2:C:51:ALA:N	2:C:52:PRO:CD	2.73	0.52
2:D:273:ASP:OD2	2:D:275:TYR:O	2.25	0.52
2:F:166:LEU:HB3	2:F:182:VAL:HG22	1.90	0.52
2:C:180:MET:HE2	2:C:244:VAL:HA	1.91	0.52
2:D:50:ARG:HB2	2:D:50:ARG:CZ	2.39	0.52
1:E:87:LEU:HD23	1:E:103:HIS:HB2	1.90	0.52
2:F:270:ARG:HH21	2:F:270:ARG:HG2	1.73	0.52
1:A:52:LEU:HB3	1:A:199:VAL:HG12	1.91	0.52
1:B:94:ASP:O	1:B:101:THR:CB	2.52	0.52
2:F:77:LEU:O	2:F:80:LEU:N	2.42	0.52
2:C:104:SER:HB3	2:C:106:HIS:CD2	2.44	0.52
2:C:189:GLU:HA	2:C:192:GLU:HB3	1.90	0.52
2:D:278:ARG:C	2:D:280:LEU:N	2.58	0.52
1:A:152:LEU:O	1:A:156:ILE:HG13	2.10	0.52
1:A:12:LYS:HE3	1:A:64:GLU:OE1	2.10	0.52
2:D:50:ARG:CB	2:D:50:ARG:NH2	2.73	0.52
2:F:21:ALA:C	2:F:23:PRO:HD3	2.30	0.52
2:D:51:ALA:H	2:D:52:PRO:CD	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:LEU:HD11	2:F:204:ALA:CB	2.27	0.52
2:F:65:ALA:HB2	2:F:202:GLY:HA2	1.91	0.52
2:C:193:CYS:O	2:C:197:CYS:N	2.33	0.52
2:D:122:PHE:HB2	2:D:123:PRO:HD3	1.91	0.52
1:A:8:TYR:CD1	1:A:8:TYR:C	2.84	0.51
1:E:20:LEU:HD22	1:E:41:LEU:HD21	1.91	0.51
2:F:177:ALA:C	2:F:179:VAL:N	2.64	0.51
2:F:94:ASP:O	2:F:95:ALA:HB3	2.10	0.51
1:B:169:LEU:N	1:B:169:LEU:HD12	2.25	0.51
2:F:247:ALA:O	2:F:248:LEU:HD22	2.09	0.51
1:A:161:LEU:CD1	1:A:161:LEU:N	2.72	0.51
2:C:247:ALA:CB	2:C:248:LEU:CD1	2.89	0.51
2:C:35:ARG:C	2:C:39:LEU:HD12	2.30	0.51
2:C:55:LEU:HD23	2:C:55:LEU:O	2.11	0.51
2:D:278:ARG:HA	2:D:281:PRO:HD3	1.89	0.51
2:D:50:ARG:HD3	2:D:53:PRO:HG3	1.92	0.51
1:B:41:LEU:O	1:B:47:ARG:NH2	2.39	0.51
2:C:204:ALA:HB2	2:C:208:GLU:OE1	2.11	0.51
2:D:212:LEU:N	2:D:212:LEU:CD1	2.73	0.51
1:A:49:ARG:NH2	1:A:78:HIS:NE2	2.59	0.51
2:C:186:LYS:NZ	2:C:237:LYS:CD	2.71	0.51
1:E:166:VAL:HG12	2:F:116:LEU:HD13	1.92	0.51
2:F:243:SER:OG	2:F:246:ARG:HB2	2.11	0.51
1:B:166:VAL:HA	1:B:169:LEU:HD13	1.92	0.51
2:C:235:ASN:N	2:C:235:ASN:OD1	2.43	0.51
2:C:88:ASP:OD2	2:C:237:LYS:NZ	2.43	0.51
2:F:288:TYR:CD2	2:F:288:TYR:C	2.85	0.51
2:D:225:LEU:CD1	2:D:244:VAL:CB	2.89	0.51
2:D:273:ASP:CB	2:D:275:TYR:HA	2.39	0.51
1:B:79:THR:O	1:B:83:VAL:HG23	2.11	0.50
2:D:38:VAL:HG22	2:D:82:ALA:CB	2.40	0.50
2:F:132:HIS:N	2:F:132:HIS:ND1	2.60	0.50
2:F:87:HIS:HA	2:F:90:LEU:HD12	1.92	0.50
1:A:109:PRO:HG3	2:C:92:CYS:O	2.11	0.50
1:A:13:ALA:C	1:A:17:ASN:HD22	2.12	0.50
2:C:4:ARG:CB	2:C:278:ARG:NH2	2.71	0.50
2:F:183:LEU:O	2:F:183:LEU:HD23	2.11	0.50
2:C:237:LYS:HG3	2:C:238:MET:H	1.76	0.50
2:C:248:LEU:CD1	2:C:248:LEU:N	2.73	0.50
2:C:283:TYR:CD1	2:C:283:TYR:C	2.84	0.50
2:D:36:TYR:OH	2:D:103:PRO:O	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:VAL:CG1	2:D:140:PRO:HD2	2.42	0.50
1:E:140:LYS:HG3	1:E:144:ARG:NH1	2.25	0.50
2:F:67:ARG:HD3	2:F:67:ARG:C	2.32	0.50
2:C:180:MET:HE1	2:C:243:SER:O	2.12	0.50
2:F:255:GLY:O	2:F:259:GLU:HG3	2.11	0.50
2:C:265:LYS:HE2	2:C:283:TYR:OH	2.11	0.50
1:A:96:ARG:HG3	1:A:97:ARG:H	1.77	0.50
1:B:95:LEU:HG	1:B:96:ARG:N	2.26	0.50
2:C:136:PRO:O	2:C:137:ASP:HB3	2.12	0.50
2:C:144:LEU:O	2:C:148:LEU:HG	2.12	0.50
2:C:174:LEU:CD2	2:C:174:LEU:H	2.24	0.50
1:B:30:PRO:HG2	2:D:162:ALA:CB	2.41	0.50
2:D:174:LEU:C	2:D:175:GLY:O	2.48	0.50
2:F:102:ARG:N	2:F:103:PRO:CD	2.75	0.50
2:F:222:LEU:HD21	2:F:286:VAL:HG11	1.92	0.50
2:F:7:TRP:C	2:F:7:TRP:CD1	2.85	0.50
1:B:84:HIS:NE2	1:B:115:GLY:HA3	2.25	0.50
2:C:199:ALA:HB2	2:C:212:LEU:HD23	1.94	0.50
2:D:233:SER:N	2:D:234:GLY:CA	2.71	0.50
2:D:278:ARG:CA	2:D:281:PRO:HD3	2.40	0.50
2:D:52:PRO:CG	2:D:53:PRO:CD	2.85	0.50
1:E:295:HIS:HA	1:E:298:ASN:HB2	1.94	0.50
2:F:69:ALA:HB3	2:F:201:LEU:HD23	1.72	0.50
2:F:225:LEU:HD13	2:F:244:VAL:CG2	2.42	0.50
2:C:22:MET:CE	2:C:38:VAL:HG21	2.42	0.50
2:F:60:CYS:HG	2:F:65:ALA:CB	2.15	0.50
2:F:85:LEU:HA	2:F:237:LYS:HZ1	1.66	0.50
2:C:62:LEU:HD22	2:C:63:LEU:CB	2.42	0.50
1:E:183:LEU:HD22	1:E:261:LEU:HD12	1.94	0.50
2:F:244:VAL:CG1	2:F:248:LEU:CG	2.73	0.49
2:F:252:ARG:NE	2:F:256:ILE:CD1	2.73	0.49
1:E:162:VAL:O	1:E:166:VAL:HG13	2.11	0.49
2:D:273:ASP:N	2:D:273:ASP:OD1	2.45	0.49
1:B:59:VAL:HA	1:B:289:THR:HB	1.95	0.49
2:C:280:LEU:O	2:C:283:TYR:N	2.45	0.49
2:C:62:LEU:O	2:C:64:GLY:N	2.45	0.49
2:D:88:ASP:O	2:D:94:ASP:OD1	2.31	0.49
2:F:36:TYR:OH	2:F:103:PRO:CG	2.60	0.49
1:B:237:THR:C	1:B:238:LYS:O	2.51	0.49
2:C:6:TYR:C	2:C:6:TYR:CD1	2.85	0.49
2:D:78:GLU:HA	2:D:78:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:LEU:CD2	2:C:75:VAL:HG12	2.35	0.49
2:C:237:LYS:HG3	2:C:238:MET:N	2.27	0.49
2:F:36:TYR:OH	2:F:103:PRO:O	2.23	0.49
2:F:14:VAL:CG1	2:F:15:GLU:N	2.76	0.49
2:F:243:SER:OG	2:F:244:VAL:HA	2.13	0.49
2:D:245:LEU:HD12	2:D:245:LEU:C	2.33	0.49
1:B:178:VAL:HB	1:B:256:THR:HG21	1.94	0.49
2:D:272:GLY:O	2:D:274:LYS:HG2	2.13	0.49
1:A:272:GLU:HG2	2:D:24:ILE:HD13	1.94	0.49
1:B:146:VAL:HG23	2:D:145:LEU:HD21	1.95	0.49
2:C:150:GLU:OE2	2:C:150:GLU:HA	2.13	0.49
2:F:21:ALA:O	2:F:23:PRO:CD	2.60	0.49
1:A:192:ALA:O	1:A:196:GLU:HG3	2.13	0.48
2:C:288:TYR:HD1	2:C:289:ALA:H	1.61	0.48
2:D:50:ARG:NE	2:D:53:PRO:CD	2.74	0.48
2:D:3:LEU:HD11	2:D:278:ARG:HD2	1.93	0.48
1:E:276:SER:HA	1:E:279:ARG:HD3	1.93	0.48
2:F:165:PHE:O	2:F:168:LEU:HB2	2.13	0.48
2:F:87:HIS:HA	2:F:90:LEU:HD11	1.95	0.48
2:D:137:ASP:OD1	2:D:137:ASP:N	2.45	0.48
2:D:212:LEU:HD13	2:D:212:LEU:H	1.76	0.48
2:D:27:PRO:O	2:D:27:PRO:HG2	2.13	0.48
2:F:104:SER:HB2	2:F:106:HIS:CD2	2.49	0.48
2:D:54:VAL:C	2:D:56:CYS:N	2.66	0.48
2:F:134:PRO:HB2	2:F:138:PRO:HG3	1.96	0.48
2:C:245:LEU:O	2:C:245:LEU:HD23	2.12	0.48
2:F:173:ALA:O	2:F:179:VAL:CG2	2.60	0.48
2:F:22:MET:O	2:F:35:ARG:HD2	2.13	0.48
2:F:277:GLU:O	2:F:280:LEU:N	2.44	0.48
1:A:155:CYS:O	1:A:161:LEU:HD13	2.13	0.48
1:B:166:VAL:CG1	2:D:113:MET:CE	2.86	0.48
1:A:30:PRO:CG	2:C:162:ALA:HB1	2.44	0.48
1:B:162:VAL:HG11	2:D:120:ALA:HB2	1.96	0.48
2:C:75:VAL:CG1	2:C:79:MET:CE	2.85	0.48
2:D:104:SER:HB2	2:D:106:HIS:CD2	2.49	0.48
2:D:192:GLU:HG3	2:D:213:ARG:HG2	1.96	0.48
1:B:296:LEU:O	1:B:300:ILE:HG13	2.14	0.48
1:B:95:LEU:HD11	1:B:99:LYS:C	2.33	0.48
2:F:243:SER:CB	2:F:246:ARG:N	2.70	0.48
2:D:264:ALA:CA	2:D:283:TYR:OH	2.62	0.48
2:F:50:ARG:CG	2:F:52:PRO:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:PHE:HB2	2:C:123:PRO:HD3	1.95	0.47
2:D:10:LEU:C	2:D:10:LEU:HD12	2.30	0.47
2:D:168:LEU:HD13	2:D:168:LEU:O	2.13	0.47
2:D:254:LEU:N	2:D:254:LEU:CD2	2.77	0.47
2:F:212:LEU:CD1	2:F:212:LEU:N	2.77	0.47
2:F:21:ALA:O	2:F:23:PRO:HD3	2.14	0.47
1:B:275:LEU:O	1:B:279:ARG:HG3	2.15	0.47
2:D:23:PRO:HG2	2:D:23:PRO:O	2.14	0.47
2:F:243:SER:HB2	2:F:246:ARG:H	1.76	0.47
1:A:84:HIS:NE2	1:A:115:GLY:HA3	2.29	0.47
1:A:291:ALA:O	1:A:295:HIS:ND1	2.42	0.47
1:A:293:LEU:HA	1:A:296:LEU:HD12	1.96	0.47
2:C:157:SER:O	2:C:162:ALA:HB2	2.13	0.47
2:C:30:ILE:HG23	2:C:31:HIS:N	2.28	0.47
2:F:213:ARG:NH2	2:F:213:ARG:CG	2.72	0.47
2:F:38:VAL:HG22	2:F:82:ALA:CB	2.44	0.47
1:A:163:ALA:O	1:A:167:VAL:HG23	2.14	0.47
1:A:296:LEU:O	1:A:300:ILE:HG13	2.13	0.47
1:A:49:ARG:HH11	1:A:78:HIS:CB	2.25	0.47
2:C:214:ARG:HD2	2:C:267:GLU:OE1	2.14	0.47
2:D:154:ALA:HB2	2:D:193:CYS:SG	2.55	0.47
2:D:245:LEU:HD12	2:D:246:ARG:HA	1.96	0.47
2:D:5:LEU:HD22	2:D:5:LEU:C	2.28	0.47
2:F:243:SER:HB2	2:F:244:VAL:C	2.34	0.47
1:A:232:ASP:HB3	1:A:257:THR:OG1	2.15	0.47
1:E:49:ARG:HH21	1:E:78:HIS:CE1	2.33	0.47
2:F:210:ALA:O	2:F:214:ARG:HG3	2.15	0.47
2:C:132:HIS:N	2:C:132:HIS:ND1	2.60	0.47
2:D:50:ARG:CB	2:D:50:ARG:HH21	2.27	0.47
1:E:148:ALA:HB1	1:E:201:ILE:HB	1.95	0.47
2:F:191:ALA:HA	2:F:194:SER:HB3	1.97	0.47
2:F:26:THR:HG23	2:F:27:PRO:HD2	1.97	0.47
2:C:131:ALA:C	2:C:132:HIS:ND1	2.68	0.47
2:C:183:LEU:HD23	2:C:183:LEU:N	2.29	0.47
2:F:23:PRO:HG2	2:F:23:PRO:O	2.14	0.47
2:F:225:LEU:HD13	2:F:244:VAL:HG21	1.97	0.47
1:A:218:MET:HA	1:A:221:ARG:HB2	1.97	0.47
2:D:178:GLU:O	2:D:181:LYS:HB2	2.14	0.47
2:D:199:ALA:HB1	2:D:212:LEU:HD23	1.95	0.47
2:D:244:VAL:HG23	2:D:245:LEU:N	2.30	0.47
2:D:63:LEU:CD2	2:D:204:ALA:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:PHE:O	2:D:168:LEU:HB3	2.14	0.47
1:B:49:ARG:HD3	1:B:194:LEU:HD22	1.96	0.47
2:C:272:GLY:O	2:C:273:ASP:HB2	2.15	0.47
2:C:5:LEU:HD22	2:C:8:THR:HG21	1.97	0.47
2:D:191:ALA:HA	2:D:194:SER:HB3	1.97	0.47
2:D:270:ARG:O	2:D:271:PHE:HB3	2.14	0.47
2:F:141:HIS:N	2:F:141:HIS:ND1	2.60	0.47
2:F:242:ALA:HB2	2:F:246:ARG:HE	1.73	0.47
2:F:261:LYS:HE3	2:F:283:TYR:CE1	2.50	0.47
1:B:143:ALA:HB2	2:D:141:HIS:CD2	2.50	0.47
2:D:225:LEU:HD13	2:D:244:VAL:CB	2.45	0.47
2:D:253:ALA:O	2:D:257:VAL:HG23	2.15	0.47
2:F:10:LEU:CD2	2:F:54:VAL:CG1	2.89	0.47
1:B:73:ALA:O	1:B:77:VAL:HG23	2.15	0.46
2:C:72:PRO:CB	2:C:133:THR:OG1	2.59	0.46
1:B:166:VAL:HG12	2:D:113:MET:SD	2.53	0.46
2:D:279:VAL:O	2:D:283:TYR:CD2	2.67	0.46
2:D:36:TYR:O	2:D:36:TYR:CG	2.68	0.46
1:E:144:ARG:HG3	1:E:204:ILE:CG2	2.45	0.46
1:E:161:LEU:O	1:E:165:GLN:HG3	2.14	0.46
2:C:7:TRP:CZ2	2:C:50:ARG:HA	2.51	0.46
1:A:5:PHE:CZ	1:A:9:MET:HE1	2.50	0.46
2:D:245:LEU:CD1	2:D:245:LEU:C	2.83	0.46
2:D:273:ASP:CA	2:D:275:TYR:H	2.29	0.46
2:D:7:TRP:HH2	2:D:51:ALA:HB2	1.80	0.46
1:B:74:VAL:HB	1:B:194:LEU:HD21	1.96	0.46
1:B:165:GLN:OE1	2:D:116:LEU:HD21	2.16	0.46
1:A:88:PRO:HD3	1:A:103:HIS:CE1	2.51	0.46
2:C:137:ASP:CG	2:C:138:PRO:CD	2.84	0.46
2:F:137:ASP:CG	2:F:138:PRO:CD	2.83	0.46
2:C:178:GLU:HG3	2:C:178:GLU:O	2.15	0.46
1:B:148:ALA:HB1	1:B:201:ILE:HB	1.97	0.46
2:C:178:GLU:OE2	2:C:178:GLU:HA	2.16	0.46
2:C:227:ASP:O	2:C:229:ILE:N	2.47	0.46
2:F:35:ARG:O	2:F:36:TYR:C	2.54	0.46
2:C:141:HIS:O	2:C:144:LEU:N	2.49	0.46
2:C:245:LEU:C	2:C:245:LEU:CD2	2.85	0.46
2:C:39:LEU:H	2:C:40:PRO:HD2	1.78	0.46
2:D:137:ASP:CG	2:D:138:PRO:CD	2.85	0.46
2:D:138:PRO:HG2	2:D:139:VAL:H	1.81	0.46
2:F:215:TYR:OH	2:F:279:VAL:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASP:HB3	1:B:257:THR:HB	1.98	0.45
2:C:271:PHE:CD1	2:C:271:PHE:N	2.85	0.45
2:D:254:LEU:HA	2:D:254:LEU:HD13	1.77	0.45
2:D:74:ALA:HA	2:D:77:LEU:HD12	1.97	0.45
2:D:87:HIS:O	2:D:93:PHE:CD2	2.69	0.45
2:F:24:ILE:C	2:F:24:ILE:HD12	2.36	0.45
2:F:23:PRO:HG2	2:F:25:ARG:HH11	1.80	0.45
2:F:25:ARG:CG	2:F:31:HIS:HE1	1.91	0.45
2:D:139:VAL:HG12	2:D:140:PRO:HD2	1.98	0.45
1:E:88:PRO:HA	1:E:92:ASP:CB	2.44	0.45
2:F:25:ARG:C	2:F:26:THR:O	2.52	0.45
1:A:30:PRO:HG2	2:C:162:ALA:HB1	1.98	0.45
2:C:150:GLU:HG3	2:C:193:CYS:HB2	1.97	0.45
2:C:193:CYS:O	2:C:196:ALA:N	2.49	0.45
2:C:36:TYR:CD2	2:C:36:TYR:O	2.70	0.45
2:D:252:ARG:NH1	2:D:259:GLU:OE2	2.35	0.45
2:D:226:VAL:HG21	2:D:286:VAL:HG22	1.97	0.45
2:F:173:ALA:C	2:F:179:VAL:HG23	2.36	0.45
2:F:52:PRO:N	2:F:53:PRO:HD2	2.31	0.45
2:C:36:TYR:CG	2:C:36:TYR:O	2.69	0.45
2:D:144:LEU:O	2:D:147:VAL:HB	2.16	0.45
2:F:55:LEU:HD12	2:F:55:LEU:C	2.33	0.45
2:F:19:ASP:OD1	2:F:20:ALA:N	2.49	0.45
1:B:199:VAL:HG21	1:B:220:ALA:HB2	1.98	0.45
2:C:93:PHE:CE2	2:C:168:LEU:CD2	2.95	0.45
2:C:94:ASP:HB2	2:C:238:MET:CE	2.46	0.45
2:D:238:MET:SD	2:D:239:ARG:CZ	3.05	0.45
2:F:69:ALA:CB	2:F:201:LEU:CG	2.79	0.45
2:F:25:ARG:O	2:F:26:THR:O	2.33	0.45
2:C:252:ARG:HG3	2:C:252:ARG:HH11	1.82	0.45
2:D:71:LEU:O	2:D:75:VAL:HG23	2.16	0.45
2:F:154:ALA:CB	2:F:193:CYS:SG	2.92	0.45
1:B:109:PRO:HG3	2:D:92:CYS:O	2.17	0.45
2:C:135:SER:OG	2:C:136:PRO:HD3	2.16	0.45
1:B:228:GLN:HA	1:B:231:ASP:HB3	1.99	0.45
2:C:52:PRO:CG	2:C:53:PRO:CD	2.86	0.45
2:D:147:VAL:HG21	2:D:201:LEU:HD11	1.98	0.45
2:D:264:ALA:HB1	2:D:283:TYR:HH	1.64	0.45
2:F:215:TYR:CE1	2:F:279:VAL:HB	2.52	0.45
2:F:52:PRO:HD2	2:F:53:PRO:HD2	1.97	0.45
2:F:7:TRP:O	2:F:7:TRP:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASP:C	1:A:101:THR:CG2	2.73	0.45
1:A:97:ARG:HB2	1:A:98:GLY:H	1.45	0.45
2:C:247:ALA:C	2:C:248:LEU:CD1	2.85	0.45
1:B:158:SER:HB2	2:D:31:HIS:NE2	2.29	0.44
2:F:80:LEU:CD1	2:F:151:LEU:HG	2.47	0.44
1:A:161:LEU:CD1	1:A:161:LEU:H	2.29	0.44
1:A:52:LEU:HB3	1:A:199:VAL:CG1	2.47	0.44
2:C:138:PRO:C	2:C:139:VAL:CG2	2.85	0.44
2:C:255:GLY:O	2:C:259:GLU:HG3	2.17	0.44
2:D:252:ARG:O	2:D:256:ILE:HG12	2.17	0.44
2:D:36:TYR:OH	2:D:103:PRO:CG	2.65	0.44
2:F:134:PRO:O	2:F:139:VAL:HG23	2.17	0.44
2:C:144:LEU:C	2:C:144:LEU:HD23	2.33	0.44
2:C:182:VAL:HG23	2:C:183:LEU:HD23	1.99	0.44
2:C:210:ALA:O	2:C:214:ARG:N	2.45	0.44
2:D:180:MET:CE	2:D:180:MET:N	2.73	0.44
2:D:210:ALA:O	2:D:214:ARG:HG3	2.18	0.44
2:D:76:ALA:O	2:D:79:MET:HB2	2.16	0.44
1:E:20:LEU:HD23	1:E:72:ALA:HB1	1.99	0.44
1:E:286:ASP:HB3	1:E:289:THR:OG1	2.17	0.44
1:B:20:LEU:HD22	1:B:41:LEU:HD21	1.99	0.44
2:D:168:LEU:CD1	2:D:168:LEU:C	2.85	0.44
2:D:52:PRO:CD	2:D:53:PRO:HD2	2.48	0.44
1:A:28:GLU:CD	1:A:29:PRO:CD	2.85	0.44
2:C:204:ALA:HB1	2:C:208:GLU:CD	2.37	0.44
1:A:28:GLU:OE1	1:A:29:PRO:HD2	2.17	0.44
2:C:138:PRO:O	2:C:139:VAL:HG23	2.18	0.44
2:C:150:GLU:OE1	2:C:193:CYS:CA	2.64	0.44
2:D:50:ARG:CD	2:D:53:PRO:CD	2.95	0.44
1:E:288:GLU:OE1	1:E:288:GLU:HA	2.17	0.44
2:F:168:LEU:CD1	2:F:168:LEU:C	2.85	0.44
2:F:35:ARG:C	2:F:37:ALA:H	2.20	0.44
1:A:178:VAL:HG21	1:A:256:THR:HG21	2.00	0.44
1:A:279:ARG:HH21	1:A:294:LEU:HD22	1.83	0.44
1:A:94:ASP:CG	1:A:95:LEU:CD2	2.85	0.44
1:B:59:VAL:HG22	1:B:285:PHE:CD1	2.53	0.44
2:D:199:ALA:CB	2:D:212:LEU:HD23	2.48	0.44
1:A:272:GLU:CG	2:D:24:ILE:CD1	2.92	0.44
2:C:5:LEU:C	2:C:7:TRP:N	2.65	0.44
1:E:9:MET:HE3	1:E:9:MET:HB2	1.82	0.44
2:F:87:HIS:CA	2:F:90:LEU:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:ASP:CA	2:D:275:TYR:N	2.79	0.44
2:F:174:LEU:HA	2:F:175:GLY:HA2	1.75	0.44
2:C:109:TYR:HA	1:E:298:ASN:HD21	1.83	0.43
1:E:301:ALA:HB1	1:E:302:TYR:CE1	2.52	0.43
2:F:244:VAL:HG11	2:F:248:LEU:HG	1.92	0.43
1:A:231:ASP:O	1:A:235:ASP:CG	2.55	0.43
1:B:168:ASP:C	1:B:170:GLU:H	2.21	0.43
2:D:140:PRO:HG2	2:D:143:VAL:HG23	1.93	0.43
2:D:280:LEU:HD23	2:D:280:LEU:HA	1.96	0.43
2:D:39:LEU:N	2:D:40:PRO:HD3	2.33	0.43
2:F:181:LYS:HD2	2:F:181:LYS:HA	1.60	0.43
2:F:242:ALA:CB	2:F:246:ARG:HB2	2.48	0.43
2:F:50:ARG:CG	2:F:52:PRO:CD	2.84	0.43
1:B:146:VAL:CG2	2:D:145:LEU:HD21	2.48	0.43
2:C:166:LEU:HD13	2:C:166:LEU:HA	1.91	0.43
2:C:55:LEU:CD2	2:C:55:LEU:C	2.87	0.43
2:D:181:LYS:HD2	2:D:181:LYS:HA	1.72	0.43
1:A:270:PHE:HE1	1:A:274:LEU:HD11	1.83	0.43
1:B:99:LYS:CD	1:B:99:LYS:C	2.86	0.43
2:F:279:VAL:HG23	2:F:280:LEU:N	2.32	0.43
2:D:137:ASP:CG	2:D:138:PRO:HD2	2.39	0.43
2:C:155:VAL:HG12	2:C:155:VAL:O	2.18	0.43
2:C:72:PRO:HG3	2:C:132:HIS:CB	2.48	0.43
2:F:22:MET:O	2:F:35:ARG:CD	2.67	0.43
2:C:176:GLU:HG3	2:C:179:VAL:HG11	0.98	0.43
2:C:5:LEU:C	2:C:8:THR:OG1	2.54	0.43
2:D:260:LEU:HD23	2:D:260:LEU:N	2.33	0.43
1:A:276:SER:HA	1:A:279:ARG:HG3	2.00	0.43
1:A:79:THR:O	1:A:83:VAL:HG23	2.17	0.43
2:C:6:TYR:OH	2:C:58:ALA:HB2	2.19	0.43
2:C:62:LEU:HD13	2:C:63:LEU:HB2	1.99	0.43
2:D:234:GLY:N	2:D:235:ASN:CA	2.81	0.43
2:D:286:VAL:C	2:D:288:TYR:HA	2.38	0.43
1:E:268:ARG:HA	1:E:268:ARG:HD2	1.74	0.43
2:F:147:VAL:HG21	2:F:201:LEU:HD11	1.99	0.43
2:F:230:ARG:HD2	2:F:230:ARG:HA	1.85	0.43
1:A:188:LEU:O	1:A:192:ALA:HB3	2.19	0.43
1:A:35:GLU:HG3	1:A:106:TYR:OH	2.18	0.43
2:F:133:THR:HG21	2:F:144:LEU:HD21	2.01	0.43
2:F:208:GLU:C	2:F:212:LEU:HD22	2.39	0.43
1:A:96:ARG:CG	1:A:97:ARG:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:C	1:B:97:ARG:CG	2.86	0.42
2:C:140:PRO:O	2:C:143:VAL:HB	2.19	0.42
2:C:269:ASP:C	2:C:271:PHE:N	2.71	0.42
2:C:59:ALA:O	2:C:62:LEU:HB3	2.19	0.42
1:E:158:SER:HB2	2:F:31:HIS:HE2	1.83	0.42
1:A:237:THR:HG22	1:A:238:LYS:HG3	2.01	0.42
2:D:235:ASN:N	2:D:235:ASN:OD1	2.51	0.42
1:E:144:ARG:HG3	1:E:204:ILE:HG23	2.01	0.42
2:F:280:LEU:N	2:F:281:PRO:HD2	2.35	0.42
1:B:78:HIS:O	1:B:81:SER:OG	2.14	0.42
2:F:26:THR:CB	2:F:27:PRO:HD2	2.49	0.42
2:D:225:LEU:CD1	2:D:244:VAL:HG21	2.50	0.42
2:F:22:MET:HE1	2:F:34:MET:HB3	2.01	0.42
2:F:36:TYR:O	2:F:36:TYR:CD1	2.73	0.42
1:B:168:ASP:C	1:B:170:GLU:N	2.73	0.42
2:D:208:GLU:HG2	2:D:208:GLU:H	1.49	0.42
2:F:160:MET:HG3	2:F:164:GLN:NE2	2.28	0.42
2:C:22:MET:HE1	2:C:38:VAL:HG21	2.00	0.42
2:D:87:HIS:O	2:D:93:PHE:CE2	2.71	0.42
1:E:35:GLU:HG3	1:E:106:TYR:OH	2.20	0.42
2:C:108:ALA:HB1	1:E:279:ARG:HH21	1.85	0.42
1:B:223:ILE:HA	1:B:226:LEU:HB3	2.02	0.42
2:C:150:GLU:CG	2:C:193:CYS:HB2	2.49	0.42
2:C:196:ALA:HB2	2:C:213:ARG:HB2	2.02	0.42
1:E:20:LEU:HD22	1:E:41:LEU:HD11	2.01	0.42
1:E:85:ASP:O	1:E:91:ASP:HB2	2.19	0.42
2:F:120:ALA:O	2:F:123:PRO:HD2	2.20	0.42
1:A:29:PRO:C	1:A:31:ALA:N	2.72	0.42
1:B:120:SER:HB2	2:D:155:VAL:HG22	2.02	0.42
1:A:302:TYR:CB	2:D:29:ARG:HG3	2.49	0.42
1:E:58:ALA:HA	1:E:62:GLY:O	2.20	0.42
2:F:55:LEU:CD1	2:F:55:LEU:C	2.87	0.42
2:F:68:GLU:OE2	2:F:68:GLU:HA	2.19	0.42
1:A:147:ARG:HG3	1:A:204:ILE:HG21	2.01	0.42
2:D:275:TYR:HA	2:D:275:TYR:HD1	1.73	0.42
2:F:270:ARG:CG	2:F:270:ARG:HH21	2.32	0.42
2:F:25:ARG:CD	2:F:31:HIS:CE1	3.00	0.42
1:B:116:ASP:OD2	2:D:87:HIS:ND1	2.46	0.42
2:D:132:HIS:N	2:D:132:HIS:ND1	2.63	0.42
2:D:133:THR:HA	2:D:134:PRO:HD2	1.75	0.42
2:D:232:ALA:HA	2:D:233:SER:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:CD	2:D:24:ILE:HD13	2.39	0.42
2:F:26:THR:CG2	2:F:27:PRO:HD2	2.50	0.42
1:A:135:ASP:O	1:A:135:ASP:CG	2.55	0.41
2:F:145:LEU:HA	2:F:148:LEU:HD12	2.02	0.41
2:F:34:MET:O	2:F:37:ALA:CA	2.67	0.41
2:F:50:ARG:CG	2:F:52:PRO:HD2	2.40	0.41
1:A:41:LEU:O	1:A:47:ARG:NH2	2.53	0.41
1:A:73:ALA:HB2	1:A:126:MET:HG3	2.02	0.41
1:B:49:ARG:HG3	1:B:49:ARG:H	1.63	0.41
2:C:176:GLU:HA	2:C:176:GLU:OE2	2.21	0.41
2:C:180:MET:O	2:C:180:MET:SD	2.79	0.41
2:D:120:ALA:O	2:D:123:PRO:HD2	2.20	0.41
1:E:100:PRO:CB	1:E:104:VAL:HG21	2.45	0.41
2:F:243:SER:CB	2:F:244:VAL:C	2.88	0.41
1:E:79:THR:O	1:E:83:VAL:HG23	2.21	0.41
2:F:245:LEU:N	2:F:245:LEU:CD2	2.72	0.41
2:D:91:PRO:HD3	2:D:106:HIS:CE1	2.55	0.41
2:D:36:TYR:OH	2:D:103:PRO:CD	2.66	0.41
1:B:156:ILE:O	1:B:162:VAL:CG2	2.67	0.41
2:D:25:ARG:O	2:D:31:HIS:CE1	2.74	0.41
1:E:129:PHE:CE2	2:F:145:LEU:HD12	2.55	0.41
2:F:52:PRO:CD	2:F:53:PRO:HD2	2.50	0.41
1:B:129:PHE:CZ	1:B:142:PRO:HG3	2.50	0.41
2:D:258:GLU:CA	2:D:258:GLU:OE1	2.68	0.41
2:D:256:ILE:O	2:D:260:LEU:HG	2.20	0.41
2:F:285:PHE:CD1	2:F:285:PHE:O	2.73	0.41
2:F:50:ARG:CZ	2:F:50:ARG:HB2	2.50	0.41
2:D:221:VAL:HG12	2:D:221:VAL:O	2.21	0.41
1:E:144:ARG:HD3	1:E:204:ILE:O	2.20	0.41
2:F:18:LEU:HA	2:F:18:LEU:HD23	1.83	0.41
2:F:69:ALA:O	2:F:201:LEU:CD2	2.68	0.41
2:F:215:TYR:OH	2:F:279:VAL:CB	2.63	0.41
1:B:50:PRO:O	1:B:54:LEU:HG	2.21	0.41
2:D:277:GLU:O	2:D:280:LEU:N	2.50	0.41
1:B:169:LEU:H	1:B:169:LEU:HD12	1.85	0.41
2:C:150:GLU:OE1	2:C:193:CYS:HB3	2.20	0.41
2:C:62:LEU:HD22	2:C:63:LEU:CD2	2.50	0.41
2:D:270:ARG:CZ	2:D:271:PHE:CD2	3.03	0.41
2:D:286:VAL:CG1	2:D:287:ASP:N	2.84	0.41
2:D:85:LEU:N	2:D:237:LYS:NZ	2.69	0.41
1:E:209:SER:OG	1:E:212:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:CG	2:D:24:ILE:HD13	2.50	0.41
1:A:28:GLU:OE1	1:A:30:PRO:CD	2.69	0.41
2:C:206:PRO:C	2:C:209:GLU:H	2.23	0.41
2:C:7:TRP:C	2:C:7:TRP:CD1	2.94	0.41
1:E:152:LEU:O	1:E:156:ILE:HG13	2.20	0.41
1:E:201:ILE:HA	1:E:204:ILE:HB	2.03	0.41
1:E:296:LEU:O	1:E:300:ILE:HG13	2.21	0.41
2:F:11:ILE:HA	2:F:14:VAL:HG12	2.02	0.41
2:F:166:LEU:HD23	2:F:166:LEU:HA	1.74	0.41
1:A:279:ARG:HH22	2:D:108:ALA:C	2.17	0.41
2:C:57:VAL:HG11	2:C:67:ARG:HD2	2.02	0.41
2:C:89:ASP:N	2:C:89:ASP:OD1	2.53	0.41
2:F:34:MET:O	2:F:35:ARG:C	2.57	0.41
2:F:60:CYS:O	2:F:65:ALA:HB2	2.19	0.41
1:B:300:ILE:O	1:B:303:ARG:HD3	2.20	0.40
2:C:35:ARG:HB3	2:C:39:LEU:HD12	2.01	0.40
2:F:172:THR:OG1	2:F:172:THR:O	2.28	0.40
2:F:252:ARG:HD2	2:F:252:ARG:C	2.42	0.40
2:C:180:MET:O	2:C:180:MET:CG	2.69	0.40
2:C:10:LEU:CD2	2:C:54:VAL:HG23	2.50	0.40
2:D:216:GLY:O	2:D:219:ILE:HG22	2.21	0.40
2:F:11:ILE:O	2:F:12:ALA:C	2.57	0.40
2:C:180:MET:HE1	2:C:242:ALA:O	2.19	0.40
2:D:272:GLY:O	2:D:274:LYS:CG	2.70	0.40
2:D:222:LEU:HD21	2:D:286:VAL:HG11	2.02	0.40
2:F:212:LEU:O	2:F:213:ARG:C	2.53	0.40
2:F:248:LEU:HD13	2:F:248:LEU:HA	1.67	0.40
1:B:152:LEU:O	1:B:156:ILE:HG13	2.21	0.40
2:D:170:GLY:O	2:D:171:ALA:CB	2.69	0.40
2:D:270:ARG:HH11	2:D:274:LYS:NZ	2.19	0.40
2:F:21:ALA:O	2:F:23:PRO:HD2	2.21	0.40
1:B:159:GLU:OE1	1:B:159:GLU:CA	2.69	0.40
1:B:187:HIS:HD2	1:B:258:TYR:HE1	1.67	0.40
2:C:133:THR:N	2:C:134:PRO:CD	2.82	0.40
2:C:23:PRO:CD	2:C:23:PRO:O	2.70	0.40
2:C:280:LEU:N	2:C:281:PRO:CD	2.84	0.40
2:C:71:LEU:HA	2:C:71:LEU:HD12	1.76	0.40
2:F:62:LEU:C	2:F:62:LEU:CD2	2.86	0.40
2:F:60:CYS:CB	2:F:70:ALA:HB2	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLN:NE2	2:F:29:ARG:NH2[1_545]	1.64	0.56
1:B:279:ARG:NH2	2:F:108:ALA:O[1_545]	2.04	0.16

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	273/305 (90%)	258 (94%)	14 (5%)	1 (0%)	38	77
1	B	267/305 (88%)	252 (94%)	14 (5%)	1 (0%)	38	77
1	E	268/305 (88%)	239 (89%)	28 (10%)	1 (0%)	38	77
2	C	248/304 (82%)	223 (90%)	20 (8%)	5 (2%)	9	49
2	D	252/304 (83%)	221 (88%)	25 (10%)	6 (2%)	7	45
2	F	247/304 (81%)	220 (89%)	19 (8%)	8 (3%)	5	38
All	All	1555/1827 (85%)	1413 (91%)	120 (8%)	22 (1%)	13	56

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	137	ASP
2	F	27	PRO
2	F	51	ALA
2	C	68	GLU
2	F	142	ALA
2	F	178	GLU
2	C	39	LEU
1	A	138	ALA
1	B	158	SER
2	D	36	TYR
2	D	168	LEU
1	E	163	ALA
2	F	177	ALA
2	F	250	MET

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Mol	Chain	Res	Type
2	F	278	ARG
2	D	55	LEU
2	C	6	TYR
2	C	51	ALA
2	D	51	ALA
2	D	279	VAL
2	F	23	PRO
2	D	23	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/239 (93%)	216 (97%)	6 (3%)	50	81
1	B	217/239 (91%)	207 (95%)	10 (5%)	31	69
1	E	219/239 (92%)	211 (96%)	8 (4%)	39	74
2	C	194/223 (87%)	160 (82%)	34 (18%)	2	15
2	D	196/223 (88%)	168 (86%)	28 (14%)	4	26
2	F	197/223 (88%)	161 (82%)	36 (18%)	2	12
All	All	1245/1386 (90%)	1123 (90%)	122 (10%)	9	42

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	49	ARG
1	A	88	PRO
1	A	89	CYS
1	A	95	LEU
1	A	211	GLU
2	C	6	TYR
2	C	8	THR
2	C	9	SER
2	C	11	ILE

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Mol	Chain	Res	Type
2	C	15	GLU
2	C	23	PRO
2	C	24	ILE
2	C	38	VAL
2	C	56	CYS
2	C	62	LEU
2	C	72	PRO
2	C	80	LEU
2	C	138	PRO
2	C	139	VAL
2	C	144	LEU
2	C	157	SER
2	C	166	LEU
2	C	174	LEU
2	C	184	THR
2	C	186	LYS
2	C	208	GLU
2	C	227	ASP
2	C	230	ARG
2	C	231	SER
2	C	235	ASN
2	C	238	MET
2	C	245	LEU
2	C	248	LEU
2	C	265	LYS
2	C	266	MET
2	C	273	ASP
2	C	283	TYR
2	C	287	ASP
2	C	288	TYR
1	B	11	GLU
1	B	91	ASP
1	B	96	ARG
1	B	97	ARG
1	B	99	LYS
1	B	166	VAL
1	B	170	GLU
1	B	171	MET
1	B	177	THR
1	B	236	VAL
2	D	4	ARG
2	D	11	ILE

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Mol	Chain	Res	Type
2	D	27	PRO
2	D	50	ARG
2	D	67	ARG
2	D	72	PRO
2	D	94	ASP
2	D	104	SER
2	D	105	THR
2	D	132	HIS
2	D	133	THR
2	D	141	HIS
2	D	155	VAL
2	D	158	THR
2	D	168	LEU
2	D	180	MET
2	D	181	LYS
2	D	184	THR
2	D	208	GLU
2	D	212	LEU
2	D	213	ARG
2	D	218	THR
2	D	239	ARG
2	D	245	LEU
2	D	258	GLU
2	D	270	ARG
2	D	273	ASP
2	D	275	TYR
1	E	28	GLU
1	E	99	LYS
1	E	140	LYS
1	E	144	ARG
1	E	166	VAL
1	E	238	LYS
1	E	257	THR
1	E	258	TYR
2	F	4	ARG
2	F	5	LEU
2	F	19	ASP
2	F	27	PRO
2	F	29	ARG
2	F	49	LYS
2	F	55	LEU
2	F	72	PRO

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Mol	Chain	Res	Type
2	F	78	GLU
2	F	85	LEU
2	F	88	ASP
2	F	89	ASP
2	F	102	ARG
2	F	104	SER
2	F	132	HIS
2	F	137	ASP
2	F	141	HIS
2	F	151	LEU
2	F	153	ARG
2	F	155	VAL
2	F	157	SER
2	F	183	LEU
2	F	209	GLU
2	F	212	LEU
2	F	213	ARG
2	F	218	THR
2	F	239	ARG
2	F	243	SER
2	F	245	LEU
2	F	251	ASP
2	F	252	ARG
2	F	258	GLU
2	F	265	LYS
2	F	275	TYR
2	F	283	TYR
2	F	288	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	304	GLN
2	C	141	HIS
2	C	235	ASN
2	C	263	GLN
1	B	6	ASN
2	D	141	HIS
2	D	224	GLN
1	E	228	GLN
2	F	106	HIS

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Mol	Chain	Res	Type
2	F	128	HIS
2	F	164	GLN
2	F	235	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	281/305 (92%)	0.27	17 (6%) 23 16	30, 84, 108, 141	0
1	B	277/305 (90%)	0.32	17 (6%) 22 16	68, 86, 112, 129	0
1	E	278/305 (91%)	0.49	18 (6%) 20 14	55, 84, 110, 142	0
2	C	262/304 (86%)	0.35	23 (8%) 11 8	50, 91, 119, 135	0
2	D	266/304 (87%)	0.27	17 (6%) 20 14	51, 90, 125, 138	0
2	F	263/304 (86%)	0.39	11 (4%) 37 26	53, 90, 119, 141	0
All	All	1627/1827 (89%)	0.35	103 (6%) 21 15	30, 88, 118, 142	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	ILE	9.2
2	F	247	ALA	7.4
2	C	202	GLY	6.4
1	B	90	MET	5.7
1	A	228	GLN	5.4
1	A	116	ASP	5.4
2	C	198	GLY	5.4
2	F	70	ALA	5.3
2	C	265	LYS	5.2
2	C	286	VAL	5.2
2	F	245	LEU	4.9
1	B	98	GLY	4.9
2	D	259	GLU	4.7
2	F	126	TYR	4.5
1	B	56	ALA	4.4
2	F	69	ALA	4.2
1	E	285	PHE	4.1
1	A	114	THR	4.0
1	B	158	SER	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	162	ALA	4.0
2	C	249	GLY	3.9
2	C	93	PHE	3.9
2	C	252	ARG	3.8
2	D	198	GLY	3.7
1	A	183	LEU	3.7
1	B	263	GLY	3.7
2	C	133	THR	3.6
1	A	223	ILE	3.6
1	B	230	VAL	3.6
2	C	187	PHE	3.6
1	B	303	ARG	3.6
2	D	52	PRO	3.6
1	A	232	ASP	3.4
2	C	154	ALA	3.4
1	A	272	GLU	3.4
2	C	30	ILE	3.4
1	E	103	HIS	3.3
2	F	190	MET	3.3
1	A	287	GLN	3.3
1	A	155	CYS	3.3
1	B	24	ILE	3.2
2	C	168	LEU	3.2
1	A	224	GLY	3.2
1	A	56	ALA	3.0
2	C	250	MET	2.9
2	D	87	HIS	2.9
2	C	186	LYS	2.9
1	A	258	TYR	2.9
1	E	268	ARG	2.9
2	F	244	VAL	2.8
2	D	283	TYR	2.7
1	A	89	CYS	2.7
1	B	25	PRO	2.7
1	B	198	SER	2.6
1	B	97	ARG	2.6
2	D	197	CYS	2.6
2	D	277	GLU	2.6
1	A	295	HIS	2.6
2	D	27	PRO	2.6
1	B	262	LEU	2.6
1	E	205	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	63	LEU	2.5
2	C	226	VAL	2.5
2	D	247	ALA	2.5
1	E	89	CYS	2.5
1	E	102	CYS	2.5
1	E	27	ASP	2.5
2	C	219	ILE	2.4
1	E	261	LEU	2.4
2	C	209	GLU	2.4
1	B	114	THR	2.4
2	C	54	VAL	2.4
2	C	71	LEU	2.4
2	F	62	LEU	2.4
1	E	258	TYR	2.4
2	D	243	SER	2.4
2	C	267	GLU	2.3
1	E	275	LEU	2.3
2	D	183	LEU	2.3
2	D	191	ALA	2.3
1	B	299	TYR	2.3
1	E	105	VAL	2.3
2	D	199	ALA	2.2
2	D	281	PRO	2.2
1	E	123	PHE	2.2
2	F	248	LEU	2.2
1	E	216	LEU	2.2
2	F	283	TYR	2.2
1	E	74	VAL	2.2
2	D	165	PHE	2.1
2	C	268	ALA	2.1
2	F	201	LEU	2.1
1	B	196	GLU	2.1
1	E	83	VAL	2.1
1	E	88	PRO	2.1
1	E	161	LEU	2.1
2	C	127	THR	2.0
1	A	275	LEU	2.0
1	B	167	VAL	2.0
1	A	187	HIS	2.0
1	E	5	PHE	2.0
2	D	159	GLY	2.0
1	A	77	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.