



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 PM UTC

PDB ID : 3MFM / pdb_00003mfm
Title : Crystal Structures and Mutational Analyses of Acyl-CoA Carboxylase Subunit of *Streptomyces coelicolor*
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Melgar, M.M.
Deposited on : 2010-04-02
Resolution : 2.38 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

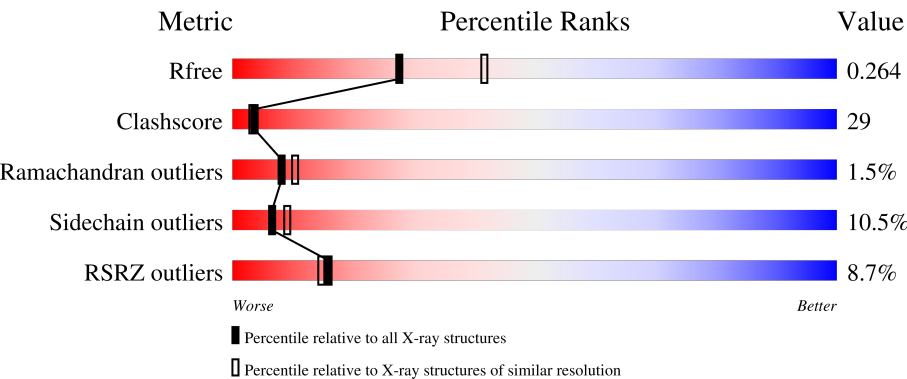
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	530	11% 48% 41% 8% .
1	B	530	11% 49% 41% 8% ..
1	C	530	7% 58% 33% 6% .
1	D	530	8% 54% 38% 6% .
1	E	530	7% 57% 34% 7% .

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Mol	Chain	Length	Quality of chain
1	F	530	7% 58% 35% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23718 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 Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	F	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	A	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	B	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	D	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	E	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			

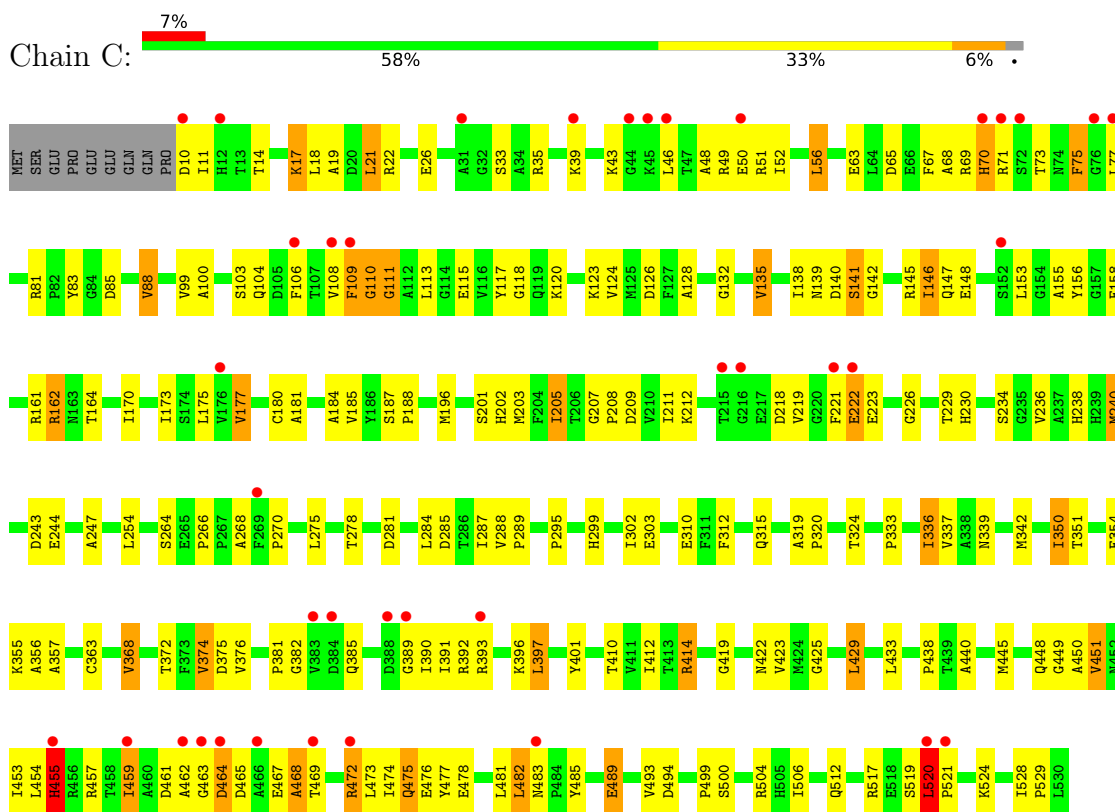
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	422	ASN	ASP	engineered mutation	UNP Q9X4K7
F	422	ASN	ASP	engineered mutation	UNP Q9X4K7
A	422	ASN	ASP	engineered mutation	UNP Q9X4K7
B	422	ASN	ASP	engineered mutation	UNP Q9X4K7
D	422	ASN	ASP	engineered mutation	UNP Q9X4K7
E	422	ASN	ASP	engineered mutation	UNP Q9X4K7

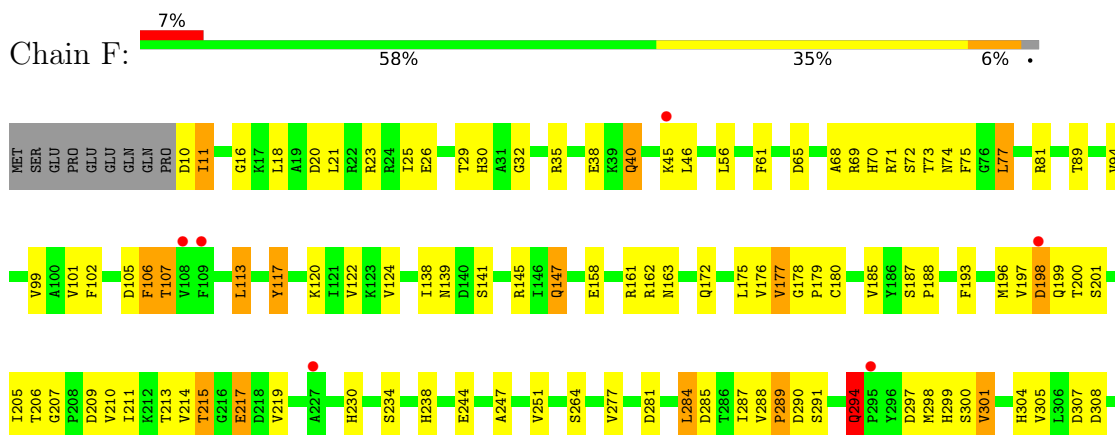
3 Residue-property plots [i](#)

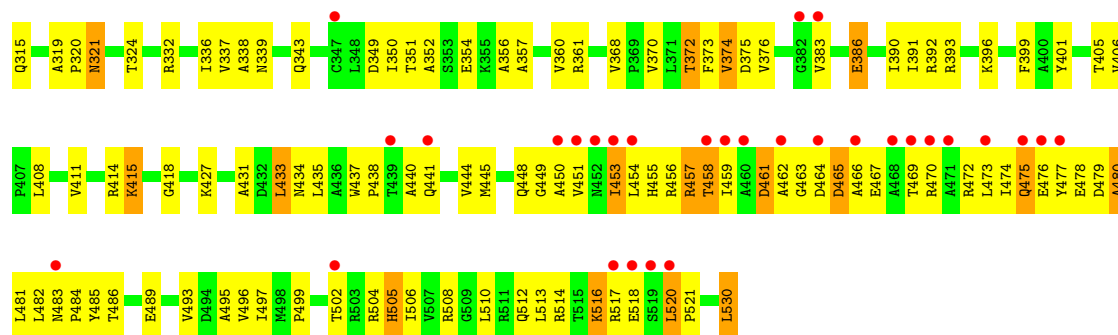
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Propionyl-CoA carboxylase complex B subunit

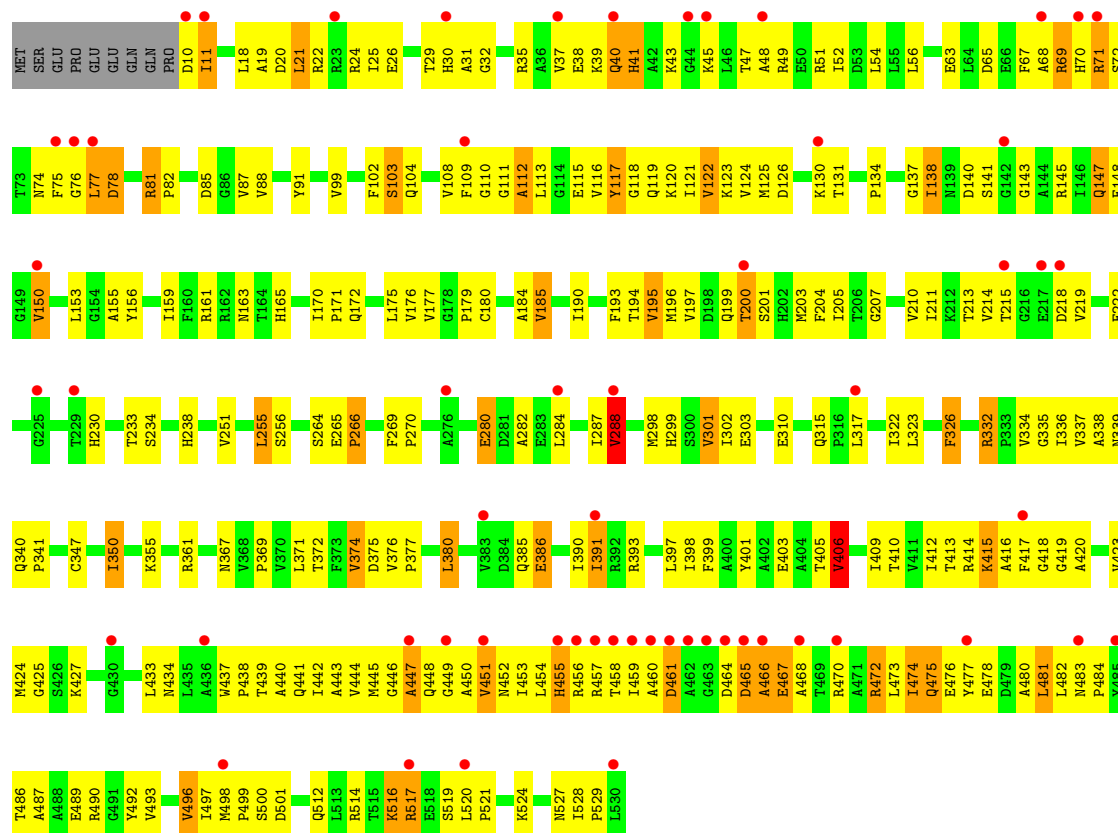


- Molecule 1: Propionyl-CoA carboxylase complex B subunit

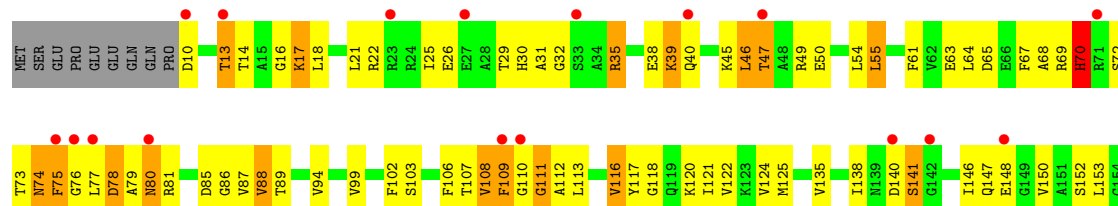


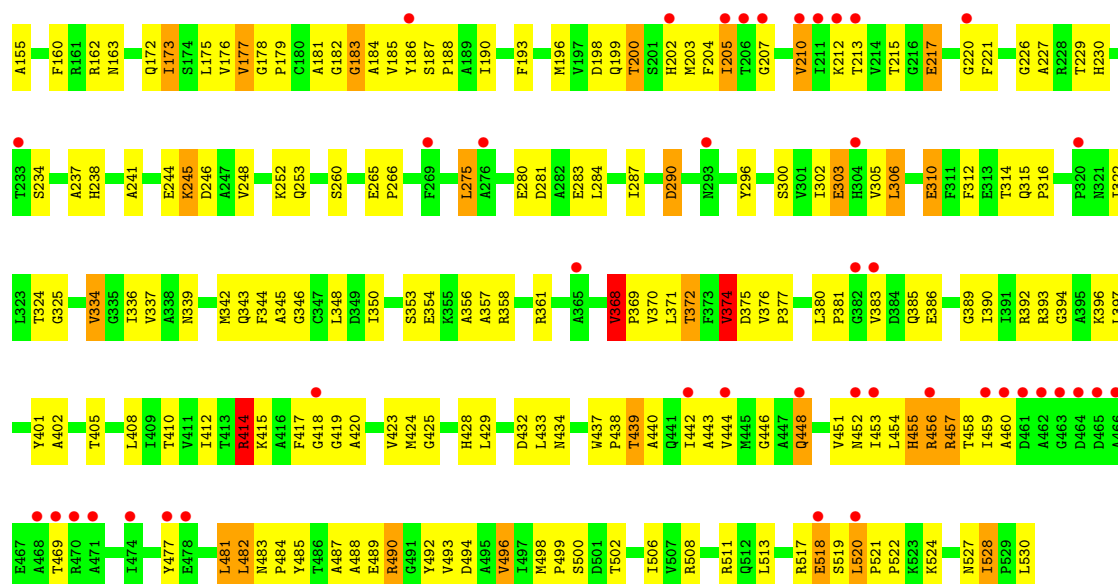


● Molecule 1: Propionyl-CoA carboxylase complex B subunit

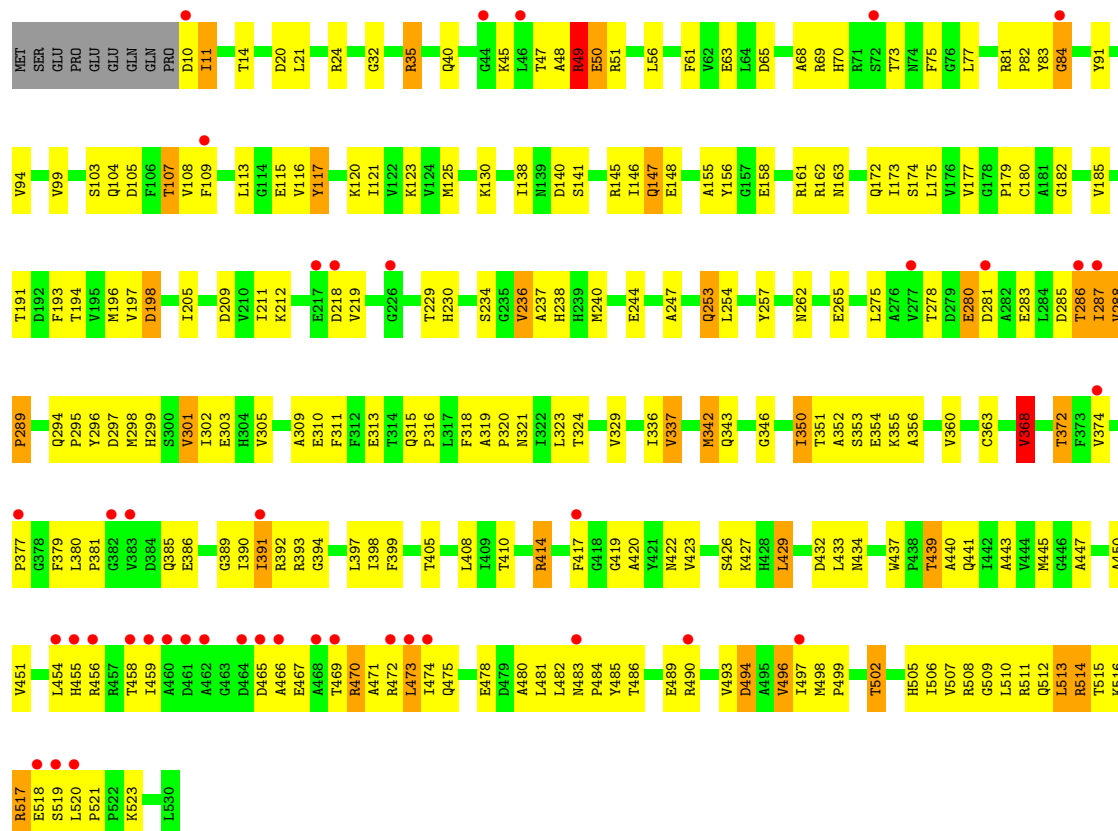


● Molecule 1: Propionyl-CoA carboxylase complex B subunit



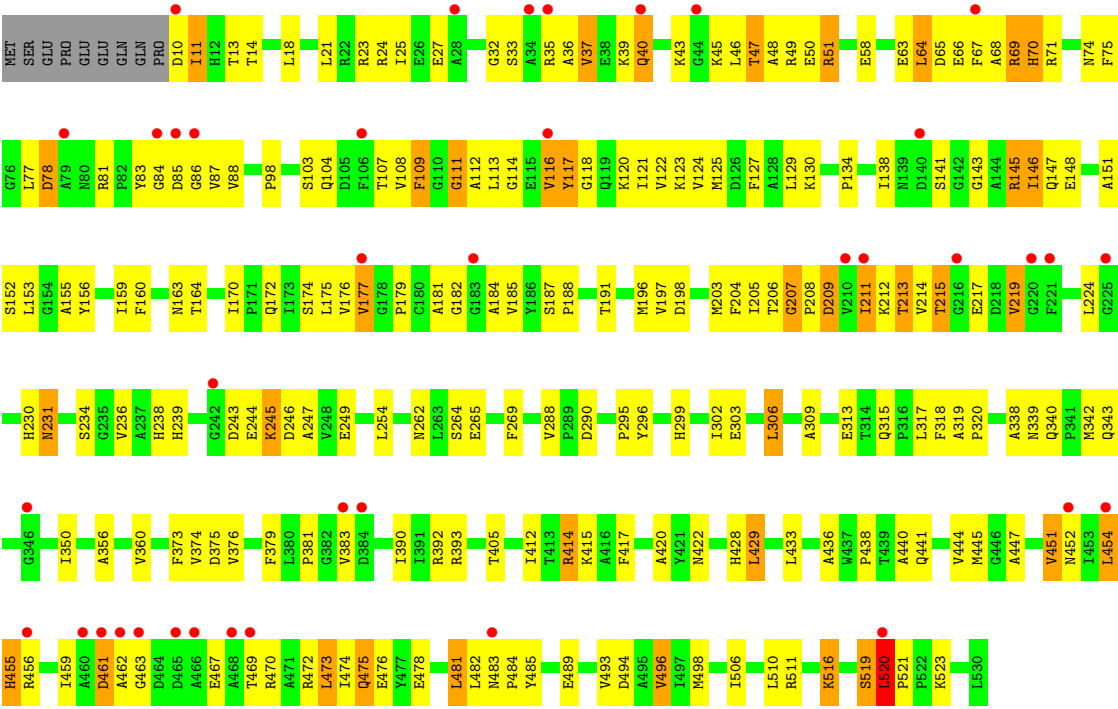


• Molecule 1: Propionyl-CoA carboxylase complex B subunit



• Molecule 1: Propionyl-CoA carboxylase complex B subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.67Å 220.96Å 136.74Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	38.82 – 2.38 38.82 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.82-2.38) 99.2 (38.82-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.268 0.219 , 0.264	Depositor DCC
R_{free} test set	9136 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	1.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23718	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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 45.90 % 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 1.2372e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.54	0/4033	0.92	7/5478 (0.1%)
1	B	0.56	0/4033	0.97	9/5478 (0.2%)
1	C	0.55	0/4033	0.93	11/5478 (0.2%)
1	D	0.57	0/4033	0.95	9/5478 (0.2%)
1	E	0.54	1/4033 (0.0%)	0.91	7/5478 (0.1%)
1	F	0.53	0/4033	0.91	6/5478 (0.1%)
All	All	0.55	1/24198 (0.0%)	0.93	49/32868 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	122	VAL	CA-CB	5.33	1.60	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	49	ARG	N-CA-C	-8.24	99.14	110.35
1	C	109	PHE	N-CA-C	-8.15	97.48	108.24
1	E	111	GLY	N-CA-C	-7.25	105.31	115.32
1	B	368	VAL	CA-C-N	7.21	127.25	119.89
1	B	368	VAL	C-N-CA	7.21	127.25	119.89
1	A	374	VAL	N-CA-C	7.09	117.87	107.37
1	E	288	VAL	N-CA-C	6.96	113.89	107.56
1	A	288	VAL	CA-C-N	6.92	126.94	119.89
1	A	288	VAL	C-N-CA	6.92	126.94	119.89
1	B	55	LEU	N-CA-C	6.55	118.42	111.28
1	F	178	GLY	CA-C-N	-6.38	113.38	120.14
1	F	178	GLY	C-N-CA	-6.38	113.38	120.14
1	D	350	ILE	CB-CA-C	-6.24	104.01	111.81
1	C	111	GLY	N-CA-C	-6.22	106.74	115.32
1	C	476	GLU	N-CA-C	-6.14	103.90	111.33
1	C	520	LEU	CA-C-N	5.86	126.41	120.38
1	C	520	LEU	C-N-CA	5.86	126.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	GLU	N-CA-C	5.83	115.98	108.34
1	C	141	SER	N-CA-C	5.76	118.04	108.13
1	A	524	LYS	N-CA-C	-5.73	104.64	111.69
1	B	524	LYS	N-CA-C	-5.63	105.29	111.82
1	E	462	ALA	N-CA-C	-5.52	106.92	113.38
1	B	511	ARG	N-CA-C	-5.48	105.31	111.28
1	D	374	VAL	N-CA-C	5.38	115.60	107.75
1	A	41	HIS	N-CA-C	-5.37	104.67	111.11
1	C	135	VAL	CB-CA-C	-5.36	102.69	110.63
1	F	415	LYS	N-CA-C	5.36	118.96	109.96
1	D	130	LYS	N-CA-C	5.35	117.11	111.28
1	E	269	PHE	CA-C-N	5.33	125.34	119.90
1	E	269	PHE	C-N-CA	5.33	125.34	119.90
1	B	374	VAL	N-CA-C	5.33	115.80	108.12
1	D	236	VAL	N-CA-C	5.29	116.77	111.00
1	F	368	VAL	N-CA-C	5.27	113.08	107.76
1	D	84	GLY	N-CA-C	-5.26	99.61	112.44
1	D	368	VAL	CA-C-N	5.25	125.54	119.92
1	D	368	VAL	C-N-CA	5.25	125.54	119.92
1	E	207	GLY	CA-C-N	5.24	124.86	119.56
1	E	207	GLY	C-N-CA	5.24	124.86	119.56
1	C	115	GLU	N-CA-C	5.21	116.65	111.07
1	B	310	GLU	N-CA-C	5.19	117.19	108.73
1	D	419	GLY	N-CA-C	-5.14	106.56	112.73
1	C	524	LYS	N-CA-C	-5.13	105.68	111.28
1	B	111	GLY	N-CA-C	-5.09	108.96	115.42
1	C	139	ASN	N-CA-C	5.07	116.87	108.20
1	C	336	ILE	N-CA-C	5.04	115.17	108.11
1	F	294	GLN	CA-C-N	5.02	125.46	120.14
1	F	294	GLN	C-N-CA	5.02	125.46	120.14
1	A	266	PRO	CA-C-N	5.01	125.01	119.90
1	A	266	PRO	C-N-CA	5.01	125.01	119.90

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	3953	0	3882	331	0
1	B	3953	0	3882	310	0
1	C	3953	0	3882	199	0
1	D	3953	0	3882	226	0
1	E	3953	0	3882	234	0
1	F	3953	0	3882	214	0
All	All	23718	0	23292	1371	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 29.

All (1371) 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:B:337:VAL:HG21	1:B:401:TYR:OH	1.46	1.15
1:E:69:ARG:HG3	1:E:69:ARG:HH11	1.01	1.13
1:B:35:ARG:HG2	1:B:35:ARG:HH11	1.06	1.13
1:C:520:LEU:HD12	1:C:521:PRO:HD2	1.16	1.12
1:A:163:ASN:HB3	1:A:190:ILE:HD11	1.23	1.11
1:E:376:VAL:HG11	1:E:420:ALA:HB1	1.34	1.08
1:A:415:LYS:HE3	1:A:416:ALA:H	1.13	1.07
1:A:415:LYS:HE3	1:A:416:ALA:N	1.69	1.07
1:A:81:ARG:HG2	1:A:81:ARG:HH11	0.95	1.06
1:E:51:ARG:HG2	1:E:51:ARG:HH11	1.17	1.06
1:B:196:MET:HE1	1:B:230:HIS:HB2	1.38	1.05
1:F:18:LEU:HG	1:E:498:MET:HE1	1.39	1.04
1:D:286:THR:O	1:D:288:VAL:HG12	1.55	1.04
1:B:339:ASN:HD21	1:B:424:MET:HE3	1.20	1.03
1:A:111:GLY:HA3	1:A:141:SER:HA	1.39	1.03
1:A:451:VAL:HG21	1:A:474:ILE:HD13	1.41	1.02
1:D:397:LEU:HD23	1:D:423:VAL:HG12	1.42	1.01
1:A:69:ARG:HG2	1:A:69:ARG:HH11	1.27	1.00
1:A:350:ILE:HD11	1:A:393:ARG:HH11	1.24	0.99
1:D:196:MET:HE1	1:D:230:HIS:HB2	1.45	0.99
1:B:35:ARG:HG2	1:B:35:ARG:NH1	1.69	0.98
1:E:295:PRO:HB2	1:E:342:MET:HE2	1.46	0.97
1:A:498:MET:HE3	1:A:500:SER:HB3	1.47	0.96
1:E:35:ARG:HG2	1:E:39:LYS:HE3	1.46	0.96
1:A:81:ARG:HG2	1:A:81:ARG:NH1	1.72	0.96
1:D:320:PRO:HB2	1:D:343:GLN:HE21	1.31	0.95
1:E:519:SER:O	1:E:520:LEU:HB2	1.66	0.95
1:D:196:MET:HE2	1:D:237:ALA:HB2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:PRO:HA	1:E:211:ILE:HG12	1.48	0.94
1:B:138:ILE:HG23	1:B:175:LEU:HD23	1.50	0.92
1:A:380:LEU:HD11	1:A:385:GLN:HG3	1.50	0.92
1:B:374:VAL:HG13	1:B:412:ILE:HD13	1.51	0.92
1:E:69:ARG:HG3	1:E:69:ARG:NH1	1.80	0.92
1:A:456:ARG:HD3	1:A:459:ILE:HG12	1.52	0.92
1:D:32:GLY:HA3	1:D:107:THR:HG23	1.52	0.92
1:F:445:MET:HE3	1:F:450:ALA:HA	1.51	0.91
1:E:113:LEU:HD23	1:E:156:TYR:CE1	2.05	0.91
1:D:32:GLY:HA3	1:D:107:THR:CG2	2.01	0.90
1:B:35:ARG:HH11	1:B:35:ARG:CG	1.83	0.90
1:C:288:VAL:O	1:D:14:THR:HG21	1.73	0.89
1:D:194:THR:H	1:D:238:HIS:HD2	1.20	0.89
1:E:295:PRO:HB2	1:E:342:MET:CE	2.01	0.89
1:A:163:ASN:HB3	1:A:190:ILE:CD1	2.03	0.88
1:B:72:SER:OG	1:B:77:LEU:HD13	1.73	0.88
1:B:72:SER:OG	1:B:77:LEU:CD1	2.21	0.88
1:A:452:ASN:HB2	1:A:456:ARG:HH21	1.38	0.88
1:E:215:THR:HB	1:E:217:GLU:HG2	1.54	0.88
1:A:350:ILE:HD11	1:A:393:ARG:NH1	1.89	0.87
1:A:391:ILE:HD12	1:A:391:ILE:H	1.37	0.87
1:C:14:THR:HG21	1:A:288:VAL:O	1.75	0.87
1:F:56:LEU:HD21	1:F:101:VAL:HG21	1.56	0.87
1:F:475:GLN:HA	1:F:478:GLU:HG2	1.56	0.86
1:F:288:VAL:O	1:B:14:THR:HG21	1.75	0.86
1:A:150:VAL:HG11	1:B:442:ILE:HG22	1.57	0.86
1:D:337:VAL:HG13	1:D:372:THR:HB	1.55	0.85
1:A:18:LEU:HD13	1:D:498:MET:HE1	1.56	0.85
1:B:305:VAL:O	1:B:306:LEU:HG	1.76	0.85
1:F:451:VAL:HA	1:F:454:LEU:HG	1.58	0.85
1:D:472:ARG:HE	1:D:475:GLN:HB3	1.39	0.85
1:B:10:ASP:O	1:B:16:GLY:HA3	1.77	0.85
1:F:497:ILE:HG21	1:F:505:HIS:CE1	2.12	0.84
1:A:465:ASP:OD2	1:A:467:GLU:HG2	1.77	0.84
1:F:32:GLY:HA3	1:F:107:THR:HG23	1.60	0.84
1:A:451:VAL:HG21	1:A:474:ILE:CD1	2.08	0.83
1:D:77:LEU:HD11	1:D:147:GLN:HG3	1.58	0.83
1:C:49:ARG:O	1:C:50:GLU:HB3	1.76	0.83
1:A:138:ILE:HG22	1:A:175:LEU:HB3	1.59	0.83
1:A:163:ASN:CB	1:A:190:ILE:HD11	2.08	0.83
1:A:380:LEU:HD11	1:A:385:GLN:CG	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:HG	1:B:521:PRO:HD2	1.59	0.82
1:E:113:LEU:HD13	1:E:117:TYR:CD2	2.14	0.82
1:C:187:SER:HB3	1:C:188:PRO:HD3	1.60	0.82
1:A:81:ARG:HH11	1:A:81:ARG:CG	1.86	0.82
1:E:520:LEU:HD22	1:E:521:PRO:HD2	1.60	0.82
1:F:458:THR:HG21	1:F:469:THR:HG21	1.62	0.82
1:B:415:LYS:HD2	1:B:417:PHE:CE1	2.15	0.81
1:E:36:ALA:HA	1:E:39:LYS:HD3	1.62	0.81
1:E:405:THR:O	1:E:516:LYS:HE3	1.79	0.81
1:C:109:PHE:C	1:C:111:GLY:H	1.88	0.81
1:D:286:THR:O	1:D:287:ILE:HG22	1.80	0.81
1:F:451:VAL:HB	1:F:470:ARG:CZ	2.10	0.81
1:A:478:GLU:HA	1:A:482:LEU:HD23	1.62	0.81
1:D:466:ALA:O	1:D:470:ARG:HB3	1.80	0.81
1:C:489:GLU:HA	1:D:68:ALA:HA	1.60	0.81
1:A:442:ILE:HG12	1:A:484:PRO:HA	1.63	0.81
1:A:112:ALA:HA	1:A:143:GLY:O	1.81	0.80
1:E:47:THR:HG22	1:E:50:GLU:HG2	1.62	0.80
1:A:288:VAL:HG21	1:A:439:THR:HG21	1.64	0.80
1:D:49:ARG:O	1:D:50:GLU:HB2	1.79	0.80
1:D:138:ILE:HD12	1:D:175:LEU:HD23	1.63	0.80
1:B:300:SER:HA	1:B:303:GLU:HG2	1.63	0.80
1:C:75:PHE:HE1	1:F:454:LEU:HD13	1.46	0.80
1:F:139:ASN:HB2	1:F:176:VAL:HG12	1.64	0.79
1:A:380:LEU:CD1	1:A:385:GLN:HG3	2.12	0.79
1:E:40:GLN:HG3	1:E:45:LYS:HB2	1.65	0.79
1:D:397:LEU:HD23	1:D:423:VAL:CG1	2.13	0.79
1:D:363:CYS:HB3	1:D:368:VAL:HG22	1.62	0.79
1:B:196:MET:HE3	1:B:227:ALA:HA	1.64	0.79
1:D:469:THR:HG22	1:D:473:LEU:HD22	1.64	0.79
1:B:21:LEU:O	1:B:25:ILE:HD12	1.82	0.79
1:B:69:ARG:HD3	1:B:81:ARG:HB2	1.65	0.79
1:D:520:LEU:HB2	1:D:521:PRO:HD2	1.65	0.79
1:D:105:ASP:OD1	1:D:107:THR:HB	1.82	0.78
1:D:286:THR:C	1:D:288:VAL:H	1.92	0.78
1:D:386:GLU:OE2	1:D:391:ILE:HD11	1.83	0.78
1:E:51:ARG:HG2	1:E:51:ARG:NH1	1.96	0.78
1:E:69:ARG:HH11	1:E:69:ARG:CG	1.91	0.78
1:E:243:ASP:HB3	1:E:246:ASP:OD1	1.84	0.78
1:E:339:ASN:OD1	1:E:376:VAL:HG23	1.84	0.78
1:A:323:LEU:HD21	1:A:340:GLN:HB2	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ARG:HD3	1:A:459:ILE:CG1	2.13	0.78
1:E:182:GLY:O	1:E:185:VAL:HG12	1.83	0.78
1:B:437:TRP:HE1	1:B:502:THR:HG21	1.49	0.78
1:A:103:SER:OG	1:A:138:ILE:HD11	1.84	0.77
1:A:369:PRO:HA	1:A:406:VAL:HG13	1.66	0.77
1:C:158:GLU:HG3	1:C:162:ARG:HH21	1.49	0.77
1:C:474:ILE:O	1:C:475:GLN:HB3	1.84	0.77
1:D:194:THR:H	1:D:238:HIS:CD2	2.03	0.77
1:A:111:GLY:HA3	1:A:141:SER:CA	2.14	0.77
1:D:354:GLU:OE2	1:D:393:ARG:HD3	1.85	0.77
1:C:39:LYS:O	1:C:43:LYS:HG3	1.83	0.76
1:F:18:LEU:HG	1:E:498:MET:CE	2.14	0.76
1:A:361:ARG:HD2	1:A:403:GLU:OE2	1.84	0.76
1:F:32:GLY:HA3	1:F:107:THR:CG2	2.15	0.76
1:A:323:LEU:CD2	1:A:340:GLN:HB2	2.16	0.76
1:A:70:HIS:HE2	1:A:148:GLU:CD	1.94	0.75
1:A:298:MET:HE3	1:A:301:VAL:HG11	1.68	0.75
1:A:211:ILE:HG21	1:B:383:VAL:HG23	1.67	0.75
1:F:448:GLN:HG2	1:F:449:GLY:H	1.51	0.75
1:B:393:ARG:O	1:B:396:LYS:HG3	1.87	0.75
1:E:203:MET:HB2	1:E:230:HIS:CE1	2.20	0.75
1:A:415:LYS:HD2	1:A:441:GLN:HB2	1.68	0.75
1:E:39:LYS:HD2	1:E:39:LYS:N	2.02	0.74
1:F:290:ASP:OD1	1:B:14:THR:HG23	1.86	0.74
1:A:380:LEU:HD12	1:A:380:LEU:O	1.86	0.74
1:C:350:ILE:HB	1:C:393:ARG:HG2	1.67	0.74
1:B:202:HIS:ND1	1:B:226:GLY:HA2	2.02	0.74
1:A:69:ARG:HG2	1:A:69:ARG:NH1	1.94	0.74
1:A:498:MET:CE	1:A:500:SER:HB3	2.15	0.74
1:A:517:ARG:CG	1:A:517:ARG:HH11	2.01	0.73
1:A:529:PRO:HA	1:B:358:ARG:NH1	2.03	0.73
1:F:94:VAL:HG23	1:F:99:VAL:HG11	1.71	0.73
1:C:75:PHE:CE1	1:F:454:LEU:HD13	2.24	0.73
1:E:113:LEU:HD12	1:E:114:GLY:N	2.03	0.73
1:C:354:GLU:CD	1:C:393:ARG:HD2	2.13	0.73
1:E:207:GLY:O	1:E:211:ILE:HG23	1.88	0.73
1:F:350:ILE:HG13	1:F:393:ARG:HD2	1.71	0.73
1:E:376:VAL:HG11	1:E:420:ALA:CB	2.15	0.73
1:C:185:VAL:HG22	1:F:391:ILE:HG23	1.69	0.72
1:C:109:PHE:O	1:C:111:GLY:N	2.21	0.72
1:A:145:ARG:HD2	1:A:148:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:VAL:HG11	1:B:506:ILE:HD12	1.71	0.72
1:D:145:ARG:HD2	1:D:148:GLU:OE2	1.89	0.72
1:D:391:ILE:CG2	1:E:185:VAL:HG22	2.19	0.72
1:B:337:VAL:CG2	1:B:401:TYR:OH	2.32	0.72
1:C:73:THR:HG21	1:B:73:THR:HG21	1.70	0.72
1:F:451:VAL:HB	1:F:470:ARG:NH2	2.05	0.72
1:B:437:TRP:HE1	1:B:502:THR:CG2	2.01	0.72
1:D:405:THR:O	1:D:516:LYS:HE2	1.90	0.72
1:D:456:ARG:O	1:D:459:ILE:HG12	1.90	0.72
1:D:350:ILE:HG23	1:D:393:ARG:HD2	1.72	0.72
1:F:73:THR:HG21	1:D:73:THR:HG21	1.72	0.71
1:F:324:THR:HA	1:F:336:ILE:O	1.89	0.71
1:A:298:MET:HE1	1:A:413:THR:HG21	1.71	0.71
1:B:389:GLY:O	1:B:393:ARG:HG2	1.91	0.71
1:A:298:MET:HE3	1:A:301:VAL:CG1	2.21	0.71
1:A:40:GLN:NE2	1:A:41:HIS:H	1.89	0.71
1:E:520:LEU:HD22	1:E:521:PRO:CD	2.20	0.71
1:C:65:ASP:OD2	1:C:123:LYS:HD3	1.91	0.71
1:A:452:ASN:HB2	1:A:456:ARG:NH2	2.06	0.71
1:A:468:ALA:O	1:A:472:ARG:HB3	1.91	0.71
1:C:208:PRO:CG	1:C:221:PHE:HE2	2.03	0.70
1:E:33:SER:O	1:E:37:VAL:HG13	1.91	0.70
1:C:397:LEU:HG	1:C:423:VAL:CG1	2.21	0.70
1:D:381:PRO:HB2	1:E:214:VAL:HG21	1.73	0.70
1:E:47:THR:HG22	1:E:50:GLU:CG	2.22	0.70
1:F:290:ASP:CG	1:B:13:THR:HG22	2.16	0.70
1:D:437:TRP:HZ2	1:D:502:THR:HG21	1.56	0.70
1:C:419:GLY:O	1:C:423:VAL:HG23	1.91	0.70
1:D:484:PRO:HD2	1:D:485:TYR:CD2	2.26	0.70
1:C:284:LEU:O	1:C:287:ILE:HG22	1.91	0.70
1:F:205:ILE:HG23	1:F:206:THR:HG23	1.73	0.70
1:A:122:VAL:HG23	1:A:159:ILE:HG13	1.73	0.70
1:B:440:ALA:HB3	1:B:484:PRO:HB3	1.73	0.70
1:C:208:PRO:CD	1:C:221:PHE:HE2	2.03	0.70
1:F:147:GLN:CD	1:F:147:GLN:H	1.98	0.70
1:B:230:HIS:HD2	1:B:234:SER:OG	1.74	0.70
1:E:211:ILE:HG13	1:E:212:LYS:N	2.07	0.69
1:E:474:ILE:HG22	1:E:475:GLN:H	1.55	0.69
1:D:230:HIS:HA	1:D:234:SER:OG	1.92	0.69
1:B:348:LEU:HD11	1:B:424:MET:HE2	1.75	0.69
1:E:467:GLU:C	1:E:469:THR:H	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:HE21	1:A:140:ASP:H	1.40	0.69
1:E:113:LEU:HD23	1:E:156:TYR:CD1	2.28	0.69
1:B:85:ASP:OD2	1:B:116:VAL:HG22	1.93	0.69
1:D:51:ARG:NH1	1:D:177:VAL:HG21	2.08	0.69
1:C:374:VAL:CG2	1:C:412:ILE:HG12	2.23	0.69
1:F:497:ILE:HG21	1:F:505:HIS:HE1	1.57	0.69
1:A:18:LEU:HD13	1:D:498:MET:CE	2.23	0.69
1:C:454:LEU:HD21	1:F:75:PHE:CZ	2.28	0.69
1:F:374:VAL:HG23	1:F:376:VAL:HG12	1.74	0.68
1:F:451:VAL:HG13	1:F:455:HIS:HB2	1.74	0.68
1:B:26:GLU:O	1:B:30:HIS:HD2	1.76	0.68
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.75	0.68
1:D:520:LEU:HB2	1:D:521:PRO:CD	2.23	0.67
1:D:437:TRP:CZ2	1:D:502:THR:HG21	2.29	0.67
1:F:187:SER:HB3	1:F:188:PRO:HD3	1.75	0.67
1:A:25:ILE:O	1:A:29:THR:HG23	1.94	0.67
1:A:299:HIS:CE1	1:A:323:LEU:HD11	2.30	0.67
1:F:287:ILE:O	1:F:289:PRO:HD3	1.93	0.67
1:A:91:TYR:CD1	1:D:512:GLN:HG3	2.30	0.67
1:A:415:LYS:NZ	1:A:441:GLN:O	2.28	0.67
1:B:343:GLN:OE1	1:B:344:PHE:HE2	1.78	0.67
1:F:18:LEU:CG	1:E:498:MET:HE1	2.20	0.66
1:A:68:ALA:HA	1:D:489:GLU:HA	1.77	0.66
1:B:374:VAL:CG1	1:B:412:ILE:HD13	2.22	0.66
1:C:69:ARG:HH11	1:C:81:ARG:HB2	1.60	0.66
1:C:397:LEU:C	1:C:397:LEU:HD12	2.21	0.66
1:F:65:ASP:HB2	1:F:120:LYS:HE3	1.77	0.66
1:B:451:VAL:HG13	1:B:455:HIS:CD2	2.29	0.66
1:A:37:VAL:O	1:A:40:GLN:NE2	2.27	0.66
1:D:320:PRO:CB	1:D:343:GLN:HE21	2.07	0.66
1:D:209:ASP:HA	1:D:212:LYS:HE3	1.78	0.66
1:E:23:ARG:O	1:E:27:GLU:HG3	1.96	0.65
1:F:451:VAL:HG22	1:F:454:LEU:HD11	1.77	0.65
1:A:405:THR:O	1:A:516:LYS:HD2	1.97	0.65
1:C:397:LEU:HG	1:C:423:VAL:HG13	1.78	0.65
1:A:103:SER:HA	1:A:138:ILE:HG13	1.77	0.65
1:B:74:ASN:HB2	1:B:77:LEU:CD1	2.27	0.65
1:E:77:LEU:HD21	1:E:147:GLN:OE1	1.96	0.65
1:A:350:ILE:HG22	1:A:385:GLN:HE22	1.60	0.65
1:B:348:LEU:HD21	1:B:424:MET:CE	2.27	0.65
1:C:339:ASN:HD22	1:C:374:VAL:HA	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:470:ARG:HH12	1:F:474:ILE:N	1.95	0.65
1:A:230:HIS:HA	1:A:234:SER:OG	1.96	0.65
1:B:519:SER:O	1:B:520:LEU:HB2	1.97	0.65
1:E:47:THR:O	1:E:51:ARG:HG3	1.97	0.65
1:B:446:GLY:HA3	1:B:448:GLN:HE21	1.61	0.65
1:E:209:ASP:O	1:E:212:LYS:HG2	1.97	0.65
1:C:21:LEU:HD12	1:C:21:LEU:O	1.97	0.65
1:F:437:TRP:HE1	1:F:502:THR:CG2	2.09	0.65
1:F:520:LEU:HD12	1:F:521:PRO:HD2	1.79	0.65
1:B:22:ARG:O	1:B:26:GLU:HG2	1.96	0.65
1:C:75:PHE:HD2	1:C:75:PHE:N	1.95	0.65
1:D:280:GLU:O	1:D:283:GLU:HG2	1.96	0.64
1:D:324:THR:HA	1:D:336:ILE:O	1.97	0.64
1:F:105:ASP:OD1	1:F:107:THR:HB	1.97	0.64
1:E:113:LEU:HD12	1:E:114:GLY:H	1.62	0.64
1:C:185:VAL:HG21	1:F:391:ILE:HG12	1.79	0.64
1:D:478:GLU:HG2	1:D:482:LEU:HD12	1.80	0.64
1:A:442:ILE:HD13	1:A:487:ALA:HB2	1.79	0.64
1:B:196:MET:CE	1:B:230:HIS:HB2	2.23	0.64
1:E:51:ARG:HH11	1:E:51:ARG:CG	2.01	0.64
1:A:165:HIS:HB3	1:B:520:LEU:HD11	1.80	0.64
1:D:478:GLU:CG	1:D:482:LEU:HD12	2.28	0.64
1:E:205:ILE:HG23	1:E:206:THR:HG23	1.78	0.64
1:B:498:MET:HE1	1:E:18:LEU:HG	1.79	0.64
1:A:265:GLU:HB2	1:A:266:PRO:HD2	1.80	0.63
1:F:453:ILE:HG13	1:F:454:LEU:N	2.13	0.63
1:A:69:ARG:HB2	1:D:489:GLU:HB2	1.81	0.63
1:A:339:ASN:O	1:A:341:PRO:HD3	1.97	0.63
1:B:376:VAL:HG21	1:B:420:ALA:HB1	1.80	0.63
1:D:288:VAL:HG21	1:D:439:THR:HG21	1.79	0.63
1:E:238:HIS:HA	1:E:315:GLN:HG2	1.79	0.63
1:C:207:GLY:O	1:C:211:ILE:HG13	1.99	0.63
1:F:386:GLU:HA	1:F:390:ILE:HG22	1.81	0.63
1:A:399:PHE:O	1:A:403:GLU:HG2	1.98	0.63
1:B:25:ILE:O	1:B:29:THR:HG23	1.98	0.63
1:B:26:GLU:O	1:B:30:HIS:CD2	2.51	0.63
1:F:504:ARG:O	1:F:508:ARG:HG3	1.97	0.63
1:A:380:LEU:HD12	1:A:380:LEU:C	2.24	0.63
1:E:234:SER:HB2	1:E:236:VAL:HG23	1.80	0.63
1:A:450:ALA:O	1:A:454:LEU:HG	1.99	0.63
1:C:464:ASP:CG	1:C:465:ASP:H	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:H	1:A:238:HIS:CD2	2.17	0.63
1:B:29:THR:HG22	1:B:49:ARG:HH12	1.64	0.63
1:B:457:ARG:O	1:B:457:ARG:HG3	1.97	0.63
1:B:140:ASP:O	1:B:141:SER:C	2.41	0.63
1:B:118:GLY:HA3	1:B:155:ALA:HB1	1.81	0.63
1:B:437:TRP:HB2	1:B:439:THR:HG23	1.81	0.63
1:A:43:LYS:HE3	1:A:45:LYS:HE2	1.80	0.62
1:B:499:PRO:O	1:B:502:THR:HG23	1.99	0.62
1:D:389:GLY:O	1:D:393:ARG:HG3	1.99	0.62
1:C:120:LYS:O	1:C:123:LYS:HB3	1.99	0.62
1:F:470:ARG:HH12	1:F:474:ILE:CA	2.12	0.62
1:F:479:ASP:O	1:F:480:ALA:HB2	1.98	0.62
1:B:414:ARG:O	1:B:440:ALA:HA	1.99	0.62
1:C:467:GLU:OE1	1:C:467:GLU:HA	1.98	0.62
1:F:207:GLY:O	1:F:211:ILE:HG12	1.99	0.62
1:F:485:TYR:HE2	1:B:17:LYS:HZ1	1.47	0.62
1:A:10:ASP:CG	1:A:11:ILE:H	2.07	0.62
1:D:69:ARG:HD3	1:D:81:ARG:O	1.99	0.62
1:A:24:ARG:HD2	1:D:485:TYR:CE1	2.34	0.62
1:D:391:ILE:HG21	1:E:185:VAL:CG2	2.30	0.62
1:A:197:VAL:HB	1:A:200:THR:HG22	1.79	0.62
1:B:55:LEU:O	1:B:252:LYS:NZ	2.32	0.62
1:B:69:ARG:HD3	1:B:81:ARG:CB	2.29	0.62
1:B:348:LEU:HD21	1:B:424:MET:HE2	1.80	0.62
1:E:340:GLN:CD	1:E:342:MET:HB2	2.25	0.62
1:C:106:PHE:HD1	1:C:140:ASP:OD1	1.83	0.62
1:F:489:GLU:HG2	1:B:69:ARG:HB2	1.80	0.62
1:B:300:SER:HA	1:B:303:GLU:CG	2.28	0.62
1:C:519:SER:O	1:C:520:LEU:CB	2.48	0.62
1:F:113:LEU:HD22	1:F:117:TYR:CE2	2.35	0.62
1:B:87:VAL:HG13	1:B:120:LYS:HD2	1.81	0.62
1:B:94:VAL:HG23	1:B:99:VAL:HG11	1.80	0.62
1:D:234:SER:O	1:E:392:ARG:NH1	2.33	0.62
1:C:49:ARG:O	1:C:50:GLU:CB	2.43	0.62
1:B:138:ILE:CG2	1:B:175:LEU:HD23	2.27	0.62
1:D:158:GLU:O	1:D:162:ARG:HG2	1.99	0.62
1:F:230:HIS:HA	1:F:234:SER:OG	2.00	0.61
1:C:14:THR:HA	1:C:17:LYS:HE2	1.82	0.61
1:F:45:LYS:HD3	1:F:200:THR:CB	2.30	0.61
1:D:363:CYS:CB	1:D:368:VAL:HG22	2.29	0.61
1:F:448:GLN:HG2	1:F:449:GLY:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:O	1:A:303:GLU:HG3	2.00	0.61
1:B:173:ILE:HG23	1:B:193:PHE:HB2	1.80	0.61
1:B:207:GLY:O	1:B:210:VAL:HG23	2.00	0.61
1:D:94:VAL:HG23	1:D:99:VAL:HG11	1.81	0.61
1:C:397:LEU:HD12	1:C:397:LEU:O	2.01	0.61
1:F:56:LEU:HD12	1:F:61:PHE:HB2	1.82	0.61
1:A:414:ARG:O	1:A:440:ALA:HA	2.00	0.61
1:B:350:ILE:HD13	1:B:390:ILE:HD13	1.81	0.61
1:E:47:THR:HG22	1:E:50:GLU:H	1.64	0.61
1:C:354:GLU:OE2	1:C:393:ARG:HD2	2.01	0.61
1:D:391:ILE:CG2	1:E:185:VAL:CG2	2.78	0.61
1:D:472:ARG:NE	1:D:475:GLN:HB3	2.14	0.61
1:C:146:ILE:HD12	1:F:445:MET:HE2	1.82	0.61
1:C:374:VAL:HG23	1:C:412:ILE:HG23	1.83	0.61
1:B:121:ILE:O	1:B:125:MET:HG3	2.01	0.61
1:D:451:VAL:HG13	1:D:455:HIS:HB2	1.83	0.61
1:E:203:MET:HB2	1:E:230:HIS:HE1	1.62	0.61
1:E:219:VAL:HG11	1:E:224:LEU:HD13	1.83	0.61
1:B:393:ARG:HA	1:B:396:LYS:HE3	1.83	0.60
1:B:437:TRP:NE1	1:B:502:THR:HG21	2.15	0.60
1:C:70:HIS:C	1:C:70:HIS:HD1	2.09	0.60
1:F:337:VAL:O	1:F:372:THR:HA	2.01	0.60
1:A:69:ARG:NH1	1:A:81:ARG:HB3	2.15	0.60
1:A:459:ILE:HG13	1:A:460:ALA:H	1.65	0.60
1:A:26:GLU:N	1:A:26:GLU:OE1	2.34	0.60
1:A:520:LEU:HG	1:A:521:PRO:HD2	1.82	0.60
1:E:474:ILE:HG22	1:E:475:GLN:N	2.15	0.60
1:C:483:ASN:ND2	1:C:485:TYR:HB2	2.17	0.60
1:D:75:PHE:HD2	1:D:147:GLN:HB3	1.66	0.60
1:D:483:ASN:ND2	1:D:485:TYR:HB2	2.15	0.60
1:E:46:LEU:HB3	1:E:50:GLU:HG3	1.82	0.60
1:E:215:THR:HB	1:E:217:GLU:CG	2.29	0.60
1:E:230:HIS:HA	1:E:234:SER:OG	2.01	0.60
1:A:442:ILE:HD13	1:A:487:ALA:CB	2.32	0.60
1:D:518:GLU:O	1:D:519:SER:HB2	2.02	0.60
1:C:109:PHE:C	1:C:111:GLY:N	2.55	0.60
1:C:374:VAL:HG22	1:C:412:ILE:HA	1.83	0.60
1:A:391:ILE:H	1:A:391:ILE:CD1	2.13	0.60
1:B:405:THR:HG22	1:B:518:GLU:OE1	2.02	0.60
1:C:187:SER:HB3	1:C:188:PRO:CD	2.31	0.60
1:B:40:GLN:OE1	1:B:45:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:MET:O	1:E:230:HIS:CE1	2.55	0.60
1:D:470:ARG:HG2	1:D:471:ALA:N	2.17	0.60
1:C:158:GLU:HG3	1:C:162:ARG:NH2	2.15	0.59
1:D:466:ALA:HB1	1:D:470:ARG:HD2	1.84	0.59
1:A:445:MET:HG3	1:A:450:ALA:HB2	1.84	0.59
1:B:456:ARG:C	1:B:458:THR:H	2.10	0.59
1:E:63:GLU:HG2	1:E:66:GLU:HB2	1.83	0.59
1:E:441:GLN:HG2	1:E:482:LEU:O	2.02	0.59
1:E:451:VAL:HB	1:E:455:HIS:HE1	1.66	0.59
1:F:45:LYS:HD2	1:F:244:GLU:OE2	2.03	0.59
1:F:479:ASP:O	1:F:480:ALA:CB	2.51	0.59
1:D:405:THR:O	1:D:516:LYS:CE	2.50	0.59
1:C:350:ILE:HG13	1:C:351:THR:N	2.16	0.59
1:A:18:LEU:HB3	1:D:498:MET:HE1	1.85	0.59
1:A:35:ARG:NH1	1:A:38:GLU:OE1	2.34	0.59
1:B:29:THR:HG22	1:B:49:ARG:NH1	2.17	0.59
1:B:496:VAL:HG13	1:E:67:PHE:CE2	2.38	0.59
1:C:451:VAL:O	1:C:454:LEU:O	2.20	0.59
1:F:457:ARG:HG3	1:F:457:ARG:HH11	1.67	0.59
1:A:214:VAL:HG21	1:B:381:PRO:HG2	1.83	0.59
1:E:163:ASN:HA	1:E:172:GLN:HE22	1.67	0.59
1:C:77:LEU:HD11	1:C:147:GLN:HG2	1.85	0.59
1:F:497:ILE:O	1:F:497:ILE:HD12	2.03	0.59
1:D:342:MET:HE2	1:D:342:MET:HA	1.83	0.59
1:E:74:ASN:HB3	1:E:75:PHE:HD1	1.67	0.59
1:D:288:VAL:CG2	1:D:439:THR:HG21	2.32	0.59
1:E:459:ILE:HD11	1:E:470:ARG:HD2	1.85	0.59
1:F:158:GLU:OE1	1:F:161:ARG:NH2	2.36	0.59
1:A:472:ARG:O	1:A:476:GLU:OE1	2.21	0.59
1:B:177:VAL:O	1:B:200:THR:O	2.20	0.59
1:D:286:THR:OG1	1:D:287:ILE:N	2.36	0.59
1:E:51:ARG:CZ	1:E:177:VAL:HG21	2.33	0.58
1:A:205:ILE:HD11	1:B:390:ILE:HG21	1.85	0.58
1:B:70:HIS:ND1	1:B:70:HIS:C	2.60	0.58
1:A:498:MET:HE2	1:A:501:ASP:OD1	2.02	0.58
1:B:334:VAL:HG21	1:B:371:LEU:HD11	1.84	0.58
1:B:380:LEU:HD23	1:B:385:GLN:CD	2.29	0.58
1:B:402:ALA:HA	1:B:429:LEU:O	2.03	0.58
1:F:456:ARG:O	1:F:459:ILE:HG13	2.03	0.58
1:A:350:ILE:HG22	1:A:385:GLN:NE2	2.17	0.58
1:D:454:LEU:HD21	1:E:75:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LYS:HG2	1:B:246:ASP:N	2.17	0.58
1:D:315:GLN:OE1	1:D:355:LYS:HG3	2.04	0.58
1:C:75:PHE:N	1:C:75:PHE:CD2	2.68	0.58
1:F:437:TRP:HE1	1:F:502:THR:HG22	1.68	0.58
1:A:51:ARG:HH11	1:A:138:ILE:CD1	2.16	0.58
1:A:52:ILE:HD11	1:A:103:SER:HB2	1.86	0.58
1:B:74:ASN:HB2	1:B:77:LEU:HD11	1.84	0.58
1:F:339:ASN:HD22	1:F:374:VAL:HA	1.67	0.58
1:F:499:PRO:O	1:F:502:THR:HG23	2.03	0.58
1:D:422:ASN:HA	1:D:426:SER:HB3	1.85	0.58
1:F:470:ARG:NH1	1:F:474:ILE:N	2.51	0.58
1:B:77:LEU:HD21	1:B:147:GLN:HG2	1.86	0.58
1:F:69:ARG:HG2	1:E:489:GLU:HG2	1.85	0.57
1:F:350:ILE:O	1:F:354:GLU:HG3	2.04	0.57
1:F:414:ARG:O	1:F:440:ALA:HA	2.04	0.57
1:E:243:ASP:OD1	1:E:244:GLU:N	2.37	0.57
1:F:176:VAL:CG2	1:F:196:MET:HG2	2.35	0.57
1:F:470:ARG:HH12	1:F:474:ILE:HA	1.69	0.57
1:A:77:LEU:HD11	1:A:147:GLN:HG3	1.87	0.57
1:A:104:GLN:HE21	1:A:140:ASP:N	2.02	0.57
1:A:288:VAL:CG2	1:A:439:THR:HG21	2.32	0.57
1:B:176:VAL:HB	1:B:196:MET:HG2	1.85	0.57
1:E:483:ASN:HB2	1:E:484:PRO:HD2	1.86	0.57
1:F:45:LYS:HD3	1:F:200:THR:HB	1.85	0.57
1:A:372:THR:HG21	1:A:401:TYR:CE1	2.39	0.57
1:B:47:THR:HG22	1:B:50:GLU:CD	2.29	0.57
1:A:372:THR:HG21	1:A:401:TYR:OH	2.04	0.57
1:A:372:THR:OG1	1:A:410:THR:HG22	2.04	0.57
1:B:182:GLY:O	1:B:184:ALA:N	2.37	0.57
1:B:203:MET:O	1:B:230:HIS:HE1	1.88	0.57
1:B:489:GLU:HB3	1:E:69:ARG:HB2	1.87	0.57
1:D:379:PHE:HZ	1:D:423:VAL:HG21	1.68	0.57
1:C:467:GLU:O	1:C:468:ALA:C	2.48	0.57
1:A:528:ILE:C	1:B:358:ARG:HH12	2.12	0.57
1:B:40:GLN:HE22	1:B:45:LYS:HE2	1.68	0.57
1:E:176:VAL:HB	1:E:196:MET:HG2	1.84	0.57
1:C:302:ILE:HD13	1:C:336:ILE:HG21	1.85	0.57
1:A:130:LYS:O	1:D:517:ARG:HD2	2.04	0.57
1:D:138:ILE:HD13	1:D:175:LEU:HB3	1.86	0.57
1:C:103:SER:HB2	1:C:138:ILE:HD12	1.85	0.57
1:C:477:TYR:CE2	1:C:481:LEU:HD12	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:H	1:A:238:HIS:HD2	1.52	0.57
1:B:54:LEU:HG	1:B:248:VAL:HG11	1.87	0.57
1:B:339:ASN:ND2	1:B:424:MET:HE3	2.04	0.57
1:E:63:GLU:OE1	1:E:88:VAL:HG13	2.04	0.57
1:F:406:VAL:C	1:F:516:LYS:HE3	2.30	0.57
1:F:451:VAL:HG13	1:F:455:HIS:CD2	2.40	0.57
1:A:185:VAL:HG11	1:A:205:ILE:HG23	1.85	0.57
1:A:380:LEU:HD11	1:A:385:GLN:CD	2.30	0.57
1:A:391:ILE:HD12	1:A:391:ILE:N	2.15	0.57
1:B:72:SER:HB2	1:B:148:GLU:OE1	2.05	0.57
1:E:339:ASN:CG	1:E:376:VAL:HG23	2.29	0.57
1:C:46:LEU:HD12	1:C:50:GLU:OE2	2.05	0.57
1:C:528:ILE:HG13	1:C:529:PRO:HD2	1.86	0.57
1:F:20:ASP:OD1	1:F:23:ARG:NH2	2.38	0.57
1:F:40:GLN:HG3	1:F:45:LYS:HB2	1.86	0.57
1:F:291:SER:HB3	1:F:294:GLN:CD	2.30	0.57
1:B:203:MET:HB2	1:B:230:HIS:CE1	2.40	0.57
1:A:150:VAL:HG12	1:A:153:LEU:HD12	1.85	0.57
1:A:454:LEU:HD21	1:B:146:ILE:CG2	2.35	0.57
1:E:451:VAL:HB	1:E:455:HIS:CE1	2.40	0.57
1:C:19:ALA:HA	1:C:22:ARG:NH1	2.20	0.56
1:C:71:ARG:HH21	1:A:490:ARG:HG2	1.70	0.56
1:A:517:ARG:HH11	1:A:517:ARG:HG3	1.70	0.56
1:B:482:LEU:N	1:B:482:LEU:HD23	2.20	0.56
1:C:410:THR:HG21	1:C:425:GLY:O	2.05	0.56
1:B:517:ARG:HG3	1:B:517:ARG:HH11	1.70	0.56
1:C:208:PRO:CG	1:C:221:PHE:CE2	2.87	0.56
1:C:472:ARG:HD3	1:C:475:GLN:HE21	1.69	0.56
1:F:475:GLN:HA	1:F:478:GLU:CG	2.33	0.56
1:A:134:PRO:HB3	1:A:171:PRO:HB2	1.86	0.56
1:D:509:GLY:O	1:D:513:LEU:HB2	2.04	0.56
1:E:47:THR:CG2	1:E:50:GLU:H	2.17	0.56
1:E:113:LEU:O	1:E:145:ARG:HB2	2.05	0.56
1:E:155:ALA:O	1:E:159:ILE:HG12	2.05	0.56
1:E:177:VAL:O	1:E:177:VAL:HG23	2.06	0.56
1:E:181:ALA:HA	1:E:204:PHE:O	2.05	0.56
1:E:245:LYS:CG	1:E:246:ASP:N	2.68	0.56
1:C:118:GLY:HA3	1:C:155:ALA:HB1	1.87	0.56
1:B:520:LEU:HG	1:B:521:PRO:CD	2.34	0.56
1:D:313:GLU:OE2	1:D:316:PRO:HA	2.04	0.56
1:D:440:ALA:HB3	1:D:484:PRO:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LEU:HD11	1:C:401:TYR:CE2	2.41	0.56
1:C:475:GLN:HA	1:C:478:GLU:HB2	1.88	0.56
1:A:520:LEU:HD12	1:A:521:PRO:HD2	1.88	0.56
1:B:314:THR:HG23	1:B:325:GLY:HA2	1.86	0.56
1:D:286:THR:C	1:D:288:VAL:N	2.64	0.56
1:C:464:ASP:OD2	1:C:468:ALA:HB2	2.06	0.56
1:A:102:PHE:CZ	1:A:137:GLY:HA3	2.40	0.56
1:C:376:VAL:O	1:C:376:VAL:HG13	2.05	0.56
1:A:69:ARG:HH11	1:A:69:ARG:CG	2.07	0.56
1:A:71:ARG:NH2	1:D:490:ARG:HE	2.04	0.56
1:B:410:THR:OG1	1:B:434:ASN:ND2	2.39	0.56
1:C:10:ASP:O	1:C:11:ILE:HD13	2.06	0.56
1:A:520:LEU:CG	1:A:521:PRO:HD2	2.35	0.56
1:B:182:GLY:HA2	1:B:205:ILE:O	2.06	0.56
1:D:356:ALA:O	1:D:360:VAL:HG23	2.05	0.56
1:F:462:ALA:HB1	1:F:465:ASP:OD2	2.05	0.56
1:A:88:VAL:O	1:A:103:SER:N	2.39	0.56
1:A:113:LEU:HD13	1:A:156:TYR:CE1	2.41	0.56
1:D:69:ARG:CD	1:D:81:ARG:O	2.54	0.56
1:D:49:ARG:HH22	1:D:63:GLU:CD	2.14	0.55
1:E:23:ARG:HG3	1:E:24:ARG:N	2.21	0.55
1:A:451:VAL:O	1:A:454:LEU:HB2	2.06	0.55
1:D:354:GLU:OE1	1:E:392:ARG:NH2	2.39	0.55
1:D:434:ASN:O	1:D:494:ASP:OD1	2.25	0.55
1:F:438:PRO:HG3	1:B:21:LEU:HD22	1.88	0.55
1:A:284:LEU:O	1:A:287:ILE:HG22	2.06	0.55
1:D:77:LEU:HD11	1:D:147:GLN:CG	2.35	0.55
1:D:297:ASP:OD1	1:D:299:HIS:HD2	1.88	0.55
1:D:323:LEU:O	1:D:337:VAL:HA	2.06	0.55
1:B:106:PHE:HB2	1:B:140:ASP:OD2	2.06	0.55
1:B:140:ASP:O	1:B:179:PRO:O	2.24	0.55
1:B:485:TYR:O	1:B:489:GLU:HG3	2.07	0.55
1:D:56:LEU:HD12	1:D:61:PHE:HB2	1.88	0.55
1:C:520:LEU:CD1	1:C:521:PRO:HD2	2.11	0.55
1:B:74:ASN:N	1:B:77:LEU:HD12	2.21	0.55
1:B:88:VAL:HG13	1:B:103:SER:HB3	1.89	0.55
1:F:105:ASP:C	1:F:107:THR:H	2.13	0.55
1:A:446:GLY:C	1:A:448:GLN:H	2.14	0.55
1:B:456:ARG:HG2	1:B:459:ILE:HG12	1.87	0.55
1:D:82:PRO:O	1:D:84:GLY:O	2.24	0.55
1:C:22:ARG:O	1:C:26:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:PRO:HA	1:C:211:ILE:HB	1.87	0.55
1:C:381:PRO:HB3	1:F:211:ILE:HD13	1.88	0.55
1:B:459:ILE:HG13	1:B:460:ALA:N	2.22	0.55
1:A:464:ASP:O	1:A:465:ASP:HB3	2.06	0.55
1:E:379:PHE:O	1:E:381:PRO:HD3	2.07	0.55
1:E:461:ASP:C	1:E:463:GLY:N	2.65	0.55
1:F:373:PHE:CD1	1:F:411:VAL:CG2	2.90	0.54
1:A:457:ARG:NH1	1:A:461:ASP:HB2	2.23	0.54
1:E:415:LYS:HE2	1:E:417:PHE:HE2	1.72	0.54
1:F:434:ASN:O	1:F:493:VAL:HG13	2.07	0.54
1:C:128:ALA:O	1:C:132:GLY:N	2.40	0.54
1:C:422:ASN:O	1:C:429:LEU:HD22	2.08	0.54
1:A:82:PRO:HG2	1:A:109:PHE:CE2	2.42	0.54
1:A:415:LYS:CD	1:A:441:GLN:HB2	2.34	0.54
1:A:451:VAL:HG11	1:A:474:ILE:HA	1.90	0.54
1:D:499:PRO:O	1:D:502:THR:CG2	2.55	0.54
1:A:457:ARG:HH22	1:A:461:ASP:CG	2.16	0.54
1:F:477:TYR:O	1:F:481:LEU:HB2	2.07	0.54
1:D:445:MET:HE3	1:D:450:ALA:HA	1.90	0.54
1:C:414:ARG:O	1:C:440:ALA:HA	2.08	0.54
1:A:88:VAL:HB	1:A:103:SER:HB3	1.90	0.54
1:E:433:LEU:HA	1:E:494:ASP:OD2	2.07	0.54
1:C:68:ALA:HA	1:A:489:GLU:HA	1.90	0.54
1:F:437:TRP:CZ2	1:F:502:THR:HG21	2.42	0.54
1:A:298:MET:HG2	1:A:338:ALA:HB1	1.90	0.54
1:A:480:ALA:O	1:A:481:LEU:HD13	2.08	0.54
1:B:350:ILE:CG2	1:B:393:ARG:NH1	2.71	0.54
1:B:520:LEU:CG	1:B:521:PRO:HD2	2.33	0.54
1:D:499:PRO:O	1:D:502:THR:HG23	2.08	0.54
1:B:489:GLU:CB	1:E:69:ARG:HB2	2.38	0.54
1:D:514:ARG:HG3	1:D:514:ARG:HH11	1.72	0.54
1:C:205:ILE:HD11	1:F:390:ILE:HG21	1.90	0.54
1:F:206:THR:OG1	1:F:211:ILE:HD11	2.08	0.54
1:F:375:ASP:OD1	1:F:415:LYS:HG2	2.08	0.54
1:F:393:ARG:HA	1:F:396:LYS:HE3	1.90	0.54
1:B:75:PHE:HD1	1:B:76:GLY:H	1.56	0.54
1:B:456:ARG:HG2	1:B:459:ILE:CD1	2.38	0.54
1:D:422:ASN:O	1:D:429:LEU:HD22	2.07	0.54
1:F:441:GLN:CG	1:F:482:LEU:HB3	2.38	0.53
1:B:140:ASP:OD1	1:B:141:SER:N	2.37	0.53
1:B:343:GLN:OE1	1:B:344:PHE:CE2	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:ARG:NH2	1:F:38:GLU:OE1	2.41	0.53
1:A:69:ARG:NH1	1:A:81:ARG:O	2.39	0.53
1:B:72:SER:OG	1:B:77:LEU:HD12	2.08	0.53
1:D:70:HIS:CE1	1:D:77:LEU:HB3	2.43	0.53
1:E:376:VAL:HG12	1:E:376:VAL:O	2.06	0.53
1:C:474:ILE:O	1:C:475:GLN:CB	2.55	0.53
1:A:163:ASN:HA	1:A:172:GLN:HE22	1.73	0.53
1:B:442:ILE:HD12	1:B:484:PRO:HA	1.90	0.53
1:B:456:ARG:HD2	1:B:456:ARG:O	2.09	0.53
1:E:185:VAL:HG23	1:E:203:MET:HE2	1.90	0.53
1:C:103:SER:HA	1:C:138:ILE:HB	1.90	0.53
1:F:175:LEU:HD11	1:F:247:ALA:HB1	1.91	0.53
1:A:70:HIS:CE1	1:A:115:GLU:HG2	2.43	0.53
1:A:104:GLN:O	1:A:140:ASP:HB3	2.08	0.53
1:B:61:PHE:CZ	1:B:63:GLU:HG3	2.43	0.53
1:B:343:GLN:C	1:B:344:PHE:HD2	2.16	0.53
1:D:125:MET:HE1	1:D:163:ASN:OD1	2.08	0.53
1:C:146:ILE:HD12	1:F:445:MET:CE	2.38	0.53
1:C:374:VAL:HG21	1:C:412:ILE:HG12	1.90	0.53
1:B:65:ASP:HB2	1:B:120:LYS:HE2	1.91	0.53
1:B:302:ILE:O	1:B:305:VAL:O	2.26	0.53
1:B:305:VAL:O	1:B:306:LEU:CG	2.54	0.53
1:B:415:LYS:HD2	1:B:417:PHE:HE1	1.65	0.53
1:D:514:ARG:HG3	1:D:514:ARG:NH1	2.23	0.53
1:E:70:HIS:O	1:E:81:ARG:HD2	2.09	0.53
1:E:231:ASN:HD21	1:E:239:HIS:CA	2.22	0.53
1:E:444:VAL:HG23	1:E:445:MET:HG2	1.88	0.53
1:F:26:GLU:O	1:F:30:HIS:HD2	1.91	0.53
1:F:486:THR:HA	1:F:489:GLU:OE1	2.08	0.53
1:A:451:VAL:HA	1:A:454:LEU:HD12	1.90	0.53
1:D:447:ALA:HB2	1:D:482:LEU:HD11	1.90	0.53
1:F:284:LEU:HD22	1:F:437:TRP:CH2	2.44	0.53
1:F:350:ILE:HD12	1:F:390:ILE:HD13	1.90	0.53
1:D:490:ARG:CZ	1:E:151:ALA:HB2	2.39	0.53
1:E:245:LYS:HG2	1:E:246:ASP:N	2.24	0.53
1:F:89:THR:HB	1:F:124:VAL:HG11	1.91	0.53
1:F:285:ASP:HB3	1:B:18:LEU:CD1	2.39	0.53
1:C:374:VAL:HG22	1:C:412:ILE:HG12	1.91	0.53
1:A:30:HIS:O	1:A:32:GLY:N	2.42	0.53
1:B:196:MET:CE	1:B:227:ALA:HA	2.35	0.53
1:D:47:THR:O	1:D:51:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ALA:HB2	1:D:351:THR:HB	1.91	0.53
1:B:284:LEU:O	1:B:287:ILE:HG22	2.09	0.53
1:D:275:LEU:HD22	1:D:508:ARG:NH1	2.24	0.53
1:E:33:SER:HB3	1:E:36:ALA:HB3	1.91	0.52
1:D:399:PHE:CD2	1:E:164:THR:HG23	2.43	0.52
1:C:164:THR:HG23	1:F:399:PHE:CD2	2.44	0.52
1:A:234:SER:O	1:B:392:ARG:HD3	2.08	0.52
1:A:361:ARG:HH21	1:B:528:ILE:HG12	1.74	0.52
1:D:417:PHE:O	1:D:420:ALA:HB3	2.08	0.52
1:C:315:GLN:OE1	1:C:355:LYS:HG3	2.09	0.52
1:A:350:ILE:CD1	1:A:393:ARG:HH11	2.11	0.52
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.91	0.52
1:A:520:LEU:CD1	1:A:521:PRO:HD2	2.39	0.52
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.90	0.52
1:E:39:LYS:N	1:E:39:LYS:CD	2.71	0.52
1:B:72:SER:CB	1:B:148:GLU:OE1	2.57	0.52
1:D:297:ASP:OD1	1:D:299:HIS:CD2	2.63	0.52
1:E:156:TYR:CE1	1:E:184:ALA:HB2	2.44	0.52
1:C:52:ILE:HG23	1:C:56:LEU:HD22	1.91	0.52
1:F:405:THR:O	1:F:516:LYS:HE3	2.10	0.52
1:D:353:SER:CB	1:D:394:GLY:HA2	2.40	0.52
1:F:470:ARG:NH1	1:F:474:ILE:HG13	2.25	0.52
1:E:70:HIS:HA	1:E:116:VAL:HG11	1.90	0.52
1:E:375:ASP:OD2	1:E:414:ARG:HD2	2.10	0.52
1:C:212:LYS:HE2	1:C:218:ASP:HB3	1.92	0.52
1:D:443:ALA:HB2	1:D:482:LEU:HD23	1.92	0.52
1:C:49:ARG:NH2	1:C:63:GLU:OE2	2.42	0.52
1:C:111:GLY:HA3	1:C:141:SER:HA	1.91	0.52
1:F:411:VAL:HG12	1:F:435:LEU:HB2	1.91	0.52
1:B:456:ARG:HG2	1:B:459:ILE:HD11	1.91	0.52
1:C:396:LYS:HE2	1:C:529:PRO:O	2.10	0.52
1:A:153:LEU:HD21	1:B:444:VAL:HA	1.92	0.52
1:B:527:ASN:O	1:B:528:ILE:C	2.53	0.52
1:E:520:LEU:CD2	1:E:521:PRO:HD2	2.36	0.52
1:C:153:LEU:HD11	1:F:444:VAL:HA	1.91	0.51
1:F:489:GLU:HA	1:B:68:ALA:HA	1.93	0.51
1:A:112:ALA:HB1	1:A:145:ARG:CA	2.41	0.51
1:C:48:ALA:C	1:C:49:ARG:O	2.48	0.51
1:C:175:LEU:HD11	1:C:247:ALA:HB1	1.92	0.51
1:A:70:HIS:HB2	1:A:85:ASP:OD1	2.10	0.51
1:B:140:ASP:O	1:B:179:PRO:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:N	1:D:35:ARG:CD	2.72	0.51
1:E:456:ARG:HA	1:E:459:ILE:HG22	1.92	0.51
1:C:104:GLN:HB3	1:C:117:TYR:OH	2.11	0.51
1:B:61:PHE:HZ	1:B:63:GLU:HG3	1.75	0.51
1:D:408:LEU:N	1:D:432:ASP:OD2	2.39	0.51
1:D:497:ILE:HD12	1:D:498:MET:H	1.75	0.51
1:E:39:LYS:HD2	1:E:39:LYS:H	1.73	0.51
1:C:177:VAL:HA	1:C:201:SER:OG	2.11	0.51
1:A:336:ILE:N	1:A:336:ILE:HD12	2.24	0.51
1:B:344:PHE:N	1:B:344:PHE:CD2	2.77	0.51
1:B:451:VAL:C	1:B:453:ILE:H	2.18	0.51
1:D:520:LEU:HD12	1:D:521:PRO:HD2	1.92	0.51
1:C:10:ASP:CG	1:C:11:ILE:H	2.19	0.51
1:C:218:ASP:O	1:C:219:VAL:HG13	2.10	0.51
1:C:454:LEU:HD21	1:F:75:PHE:CE2	2.46	0.51
1:F:356:ALA:O	1:F:360:VAL:HG23	2.11	0.51
1:F:451:VAL:CG1	1:F:455:HIS:HB2	2.39	0.51
1:A:418:GLY:HA2	1:B:153:LEU:HD21	1.91	0.51
1:B:483:ASN:HB2	1:B:485:TYR:CD1	2.46	0.51
1:A:18:LEU:CD1	1:D:285:ASP:HB3	2.40	0.51
1:A:529:PRO:CA	1:B:358:ARG:NH1	2.72	0.51
1:B:230:HIS:HA	1:B:234:SER:OG	2.11	0.51
1:D:321:ASN:HD21	1:D:352:ALA:HB2	1.74	0.51
1:D:486:THR:O	1:D:489:GLU:HG2	2.10	0.51
1:C:339:ASN:ND2	1:C:374:VAL:HA	2.24	0.51
1:F:138:ILE:HG12	1:F:175:LEU:HD23	1.93	0.51
1:B:432:ASP:OD1	1:E:130:LYS:HE3	2.11	0.51
1:E:48:ALA:HA	1:E:51:ARG:HD2	1.93	0.51
1:A:112:ALA:HB1	1:A:145:ARG:HA	1.93	0.51
1:A:332:ARG:NE	1:A:514:ARG:HH12	2.08	0.51
1:A:391:ILE:HG23	1:B:185:VAL:CG2	2.41	0.51
1:D:45:LYS:HB2	1:D:244:GLU:OE2	2.10	0.51
1:C:19:ALA:HA	1:C:22:ARG:HH11	1.75	0.51
1:F:472:ARG:HG2	1:F:476:GLU:HG2	1.93	0.51
1:B:45:LYS:HD2	1:B:200:THR:HG22	1.93	0.51
1:B:111:GLY:C	1:B:141:SER:HB2	2.35	0.51
1:E:39:LYS:CD	1:E:39:LYS:H	2.22	0.51
1:E:374:VAL:HB	1:E:412:ILE:HD13	1.93	0.51
1:C:475:GLN:H	1:C:477:TYR:H	1.59	0.51
1:F:45:LYS:HD3	1:F:200:THR:HG21	1.93	0.51
1:F:475:GLN:O	1:F:479:ASP:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ASP:OD1	1:E:130:LYS:CE	2.59	0.51
1:D:329:VAL:HG11	1:D:510:LEU:HD12	1.93	0.51
1:E:51:ARG:HD3	1:E:138:ILE:HG21	1.92	0.51
1:E:456:ARG:O	1:E:459:ILE:HG22	2.11	0.51
1:C:397:LEU:CD1	1:C:401:TYR:CD2	2.93	0.50
1:C:519:SER:O	1:C:520:LEU:HB2	2.11	0.50
1:A:118:GLY:HA3	1:A:155:ALA:HB1	1.92	0.50
1:A:207:GLY:O	1:A:211:ILE:HD12	2.10	0.50
1:D:280:GLU:HG3	1:D:281:ASP:H	1.76	0.50
1:C:14:THR:O	1:C:18:LEU:HD13	2.12	0.50
1:F:238:HIS:HA	1:F:315:GLN:HG2	1.93	0.50
1:A:528:ILE:HG21	1:B:528:ILE:HD11	1.92	0.50
1:B:459:ILE:HG13	1:B:460:ALA:H	1.75	0.50
1:D:194:THR:N	1:D:238:HIS:HD2	1.99	0.50
1:A:153:LEU:HD22	1:B:418:GLY:O	2.12	0.50
1:B:21:LEU:HG	1:B:25:ILE:HD11	1.94	0.50
1:E:187:SER:HB3	1:E:188:PRO:HD3	1.94	0.50
1:E:203:MET:O	1:E:230:HIS:HE1	1.93	0.50
1:C:71:ARG:NH2	1:A:490:ARG:HG2	2.26	0.50
1:F:441:GLN:HG2	1:F:482:LEU:HB3	1.94	0.50
1:A:22:ARG:O	1:A:26:GLU:OE1	2.30	0.50
1:A:82:PRO:HG2	1:A:109:PHE:HE2	1.77	0.50
1:A:341:PRO:HG3	1:A:375:ASP:HB3	1.93	0.50
1:B:353:SER:HB3	1:B:394:GLY:HA2	1.94	0.50
1:B:457:ARG:O	1:B:457:ARG:CG	2.59	0.50
1:E:141:SER:O	1:E:179:PRO:HG2	2.11	0.50
1:B:74:ASN:HB2	1:B:77:LEU:HD12	1.94	0.50
1:D:145:ARG:HG2	1:D:147:GLN:HG2	1.93	0.50
1:D:353:SER:OG	1:D:394:GLY:HA2	2.12	0.50
1:D:465:ASP:OD1	1:D:466:ALA:N	2.45	0.50
1:E:474:ILE:O	1:E:475:GLN:HG3	2.11	0.50
1:A:10:ASP:CG	1:A:11:ILE:N	2.70	0.50
1:F:215:THR:HG21	1:F:217:GLU:OE2	2.12	0.50
1:A:213:THR:O	1:A:213:THR:HG22	2.12	0.50
1:B:184:ALA:C	1:B:186:TYR:H	2.20	0.50
1:B:377:PRO:O	1:B:417:PHE:HD1	1.95	0.50
1:E:461:ASP:C	1:E:463:GLY:H	2.20	0.50
1:C:69:ARG:NH1	1:C:81:ARG:HB2	2.25	0.50
1:A:177:VAL:HG12	1:A:197:VAL:HG23	1.93	0.50
1:B:419:GLY:O	1:B:423:VAL:HG23	2.12	0.50
1:B:456:ARG:HG2	1:B:459:ILE:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LYS:HE2	1:F:200:THR:HB	1.92	0.49
1:A:69:ARG:HH12	1:A:81:ARG:HB3	1.76	0.49
1:A:251:VAL:O	1:A:255:LEU:HD22	2.12	0.49
1:B:496:VAL:CG1	1:E:67:PHE:HD2	2.24	0.49
1:D:507:VAL:O	1:D:511:ARG:HG3	2.12	0.49
1:C:106:PHE:O	1:C:106:PHE:CD2	2.65	0.49
1:F:437:TRP:HE1	1:F:502:THR:HG21	1.77	0.49
1:A:205:ILE:HD13	1:B:390:ILE:HG12	1.94	0.49
1:B:410:THR:HG21	1:B:425:GLY:O	2.12	0.49
1:D:104:GLN:HG3	1:D:138:ILE:O	2.12	0.49
1:C:396:LYS:HD3	1:F:530:LEU:HG	1.94	0.49
1:F:285:ASP:HB3	1:B:18:LEU:HD11	1.94	0.49
1:F:163:ASN:HA	1:F:172:GLN:HE22	1.75	0.49
1:F:321:ASN:HA	1:F:343:GLN:HB2	1.94	0.49
1:A:70:HIS:NE2	1:A:148:GLU:CD	2.67	0.49
1:A:75:PHE:CE2	1:B:454:LEU:HD13	2.47	0.49
1:A:445:MET:HE3	1:B:146:ILE:CD1	2.42	0.49
1:E:376:VAL:CG1	1:E:420:ALA:HB1	2.25	0.49
1:F:281:ASP:O	1:F:284:LEU:HB2	2.13	0.49
1:A:326:PHE:HB3	1:A:334:VAL:O	2.12	0.49
1:D:10:ASP:CG	1:D:11:ILE:H	2.20	0.49
1:D:146:ILE:HG23	1:E:444:VAL:HG21	1.94	0.49
1:B:489:GLU:HG2	1:E:69:ARG:HB2	1.95	0.49
1:B:517:ARG:HG3	1:B:517:ARG:NH1	2.27	0.49
1:E:47:THR:HG23	1:E:49:ARG:H	1.77	0.49
1:E:447:ALA:HB1	1:E:474:ILE:HG23	1.95	0.49
1:C:208:PRO:HG3	1:C:221:PHE:CE2	2.47	0.49
1:C:350:ILE:HD13	1:C:393:ARG:NH1	2.27	0.49
1:F:290:ASP:OD1	1:B:13:THR:HG22	2.13	0.49
1:F:375:ASP:CG	1:F:414:ARG:HB3	2.38	0.49
1:A:49:ARG:HG3	1:A:88:VAL:HG21	1.94	0.49
1:A:163:ASN:HB3	1:A:190:ILE:CG1	2.43	0.49
1:A:498:MET:HE3	1:A:500:SER:CB	2.31	0.49
1:A:161:ARG:HD3	1:B:428:HIS:O	2.12	0.49
1:A:176:VAL:O	1:A:196:MET:HA	2.13	0.49
1:A:393:ARG:HH22	1:B:393:ARG:NH1	2.11	0.49
1:B:89:THR:HB	1:B:124:VAL:HG11	1.95	0.49
1:B:397:LEU:HD23	1:B:423:VAL:CG1	2.43	0.49
1:B:498:MET:CE	1:E:18:LEU:HG	2.43	0.49
1:E:520:LEU:HD13	1:E:521:PRO:HD2	1.94	0.49
1:F:213:THR:O	1:F:213:THR:HG22	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:496:VAL:HB	1:B:67:PHE:HE2	1.76	0.49
1:A:377:PRO:HA	1:A:417:PHE:HD2	1.78	0.49
1:D:410:THR:HB	1:D:434:ASN:ND2	2.27	0.49
1:C:208:PRO:HD3	1:C:221:PHE:CE2	2.47	0.49
1:A:40:GLN:NE2	1:A:41:HIS:N	2.59	0.49
1:B:46:LEU:HB3	1:B:50:GLU:HB2	1.94	0.49
1:D:337:VAL:O	1:D:372:THR:HA	2.12	0.49
1:E:175:LEU:HD11	1:E:247:ALA:HB1	1.95	0.49
1:C:208:PRO:HD3	1:C:221:PHE:HE2	1.75	0.48
1:C:482:LEU:N	1:C:482:LEU:HD23	2.28	0.48
1:A:40:GLN:CD	1:A:41:HIS:H	2.20	0.48
1:D:121:ILE:O	1:D:125:MET:HG3	2.13	0.48
1:E:109:PHE:C	1:E:111:GLY:H	2.21	0.48
1:E:356:ALA:O	1:E:360:VAL:HG23	2.12	0.48
1:C:70:HIS:C	1:C:70:HIS:ND1	2.68	0.48
1:F:21:LEU:HD22	1:E:438:PRO:HG3	1.95	0.48
1:D:302:ILE:HD13	1:D:336:ILE:HG21	1.95	0.48
1:C:391:ILE:HG23	1:F:185:VAL:HG22	1.96	0.48
1:B:350:ILE:HG21	1:B:393:ARG:NH1	2.29	0.48
1:B:455:HIS:CD2	1:B:455:HIS:N	2.81	0.48
1:E:302:ILE:HG22	1:E:306:LEU:HD22	1.94	0.48
1:E:303:GLU:HG2	1:E:309:ALA:O	2.13	0.48
1:C:208:PRO:CD	1:C:221:PHE:CE2	2.93	0.48
1:C:234:SER:O	1:F:392:ARG:NH1	2.46	0.48
1:B:494:ASP:HB3	1:E:64:LEU:HD12	1.95	0.48
1:D:196:MET:HE1	1:D:230:HIS:CB	2.29	0.48
1:E:51:ARG:NH1	1:E:51:ARG:CG	2.66	0.48
1:F:77:LEU:HD13	1:F:147:GLN:HG3	1.94	0.48
1:F:289:PRO:HB2	1:F:294:GLN:HG3	1.96	0.48
1:E:21:LEU:O	1:E:25:ILE:HG13	2.13	0.48
1:E:234:SER:CB	1:E:236:VAL:HG23	2.43	0.48
1:C:202:HIS:HE1	1:C:222:GLU:HA	1.78	0.48
1:C:285:ASP:OD2	1:C:500:SER:HB3	2.14	0.48
1:A:40:GLN:HB2	1:A:45:LYS:HD2	1.96	0.48
1:B:89:THR:HG22	1:B:102:PHE:HB2	1.95	0.48
1:A:459:ILE:CG1	1:A:460:ALA:N	2.77	0.48
1:B:496:VAL:CG1	1:E:67:PHE:CD2	2.97	0.48
1:C:106:PHE:O	1:C:106:PHE:HD2	1.97	0.48
1:C:461:ASP:C	1:C:463:GLY:N	2.71	0.48
1:F:297:ASP:OD1	1:F:299:HIS:HD2	1.97	0.48
1:B:357:ALA:O	1:B:361:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASP:HB2	1:D:120:LYS:HE3	1.94	0.48
1:D:295:PRO:HB2	1:D:342:MET:HE3	1.96	0.48
1:C:243:ASP:OD2	1:C:244:GLU:N	2.47	0.48
1:A:442:ILE:HD11	1:A:487:ALA:H	1.79	0.48
1:D:302:ILE:O	1:D:305:VAL:HG22	2.13	0.48
1:E:350:ILE:HG13	1:E:390:ILE:HD13	1.95	0.48
1:C:126:ASP:OD1	1:C:162:ARG:HD3	2.14	0.48
1:C:461:ASP:O	1:C:462:ALA:C	2.57	0.48
1:C:469:THR:O	1:C:473:LEU:HG	2.13	0.48
1:F:357:ALA:O	1:F:361:ARG:HG3	2.14	0.48
1:F:458:THR:HA	1:F:461:ASP:HB2	1.96	0.48
1:A:391:ILE:HG23	1:B:185:VAL:HG23	1.95	0.48
1:A:465:ASP:O	1:A:466:ALA:C	2.57	0.48
1:B:370:VAL:HB	1:B:408:LEU:HD23	1.95	0.48
1:D:104:GLN:HE21	1:D:140:ASP:H	1.62	0.48
1:E:47:THR:HG23	1:E:49:ARG:N	2.29	0.48
1:E:211:ILE:HG13	1:E:212:LYS:H	1.79	0.48
1:C:51:ARG:HH12	1:C:140:ASP:HB2	1.78	0.47
1:F:10:ASP:O	1:F:16:GLY:HA3	2.14	0.47
1:F:138:ILE:HA	1:F:175:LEU:O	2.14	0.47
1:A:322:ILE:CG2	1:A:355:LYS:HD3	2.44	0.47
1:A:517:ARG:HH11	1:A:517:ARG:HG2	1.77	0.47
1:E:245:LYS:HG2	1:E:246:ASP:H	1.77	0.47
1:C:158:GLU:OE2	1:C:161:ARG:NH2	2.46	0.47
1:C:295:PRO:HB2	1:C:342:MET:HE2	1.96	0.47
1:A:369:PRO:HA	1:A:406:VAL:CG1	2.40	0.47
1:A:454:LEU:HD21	1:B:146:ILE:HG21	1.95	0.47
1:B:109:PHE:C	1:B:111:GLY:H	2.21	0.47
1:B:496:VAL:HG13	1:E:67:PHE:CD2	2.49	0.47
1:E:74:ASN:HB3	1:E:75:PHE:CD1	2.47	0.47
1:E:103:SER:HB2	1:E:138:ILE:HD12	1.95	0.47
1:E:185:VAL:C	1:E:188:PRO:HD2	2.40	0.47
1:C:110:GLY:O	1:C:142:GLY:N	2.40	0.47
1:A:104:GLN:HB2	1:A:140:ASP:H	1.78	0.47
1:A:332:ARG:CZ	1:A:514:ARG:NH1	2.78	0.47
1:B:21:LEU:HG	1:B:25:ILE:CD1	2.44	0.47
1:B:73:THR:O	1:B:75:PHE:N	2.47	0.47
1:B:374:VAL:HG23	1:B:376:VAL:HG12	1.96	0.47
1:D:173:ILE:HD13	1:D:254:LEU:HD23	1.95	0.47
1:C:517:ARG:O	1:C:517:ARG:HG3	2.14	0.47
1:A:18:LEU:CD1	1:D:498:MET:HE1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD11	1:D:285:ASP:HB3	1.96	0.47
1:A:238:HIS:CE1	1:A:315:GLN:HE21	2.32	0.47
1:A:410:THR:OG1	1:A:434:ASN:ND2	2.47	0.47
1:A:527:ASN:O	1:B:358:ARG:NH1	2.47	0.47
1:B:77:LEU:HD21	1:B:147:GLN:HB3	1.97	0.47
1:E:112:ALA:HA	1:E:143:GLY:O	2.15	0.47
1:A:141:SER:O	1:A:179:PRO:O	2.33	0.47
1:B:451:VAL:O	1:B:455:HIS:HD2	1.98	0.47
1:E:414:ARG:O	1:E:440:ALA:HA	2.14	0.47
1:F:217:GLU:O	1:F:217:GLU:HG2	2.14	0.47
1:A:371:LEU:CD2	1:A:409:ILE:HB	2.45	0.47
1:B:375:ASP:OD2	1:B:414:ARG:HD2	2.14	0.47
1:B:530:LEU:HA	1:B:530:LEU:HD23	1.58	0.47
1:D:161:ARG:HD3	1:E:428:HIS:O	2.14	0.47
1:E:14:THR:O	1:E:18:LEU:HD13	2.14	0.47
1:C:83:TYR:C	1:C:85:ASP:H	2.23	0.47
1:C:381:PRO:HG2	1:F:214:VAL:HG21	1.95	0.47
1:C:433:LEU:HA	1:C:494:ASP:OD2	2.14	0.47
1:C:512:GLN:HG3	1:D:91:TYR:CE1	2.49	0.47
1:F:177:VAL:HA	1:F:201:SER:OG	2.14	0.47
1:A:40:GLN:CD	1:A:40:GLN:H	2.22	0.47
1:A:393:ARG:NH2	1:B:393:ARG:NH1	2.62	0.47
1:A:401:TYR:CD1	1:A:425:GLY:HA2	2.49	0.47
1:A:459:ILE:HG13	1:A:460:ALA:N	2.30	0.47
1:E:214:VAL:HG23	1:E:215:THR:N	2.28	0.47
1:E:470:ARG:O	1:E:474:ILE:HG13	2.14	0.47
1:C:99:VAL:HG12	1:C:100:ALA:N	2.30	0.47
1:F:45:LYS:HD3	1:F:200:THR:CG2	2.45	0.47
1:A:35:ARG:NH2	1:A:39:LYS:CE	2.78	0.47
1:A:218:ASP:O	1:A:219:VAL:HG23	2.14	0.47
1:B:198:ASP:OD1	1:B:199:GLN:HG2	2.15	0.47
1:D:350:ILE:HD13	1:D:390:ILE:HD13	1.96	0.47
1:E:299:HIS:HE1	1:E:313:GLU:OE1	1.97	0.47
1:C:202:HIS:ND1	1:C:226:GLY:HA2	2.29	0.47
1:F:441:GLN:HG3	1:F:482:LEU:O	2.15	0.47
1:F:483:ASN:HB2	1:F:484:PRO:HD2	1.97	0.47
1:A:35:ARG:NH2	1:A:39:LYS:NZ	2.63	0.47
1:A:361:ARG:CD	1:A:403:GLU:OE2	2.61	0.47
1:A:386:GLU:OE2	1:B:204:PHE:HA	2.15	0.47
1:A:445:MET:HE3	1:B:146:ILE:HD11	1.96	0.47
1:A:447:ALA:O	1:A:474:ILE:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ASN:ND2	1:E:523:LYS:HA	2.29	0.47
1:D:296:TYR:O	1:D:342:MET:HG2	2.15	0.47
1:D:319:ALA:N	1:D:320:PRO:HD3	2.30	0.47
1:E:87:VAL:HG23	1:E:104:GLN:HA	1.97	0.47
1:E:472:ARG:O	1:E:476:GLU:HB2	2.15	0.47
1:F:25:ILE:O	1:F:29:THR:HG23	2.14	0.46
1:F:105:ASP:C	1:F:107:THR:N	2.72	0.46
1:A:445:MET:SD	1:A:450:ALA:HA	2.55	0.46
1:A:449:GLY:HA2	1:A:452:ASN:ND2	2.29	0.46
1:A:517:ARG:HG2	1:A:517:ARG:NH1	2.31	0.46
1:E:320:PRO:HB2	1:E:343:GLN:HG3	1.96	0.46
1:C:459:ILE:C	1:C:459:ILE:HD13	2.41	0.46
1:D:51:ARG:HH11	1:D:51:ARG:HG2	1.80	0.46
1:F:457:ARG:NH1	1:F:458:THR:OG1	2.45	0.46
1:A:47:THR:O	1:A:48:ALA:HB3	2.15	0.46
1:B:86:GLY:HA2	1:B:108:VAL:HB	1.96	0.46
1:B:281:ASP:O	1:B:500:SER:HA	2.16	0.46
1:B:337:VAL:CG2	1:B:372:THR:HG22	2.45	0.46
1:D:21:LEU:O	1:D:21:LEU:HD12	2.15	0.46
1:C:153:LEU:HD21	1:F:418:GLY:HA2	1.97	0.46
1:A:67:PHE:CE2	1:D:496:VAL:HG13	2.50	0.46
1:A:153:LEU:HG	1:B:444:VAL:HG12	1.97	0.46
1:B:344:PHE:C	1:B:346:GLY:H	2.23	0.46
1:B:490:ARG:HD3	1:B:492:TYR:CZ	2.50	0.46
1:D:182:GLY:C	1:D:205:ILE:HD12	2.40	0.46
1:D:286:THR:O	1:D:287:ILE:CG2	2.56	0.46
1:C:209:ASP:OD1	1:C:209:ASP:N	2.47	0.46
1:A:466:ALA:O	1:A:467:GLU:C	2.59	0.46
1:B:77:LEU:O	1:B:79:ALA:N	2.49	0.46
1:B:80:ASN:ND2	1:B:80:ASN:O	2.49	0.46
1:B:455:HIS:HE1	1:B:477:TYR:CE2	2.33	0.46
1:D:107:THR:CG2	1:D:107:THR:O	2.62	0.46
1:D:441:GLN:HG2	1:D:482:LEU:O	2.16	0.46
1:E:84:GLY:C	1:E:86:GLY:H	2.24	0.46
1:C:285:ASP:OD1	1:C:499:PRO:HD2	2.16	0.46
1:A:334:VAL:CG2	1:A:371:LEU:HG	2.45	0.46
1:B:496:VAL:HG13	1:E:67:PHE:HE2	1.80	0.46
1:D:350:ILE:HG21	1:D:393:ARG:NH1	2.31	0.46
1:D:458:THR:HG22	1:D:458:THR:O	2.16	0.46
1:D:513:LEU:HD12	1:D:513:LEU:HA	1.64	0.46
1:C:382:GLY:O	1:C:385:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:O	1:A:47:THR:HG22	2.16	0.46
1:A:442:ILE:CD1	1:A:487:ALA:H	2.28	0.46
1:B:305:VAL:O	1:B:306:LEU:CB	2.63	0.46
1:D:354:GLU:OE2	1:D:393:ARG:CD	2.59	0.46
1:E:51:ARG:NH2	1:E:177:VAL:HG21	2.31	0.46
1:C:145:ARG:HG3	1:C:148:GLU:HG3	1.98	0.46
1:F:102:PHE:CD1	1:F:102:PHE:C	2.93	0.46
1:F:517:ARG:O	1:F:518:GLU:HB3	2.15	0.46
1:A:175:LEU:HA	1:A:195:VAL:HG13	1.98	0.46
1:B:280:GLU:O	1:B:283:GLU:HG3	2.16	0.46
1:D:197:VAL:HG12	1:D:247:ALA:HB2	1.96	0.46
1:E:36:ALA:HA	1:E:39:LYS:CD	2.41	0.46
1:E:47:THR:HG22	1:E:50:GLU:N	2.29	0.46
1:C:363:CYS:HB3	1:C:368:VAL:HG22	1.98	0.46
1:A:350:ILE:HG13	1:A:393:ARG:HD2	1.96	0.46
1:A:372:THR:HG21	1:A:401:TYR:HE1	1.79	0.46
1:B:69:ARG:NE	1:B:81:ARG:O	2.48	0.46
1:D:211:ILE:HG21	1:E:383:VAL:HG23	1.97	0.46
1:D:381:PRO:HB2	1:E:214:VAL:CG2	2.45	0.46
1:F:458:THR:CG2	1:F:469:THR:HG21	2.41	0.46
1:F:464:ASP:C	1:F:466:ALA:H	2.24	0.46
1:F:493:VAL:HG12	1:F:495:ALA:H	1.80	0.46
1:A:376:VAL:HG21	1:A:420:ALA:HB1	1.98	0.46
1:A:443:ALA:O	1:B:153:LEU:HD11	2.16	0.46
1:B:350:ILE:HG21	1:B:393:ARG:HH12	1.81	0.46
1:E:69:ARG:NH1	1:E:69:ARG:CG	2.60	0.46
1:C:397:LEU:C	1:C:397:LEU:CD1	2.89	0.45
1:A:113:LEU:HD23	1:A:113:LEU:O	2.15	0.45
1:A:393:ARG:HH12	1:B:393:ARG:NH2	2.14	0.45
1:A:437:TRP:CE2	1:A:499:PRO:HA	2.50	0.45
1:A:459:ILE:HD12	1:A:460:ALA:N	2.32	0.45
1:B:108:VAL:HG12	1:B:109:PHE:CD1	2.50	0.45
1:D:47:THR:O	1:D:49:ARG:O	2.34	0.45
1:D:480:ALA:O	1:D:481:LEU:HD23	2.16	0.45
1:E:459:ILE:HD11	1:E:470:ARG:HB2	1.98	0.45
1:F:461:ASP:O	1:F:462:ALA:C	2.58	0.45
1:D:303:GLU:O	1:D:309:ALA:HA	2.16	0.45
1:E:68:ALA:HB3	1:E:85:ASP:OD2	2.17	0.45
1:E:156:TYR:HE1	1:E:184:ALA:HB2	1.81	0.45
1:C:474:ILE:O	1:C:474:ILE:HG22	2.16	0.45
1:F:451:VAL:C	1:F:453:ILE:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:HB	1:A:412:ILE:HG12	1.98	0.45
1:D:198:ASP:HA	1:D:240:MET:SD	2.57	0.45
1:E:36:ALA:CA	1:E:39:LYS:HD3	2.41	0.45
1:A:138:ILE:HG22	1:A:175:LEU:CB	2.39	0.45
1:A:288:VAL:O	1:A:288:VAL:HG22	2.16	0.45
1:A:516:LYS:HE2	1:A:516:LYS:HB2	1.78	0.45
1:D:311:PHE:CE2	1:D:313:GLU:HB2	2.51	0.45
1:E:436:ALA:O	1:E:496:VAL:HA	2.16	0.45
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.68	0.45
1:F:187:SER:HB3	1:F:188:PRO:CD	2.45	0.45
1:A:475:GLN:NE2	1:A:475:GLN:HA	2.31	0.45
1:B:296:TYR:O	1:B:342:MET:HG2	2.17	0.45
1:E:47:THR:H	1:E:50:GLU:CD	2.25	0.45
1:E:481:LEU:C	1:E:483:ASN:H	2.24	0.45
1:F:70:HIS:O	1:F:81:ARG:NH1	2.49	0.45
1:A:77:LEU:HD21	1:A:147:GLN:HG3	1.98	0.45
1:A:104:GLN:HB3	1:A:117:TYR:OH	2.16	0.45
1:A:116:VAL:HA	1:A:119:GLN:OE1	2.16	0.45
1:D:113:LEU:HD21	1:D:155:ALA:HB3	1.98	0.45
1:D:253:GLN:NE2	1:D:257:TYR:HE2	2.15	0.45
1:E:27:GLU:OE1	1:E:83:TYR:HE2	1.99	0.45
1:E:485:TYR:O	1:E:489:GLU:HG3	2.17	0.45
1:F:45:LYS:NZ	1:F:244:GLU:OE2	2.49	0.45
1:F:298:MET:O	1:F:301:VAL:HG13	2.17	0.45
1:A:372:THR:CG2	1:A:401:TYR:OH	2.64	0.45
1:D:103:SER:HA	1:D:138:ILE:HB	1.99	0.45
1:D:280:GLU:HG3	1:D:281:ASP:N	2.32	0.45
1:D:414:ARG:HA	1:D:439:THR:O	2.17	0.45
1:E:87:VAL:O	1:E:120:LYS:NZ	2.43	0.45
1:F:180:CYS:SG	1:F:185:VAL:HA	2.57	0.45
1:F:411:VAL:HG12	1:F:435:LEU:HD12	1.98	0.45
1:A:418:GLY:HA2	1:B:153:LEU:CD2	2.45	0.45
1:B:31:ALA:HB1	1:B:108:VAL:HG22	1.99	0.45
1:B:322:ILE:HD13	1:B:356:ALA:HB2	1.98	0.45
1:B:451:VAL:HG13	1:B:455:HIS:NE2	2.32	0.45
1:D:48:ALA:HA	1:D:51:ARG:HD2	1.99	0.45
1:E:182:GLY:O	1:E:185:VAL:CG1	2.61	0.45
1:C:67:PHE:CD2	1:A:496:VAL:CG2	3.00	0.45
1:A:113:LEU:HD23	1:A:113:LEU:C	2.42	0.45
1:B:87:VAL:HG13	1:B:120:LYS:CD	2.45	0.45
1:E:422:ASN:O	1:E:429:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:ARG:O	1:E:474:ILE:O	2.35	0.45
1:C:319:ALA:N	1:C:320:PRO:HD3	2.33	0.44
1:A:43:LYS:HE3	1:A:45:LYS:CE	2.45	0.44
1:A:76:GLY:O	1:A:77:LEU:C	2.60	0.44
1:B:110:GLY:C	1:B:112:ALA:H	2.26	0.44
1:B:238:HIS:HA	1:B:315:GLN:HG3	1.99	0.44
1:D:520:LEU:CB	1:D:521:PRO:CD	2.92	0.44
1:F:141:SER:O	1:F:179:PRO:HG2	2.18	0.44
1:A:19:ALA:O	1:A:20:ASP:C	2.60	0.44
1:B:32:GLY:H	1:B:107:THR:CG2	2.29	0.44
1:B:196:MET:HE2	1:B:237:ALA:CB	2.47	0.44
1:D:108:VAL:HG12	1:D:109:PHE:CD1	2.52	0.44
1:D:447:ALA:HB2	1:D:478:GLU:HG3	2.00	0.44
1:F:478:GLU:HB3	1:F:482:LEU:HD22	1.99	0.44
1:A:70:HIS:ND1	1:A:71:ARG:N	2.59	0.44
1:A:196:MET:HB3	1:A:201:SER:OG	2.17	0.44
1:B:14:THR:O	1:B:18:LEU:HG	2.17	0.44
1:B:182:GLY:C	1:B:184:ALA:N	2.75	0.44
1:D:298:MET:SD	1:D:301:VAL:HG11	2.57	0.44
1:E:455:HIS:ND1	1:E:455:HIS:N	2.64	0.44
1:F:70:HIS:HE1	1:F:72:SER:O	2.00	0.44
1:F:510:LEU:O	1:F:514:ARG:HG3	2.18	0.44
1:A:115:GLU:HG3	1:A:116:VAL:N	2.33	0.44
1:D:107:THR:HG23	1:D:107:THR:O	2.16	0.44
1:D:321:ASN:ND2	1:D:352:ALA:HB2	2.33	0.44
1:D:422:ASN:HA	1:D:426:SER:CB	2.46	0.44
1:E:467:GLU:C	1:E:469:THR:N	2.68	0.44
1:F:45:LYS:CE	1:F:200:THR:HB	2.48	0.44
1:A:70:HIS:HE1	1:A:115:GLU:HG2	1.80	0.44
1:A:71:ARG:HH21	1:D:490:ARG:HE	1.65	0.44
1:A:347:CYS:SG	1:A:380:LEU:HB3	2.58	0.44
1:A:380:LEU:CD1	1:A:380:LEU:C	2.91	0.44
1:B:77:LEU:HD21	1:B:147:GLN:CB	2.48	0.44
1:B:230:HIS:CD2	1:B:234:SER:OG	2.63	0.44
1:B:253:GLN:HG2	1:B:312:PHE:CE1	2.53	0.44
1:B:368:VAL:HA	1:B:369:PRO:HD3	1.88	0.44
1:D:483:ASN:HB2	1:D:484:PRO:CD	2.47	0.44
1:E:473:LEU:HD13	1:E:473:LEU:HA	1.87	0.44
1:C:438:PRO:HG3	1:D:21:LEU:HD22	1.99	0.44
1:D:51:ARG:NH1	1:D:51:ARG:HG2	2.33	0.44
1:D:398:ILE:HG21	1:E:160:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:TRP:NE1	1:F:502:THR:HG21	2.32	0.44
1:D:399:PHE:CE2	1:E:164:THR:HG23	2.53	0.44
1:F:106:PHE:O	1:F:106:PHE:CD2	2.70	0.44
1:F:370:VAL:HB	1:F:408:LEU:HD23	1.99	0.44
1:B:113:LEU:HD21	1:B:155:ALA:HB3	2.00	0.44
1:D:447:ALA:HB1	1:D:474:ILE:HG23	1.99	0.44
1:D:506:ILE:O	1:D:510:LEU:HG	2.18	0.44
1:E:187:SER:O	1:E:191:THR:HG23	2.18	0.44
1:E:414:ARG:O	1:E:441:GLN:N	2.39	0.44
1:C:181:ALA:O	1:C:184:ALA:HB3	2.18	0.44
1:C:397:LEU:HD11	1:C:401:TYR:HE2	1.82	0.44
1:F:319:ALA:N	1:F:320:PRO:HD3	2.32	0.44
1:A:302:ILE:HD13	1:A:336:ILE:HG21	1.99	0.44
1:A:528:ILE:O	1:A:529:PRO:C	2.59	0.44
1:B:75:PHE:HD1	1:B:76:GLY:N	2.16	0.44
1:B:417:PHE:HA	1:B:443:ALA:O	2.18	0.44
1:E:78:ASP:OD1	1:E:78:ASP:N	2.50	0.44
1:C:254:LEU:HD13	1:C:312:PHE:HE2	1.82	0.43
1:C:482:LEU:N	1:C:482:LEU:CD2	2.81	0.43
1:F:497:ILE:HD12	1:F:497:ILE:C	2.42	0.43
1:A:487:ALA:HB1	1:A:492:TYR:HB2	2.00	0.43
1:B:89:THR:HG22	1:B:102:PHE:CB	2.48	0.43
1:B:377:PRO:HB3	1:B:415:LYS:HE3	1.99	0.43
1:D:24:ARG:NH1	1:D:83:TYR:OH	2.43	0.43
1:D:318:PHE:O	1:D:319:ALA:C	2.60	0.43
1:E:318:PHE:O	1:E:319:ALA:C	2.61	0.43
1:C:449:GLY:O	1:C:453:ILE:HD13	2.19	0.43
1:F:11:ILE:N	1:F:11:ILE:HD12	2.33	0.43
1:F:163:ASN:ND2	1:F:187:SER:OG	2.46	0.43
1:A:51:ARG:NH1	1:A:138:ILE:HD12	2.33	0.43
1:A:102:PHE:CE2	1:A:137:GLY:HA3	2.53	0.43
1:A:238:HIS:HA	1:A:315:GLN:HG3	2.00	0.43
1:A:459:ILE:HG21	1:A:470:ARG:HE	1.83	0.43
1:A:529:PRO:HG3	1:B:190:ILE:HA	1.99	0.43
1:B:343:GLN:C	1:B:344:PHE:CD2	2.96	0.43
1:D:196:MET:HE2	1:D:237:ALA:CB	2.35	0.43
1:D:440:ALA:HB3	1:D:484:PRO:HG3	2.00	0.43
1:F:46:LEU:HB2	1:F:244:GLU:OE1	2.18	0.43
1:F:483:ASN:HB2	1:F:485:TYR:HD2	1.83	0.43
1:A:35:ARG:NH2	1:A:39:LYS:HE2	2.33	0.43
1:A:350:ILE:HG13	1:A:393:ARG:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLY:O	1:A:423:VAL:HG23	2.18	0.43
1:A:449:GLY:HA2	1:A:452:ASN:HD21	1.83	0.43
1:D:47:THR:C	1:D:49:ARG:O	2.60	0.43
1:D:141:SER:O	1:D:179:PRO:HG2	2.17	0.43
1:D:294:GLN:OE1	1:D:295:PRO:HD2	2.18	0.43
1:E:295:PRO:CB	1:E:342:MET:HE2	2.33	0.43
1:C:230:HIS:HA	1:C:234:SER:OG	2.19	0.43
1:C:288:VAL:HG12	1:C:289:PRO:O	2.19	0.43
1:F:476:GLU:OE1	1:F:476:GLU:HA	2.17	0.43
1:A:51:ARG:HH11	1:A:138:ILE:HD13	1.82	0.43
1:A:298:MET:HE3	1:A:301:VAL:HG13	1.98	0.43
1:A:374:VAL:CG1	1:A:376:VAL:HG12	2.48	0.43
1:B:405:THR:HA	1:B:518:GLU:OE1	2.17	0.43
1:E:86:GLY:HA2	1:E:108:VAL:HB	1.99	0.43
1:C:392:ARG:NH1	1:F:234:SER:O	2.52	0.43
1:F:485:TYR:HE2	1:B:17:LYS:NZ	2.16	0.43
1:A:126:ASP:O	1:A:130:LYS:HB3	2.18	0.43
1:A:153:LEU:CD2	1:B:444:VAL:HG12	2.49	0.43
1:B:448:GLN:O	1:B:452:ASN:OD1	2.36	0.43
1:E:47:THR:HG22	1:E:50:GLU:CB	2.48	0.43
1:C:63:GLU:OE2	1:C:88:VAL:HG23	2.17	0.43
1:C:135:VAL:HG23	1:C:170:ILE:HD12	2.00	0.43
1:C:324:THR:HA	1:C:336:ILE:O	2.18	0.43
1:C:472:ARG:HD3	1:C:472:ARG:HA	1.61	0.43
1:F:210:VAL:O	1:F:214:VAL:HG23	2.18	0.43
1:F:338:ALA:HB1	1:F:373:PHE:HB2	2.00	0.43
1:B:372:THR:OG1	1:B:410:THR:HG22	2.18	0.43
1:A:156:TYR:CE1	1:A:184:ALA:HB2	2.54	0.43
1:A:205:ILE:CD1	1:B:390:ILE:HG12	2.49	0.43
1:A:478:GLU:O	1:A:482:LEU:HB2	2.18	0.43
1:B:78:ASP:OD1	1:B:78:ASP:N	2.51	0.43
1:B:135:VAL:HG12	1:B:172:GLN:HA	2.00	0.43
1:B:177:VAL:HG23	1:B:178:GLY:H	1.83	0.43
1:B:212:LYS:HG3	1:B:213:THR:N	2.34	0.43
1:B:477:TYR:O	1:B:481:LEU:HB2	2.19	0.43
1:E:23:ARG:HG3	1:E:24:ARG:H	1.83	0.43
1:E:340:GLN:O	1:E:340:GLN:HG3	2.18	0.43
1:E:474:ILE:O	1:E:476:GLU:N	2.46	0.43
1:C:146:ILE:H	1:C:146:ILE:HG12	1.30	0.43
1:F:45:LYS:CD	1:F:200:THR:HB	2.49	0.43
1:F:437:TRP:NE1	1:F:502:THR:CG2	2.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:462:ALA:HB1	1:F:465:ASP:CG	2.44	0.43
1:B:275:LEU:HD11	1:B:508:ARG:NH2	2.33	0.43
1:B:290:ASP:OD2	1:B:290:ASP:N	2.51	0.43
1:D:193:PHE:HA	1:D:238:HIS:CD2	2.54	0.43
1:E:483:ASN:HB2	1:E:484:PRO:CD	2.49	0.43
1:C:268:ALA:C	1:C:270:PRO:HD3	2.44	0.43
1:C:350:ILE:HG22	1:C:390:ILE:CD1	2.48	0.43
1:A:52:ILE:HG23	1:A:56:LEU:HD12	2.01	0.43
1:E:375:ASP:CG	1:E:414:ARG:HB3	2.44	0.43
1:E:451:VAL:HA	1:E:454:LEU:HB2	2.00	0.43
1:C:113:LEU:HD12	1:C:117:TYR:CE2	2.53	0.43
1:C:238:HIS:HA	1:C:315:GLN:HG2	2.00	0.43
1:C:472:ARG:CD	1:C:475:GLN:HE21	2.31	0.43
1:A:399:PHE:CG	1:A:528:ILE:HG13	2.54	0.43
1:A:451:VAL:HG13	1:A:477:TYR:CD1	2.54	0.43
1:B:150:VAL:C	1:B:152:SER:N	2.77	0.43
1:B:437:TRP:NE1	1:B:502:THR:CG2	2.76	0.43
1:D:288:VAL:O	1:D:288:VAL:HG22	2.18	0.43
1:E:118:GLY:HA3	1:E:155:ALA:HB1	2.01	0.43
1:C:196:MET:HE1	1:C:203:MET:HE2	2.00	0.42
1:F:141:SER:O	1:F:179:PRO:O	2.37	0.42
1:F:451:VAL:HG13	1:F:455:HIS:CB	2.47	0.42
1:A:121:ILE:O	1:A:125:MET:HG3	2.20	0.42
1:A:374:VAL:HG22	1:A:424:MET:HB3	2.01	0.42
1:B:74:ASN:H	1:B:77:LEU:HD12	1.84	0.42
1:D:342:MET:HA	1:D:342:MET:CE	2.47	0.42
1:E:129:LEU:HA	1:E:170:ILE:HD13	2.00	0.42
1:E:141:SER:O	1:E:179:PRO:O	2.36	0.42
1:C:337:VAL:O	1:C:372:THR:HA	2.19	0.42
1:F:320:PRO:HB2	1:F:343:GLN:HG3	2.01	0.42
1:A:528:ILE:O	1:B:358:ARG:NH1	2.52	0.42
1:B:477:TYR:O	1:B:481:LEU:N	2.52	0.42
1:E:246:ASP:O	1:E:249:GLU:N	2.51	0.42
1:E:510:LEU:O	1:E:511:ARG:C	2.61	0.42
1:C:180:CYS:HB3	1:C:203:MET:HG2	2.01	0.42
1:F:45:LYS:HE3	1:F:177:VAL:O	2.19	0.42
1:F:456:ARG:HG3	1:F:457:ARG:N	2.34	0.42
1:A:398:ILE:HD13	1:B:160:PHE:CD2	2.54	0.42
1:A:438:PRO:HD3	1:A:497:ILE:O	2.19	0.42
1:B:77:LEU:HD21	1:B:147:GLN:CG	2.48	0.42
1:B:290:ASP:HB3	1:E:13:THR:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:TYR:C	1:D:117:TYR:CD2	2.97	0.42
1:D:437:TRP:CE2	1:D:499:PRO:HA	2.54	0.42
1:D:523:LYS:HA	1:E:262:ASN:ND2	2.33	0.42
1:E:98:PRO:O	1:E:134:PRO:HD2	2.19	0.42
1:C:389:GLY:C	1:C:391:ILE:N	2.74	0.42
1:F:475:GLN:O	1:F:475:GLN:HG2	2.18	0.42
1:A:199:GLN:HG3	1:A:222:GLU:OE1	2.19	0.42
1:A:204:PHE:HA	1:B:386:GLU:OE2	2.19	0.42
1:A:238:HIS:CE1	1:A:315:GLN:NE2	2.87	0.42
1:A:459:ILE:CG1	1:A:460:ALA:H	2.32	0.42
1:B:483:ASN:HB2	1:B:485:TYR:HD1	1.83	0.42
1:D:262:ASN:HD21	1:E:523:LYS:HA	1.85	0.42
1:C:108:VAL:O	1:C:109:PHE:CG	2.73	0.42
1:C:164:THR:HG23	1:F:399:PHE:CE2	2.54	0.42
1:C:414:ARG:HA	1:C:440:ALA:HA	2.02	0.42
1:C:481:LEU:C	1:C:483:ASN:H	2.26	0.42
1:F:305:VAL:HG11	1:F:506:ILE:CD1	2.49	0.42
1:A:76:GLY:O	1:A:78:ASP:N	2.52	0.42
1:A:176:VAL:HG12	1:A:201:SER:HB2	2.02	0.42
1:B:344:PHE:C	1:B:346:GLY:N	2.77	0.42
1:D:35:ARG:N	1:D:35:ARG:HD2	2.33	0.42
1:D:65:ASP:OD1	1:D:123:LYS:NZ	2.47	0.42
1:D:391:ILE:HG21	1:E:185:VAL:HG21	2.01	0.42
1:E:113:LEU:CD1	1:E:117:TYR:CD2	2.95	0.42
1:C:170:ILE:O	1:C:170:ILE:HG13	2.18	0.42
1:F:451:VAL:HG13	1:F:455:HIS:HD2	1.83	0.42
1:A:367:ASN:HA	1:A:406:VAL:CG2	2.50	0.42
1:B:111:GLY:O	1:B:141:SER:HB2	2.19	0.42
1:B:148:GLU:HB2	1:B:152:SER:OG	2.19	0.42
1:B:489:GLU:CG	1:E:69:ARG:HB2	2.49	0.42
1:D:520:LEU:CB	1:D:521:PRO:HD2	2.42	0.42
1:C:201:SER:C	1:C:202:HIS:CD2	2.98	0.42
1:C:339:ASN:HD22	1:C:375:ASP:H	1.68	0.42
1:C:454:LEU:O	1:C:455:HIS:HD2	2.03	0.42
1:F:472:ARG:O	1:F:476:GLU:HG2	2.19	0.42
1:A:337:VAL:O	1:A:372:THR:HA	2.19	0.42
1:B:32:GLY:H	1:B:107:THR:HG21	1.85	0.42
1:D:454:LEU:HD21	1:E:75:PHE:CZ	2.53	0.42
1:D:465:ASP:CG	1:D:467:GLU:H	2.28	0.42
1:E:121:ILE:O	1:E:125:MET:HG3	2.20	0.42
1:E:447:ALA:HB2	1:E:478:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:SER:O	1:C:520:LEU:HB3	2.20	0.42
1:F:89:THR:HG22	1:F:102:PHE:HB2	2.02	0.42
1:A:108:VAL:O	1:A:110:GLY:O	2.38	0.42
1:A:185:VAL:HG22	1:A:203:MET:HE2	2.02	0.42
1:B:163:ASN:HD22	1:B:172:GLN:HE22	1.68	0.42
1:B:372:THR:CG2	1:B:410:THR:HG22	2.49	0.42
1:B:456:ARG:C	1:B:458:THR:N	2.78	0.42
1:B:488:ALA:O	1:E:68:ALA:HA	2.19	0.42
1:E:254:LEU:HD12	1:E:254:LEU:HA	1.74	0.42
1:C:372:THR:HB	1:C:410:THR:HB	2.02	0.42
1:C:445:MET:HG3	1:C:450:ALA:HB2	2.01	0.42
1:F:307:ASP:O	1:F:308:ASP:HB2	2.20	0.42
1:F:427:LYS:CD	1:F:431:ALA:O	2.68	0.42
1:A:21:LEU:HD12	1:A:21:LEU:O	2.20	0.42
1:A:193:PHE:HA	1:A:238:HIS:CD2	2.55	0.42
1:B:315:GLN:N	1:B:316:PRO:HD3	2.34	0.42
1:B:324:THR:HA	1:B:336:ILE:O	2.20	0.42
1:B:482:LEU:N	1:B:482:LEU:CD2	2.83	0.42
1:D:287:ILE:O	1:D:289:PRO:HD3	2.19	0.42
1:C:240:MET:O	1:C:240:MET:HG3	2.18	0.42
1:C:397:LEU:HG	1:C:423:VAL:HG12	1.97	0.42
1:F:122:VAL:HG13	1:F:162:ARG:NE	2.35	0.42
1:F:349:ASP:H	1:F:352:ALA:HB3	1.85	0.42
1:F:458:THR:HA	1:F:461:ASP:CB	2.50	0.42
1:A:65:ASP:OD2	1:A:123:LYS:HD3	2.20	0.42
1:A:405:THR:O	1:A:516:LYS:CD	2.68	0.42
1:E:461:ASP:C	1:E:461:ASP:OD1	2.62	0.42
1:C:33:SER:OG	1:C:35:ARG:HG3	2.20	0.41
1:C:464:ASP:CG	1:C:465:ASP:N	2.74	0.41
1:A:340:GLN:O	1:A:340:GLN:HG3	2.19	0.41
1:B:150:VAL:C	1:B:152:SER:H	2.28	0.41
1:B:265:GLU:HB2	1:B:266:PRO:CD	2.50	0.41
1:E:66:GLU:HG2	1:E:67:PHE:CE1	2.55	0.41
1:C:70:HIS:CE1	1:C:81:ARG:HG2	2.55	0.41
1:C:278:THR:O	1:C:281:ASP:HB2	2.20	0.41
1:C:397:LEU:HD11	1:C:401:TYR:CD2	2.55	0.41
1:A:335:GLY:C	1:A:336:ILE:HD12	2.46	0.41
1:D:346:GLY:O	1:D:377:PRO:HD2	2.20	0.41
1:E:146:ILE:H	1:E:146:ILE:HG13	1.50	0.41
1:C:299:HIS:O	1:C:303:GLU:HG3	2.21	0.41
1:C:397:LEU:CD1	1:C:401:TYR:CE2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:LEU:HD12	1:F:433:LEU:HA	1.89	0.41
1:A:87:VAL:HG23	1:A:104:GLN:HA	2.02	0.41
1:A:131:THR:O	1:D:515:THR:OG1	2.34	0.41
1:A:177:VAL:HG12	1:A:197:VAL:CG2	2.51	0.41
1:A:455:HIS:ND1	1:A:455:HIS:N	2.67	0.41
1:A:529:PRO:N	1:B:358:ARG:HH12	2.19	0.41
1:B:241:ALA:HB1	1:B:246:ASP:HB2	2.03	0.41
1:D:380:LEU:O	1:D:385:GLN:HG3	2.21	0.41
1:D:478:GLU:HG3	1:D:482:LEU:HD12	2.02	0.41
1:E:32:GLY:O	1:E:33:SER:C	2.62	0.41
1:F:319:ALA:HB2	1:F:351:THR:HB	2.02	0.41
1:A:74:ASN:O	1:A:75:PHE:CD1	2.74	0.41
1:A:442:ILE:CD1	1:A:487:ALA:HB2	2.50	0.41
1:A:450:ALA:O	1:A:451:VAL:C	2.64	0.41
1:B:215:THR:OG1	1:B:217:GLU:OE1	2.38	0.41
1:B:238:HIS:HA	1:B:315:GLN:CG	2.50	0.41
1:D:193:PHE:CB	1:D:254:LEU:HD21	2.50	0.41
1:C:106:PHE:O	1:C:109:PHE:O	2.39	0.41
1:C:356:ALA:O	1:C:357:ALA:C	2.62	0.41
1:F:300:SER:O	1:F:304:HIS:ND1	2.53	0.41
1:F:438:PRO:O	1:B:17:LYS:HG3	2.20	0.41
1:A:153:LEU:HD21	1:B:418:GLY:HA2	2.02	0.41
1:E:103:SER:HA	1:E:138:ILE:HB	2.03	0.41
1:E:214:VAL:CG2	1:E:215:THR:N	2.84	0.41
1:F:372:THR:HG21	1:F:401:TYR:CE1	2.55	0.41
1:A:77:LEU:HD11	1:A:147:GLN:CG	2.50	0.41
1:A:269:PHE:O	1:A:270:PRO:C	2.63	0.41
1:A:442:ILE:O	1:A:442:ILE:HG13	2.19	0.41
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.51	0.41
1:B:181:ALA:HA	1:B:204:PHE:O	2.21	0.41
1:D:70:HIS:HA	1:D:116:VAL:HG21	2.01	0.41
1:D:180:CYS:SG	1:D:185:VAL:HA	2.60	0.41
1:F:473:LEU:HA	1:F:476:GLU:HB2	2.01	0.41
1:A:70:HIS:HA	1:A:116:VAL:HG21	2.02	0.41
1:A:440:ALA:HB3	1:A:484:PRO:HB3	2.02	0.41
1:B:29:THR:HA	1:B:49:ARG:CZ	2.51	0.41
1:B:69:ARG:O	1:B:70:HIS:C	2.64	0.41
1:B:70:HIS:O	1:B:81:ARG:HD2	2.21	0.41
1:B:241:ALA:HB1	1:B:246:ASP:CB	2.49	0.41
1:B:442:ILE:HG21	1:B:487:ALA:HB2	2.03	0.41
1:C:156:TYR:CE1	1:C:184:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:427:LYS:HD3	1:F:427:LYS:HA	1.66	0.41
1:B:122:VAL:HG13	1:B:162:ARG:NE	2.36	0.41
1:B:354:GLU:OE2	1:B:393:ARG:HD2	2.20	0.41
1:B:451:VAL:C	1:B:453:ILE:N	2.78	0.41
1:E:32:GLY:HA3	1:E:107:THR:OG1	2.20	0.41
1:E:159:ILE:O	1:E:160:PHE:C	2.64	0.41
1:E:197:VAL:O	1:E:198:ASP:C	2.63	0.41
1:C:266:PRO:HB2	1:C:333:PRO:HG2	2.02	0.41
1:A:103:SER:HA	1:A:138:ILE:CG1	2.47	0.41
1:A:125:MET:HE1	1:A:163:ASN:OD1	2.21	0.41
1:A:180:CYS:SG	1:A:185:VAL:HA	2.60	0.41
1:A:190:ILE:HD12	1:A:190:ILE:C	2.46	0.41
1:A:372:THR:HG21	1:A:401:TYR:CZ	2.55	0.41
1:B:35:ARG:HB3	1:B:39:LYS:NZ	2.35	0.41
1:B:88:VAL:CG1	1:B:103:SER:HB3	2.51	0.41
1:B:414:ARG:HD2	1:B:414:ARG:HH11	1.72	0.41
1:B:513:LEU:HD21	1:E:127:PHE:HE1	1.86	0.41
1:D:20:ASP:O	1:D:24:ARG:HG2	2.21	0.41
1:E:414:ARG:HA	1:E:440:ALA:HA	2.02	0.41
1:F:70:HIS:ND1	1:F:71:ARG:N	2.69	0.41
1:A:205:ILE:CD1	1:B:390:ILE:HG21	2.51	0.41
1:D:163:ASN:HA	1:D:172:GLN:HE22	1.85	0.41
1:E:10:ASP:O	1:E:11:ILE:HB	2.21	0.41
1:E:209:ASP:O	1:E:213:THR:HG23	2.20	0.41
1:E:296:TYR:O	1:E:342:MET:HG2	2.21	0.41
1:C:275:LEU:O	1:C:504:ARG:HD2	2.20	0.40
1:C:393:ARG:HD3	1:C:393:ARG:HA	1.82	0.40
1:F:77:LEU:CD1	1:F:147:GLN:HG3	2.50	0.40
1:A:170:ILE:HG13	1:A:170:ILE:O	2.20	0.40
1:A:390:ILE:O	1:A:390:ILE:HG13	2.21	0.40
1:B:182:GLY:O	1:B:183:GLY:C	2.64	0.40
1:D:481:LEU:C	1:D:483:ASN:H	2.29	0.40
1:F:10:ASP:OD1	1:F:11:ILE:N	2.43	0.40
1:F:74:ASN:HB3	1:F:75:PHE:CD1	2.57	0.40
1:A:70:HIS:CD2	1:A:72:SER:HB3	2.57	0.40
1:A:280:GLU:H	1:A:280:GLU:HG3	1.50	0.40
1:A:457:ARG:HG3	1:A:457:ARG:O	2.20	0.40
1:B:35:ARG:NH1	1:B:38:GLU:OE1	2.54	0.40
1:D:49:ARG:NH2	1:D:63:GLU:OE1	2.51	0.40
1:D:197:VAL:CG1	1:D:247:ALA:HB2	2.50	0.40
1:D:278:THR:OG1	1:D:280:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:VAL:CG1	1:E:120:LYS:HD3	2.51	0.40
1:E:208:PRO:CA	1:E:211:ILE:HG12	2.35	0.40
1:E:338:ALA:HA	1:E:373:PHE:O	2.21	0.40
1:E:516:LYS:O	1:E:516:LYS:HG3	2.20	0.40
1:F:370:VAL:HG12	1:F:372:THR:HG22	2.03	0.40
1:F:375:ASP:OD2	1:F:414:ARG:HB3	2.20	0.40
1:F:451:VAL:C	1:F:453:ILE:H	2.27	0.40
1:A:65:ASP:HB3	1:A:68:ALA:HB2	2.03	0.40
1:A:91:TYR:CE1	1:D:512:GLN:HG3	2.55	0.40
1:A:108:VAL:HG12	1:A:109:PHE:HD2	1.87	0.40
1:A:446:GLY:C	1:A:448:GLN:N	2.79	0.40
1:B:458:THR:O	1:B:458:THR:HG22	2.21	0.40
1:D:113:LEU:HD13	1:D:156:TYR:CE1	2.55	0.40
1:F:68:ALA:HA	1:E:489:GLU:HA	2.02	0.40
1:F:197:VAL:O	1:F:198:ASP:C	2.63	0.40
1:A:397:LEU:HD22	1:A:401:TYR:CE2	2.56	0.40
1:A:415:LYS:HZ1	1:A:441:GLN:C	2.23	0.40
1:B:75:PHE:CD1	1:B:76:GLY:N	2.89	0.40
1:B:350:ILE:HD13	1:B:390:ILE:CD1	2.50	0.40
1:B:438:PRO:HG3	1:E:21:LEU:HD22	2.02	0.40
1:D:174:SER:OG	1:D:191:THR:HG21	2.21	0.40
1:D:319:ALA:C	1:D:321:ASN:H	2.29	0.40
1:E:65:ASP:OD2	1:E:123:LYS:HD2	2.21	0.40
1:C:111:GLY:O	1:C:141:SER:HB2	2.20	0.40
1:F:193:PHE:HA	1:F:238:HIS:CE1	2.56	0.40
1:A:282:ALA:HA	1:A:500:SER:OG	2.21	0.40
1:A:457:ARG:CZ	1:A:461:ASP:HB2	2.51	0.40
1:B:140:ASP:O	1:B:179:PRO:CD	2.69	0.40
1:B:146:ILE:O	1:B:147:GLN:C	2.65	0.40
1:B:220:GLY:O	1:B:221:PHE:C	2.65	0.40
1:D:108:VAL:HG12	1:D:109:PHE:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/530 (98%)	470 (91%)	38 (7%)	11 (2%)	5	6
1	B	519/530 (98%)	455 (88%)	52 (10%)	12 (2%)	5	5
1	C	519/530 (98%)	475 (92%)	37 (7%)	7 (1%)	9	12
1	D	519/530 (98%)	472 (91%)	41 (8%)	6 (1%)	10	14
1	E	519/530 (98%)	476 (92%)	39 (8%)	4 (1%)	16	23
1	F	519/530 (98%)	479 (92%)	33 (6%)	7 (1%)	9	12
All	All	3114/3180 (98%)	2827 (91%)	240 (8%)	47 (2%)	8	10

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	520	LEU
1	F	480	ALA
1	B	75	PHE
1	B	306	LEU
1	D	198	ASP
1	E	11	ILE
1	E	520	LEU
1	C	110	GLY
1	C	455	HIS
1	C	464	ASP
1	C	468	ALA
1	C	475	GLN
1	F	198	ASP
1	A	31	ALA
1	A	451	VAL
1	B	141	SER
1	B	183	GLY
1	D	11	ILE
1	D	50	GLU
1	D	287	ILE
1	D	289	PRO
1	D	414	ARG
1	F	106	PHE
1	A	78	ASP
1	A	112	ALA
1	A	466	ALA
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	78	ASP
1	B	414	ARG
1	E	414	ARG
1	F	289	PRO
1	A	11	ILE
1	A	77	LEU
1	A	406	VAL
1	A	447	ALA
1	A	465	ASP
1	B	70	HIS
1	B	109	PHE
1	E	109	PHE
1	F	145	ARG
1	F	465	ASP
1	A	467	GLU
1	B	345	ALA
1	B	520	LEU
1	C	414	ARG
1	F	463	GLY
1	B	528	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/421 (98%)	356 (86%)	56 (14%)	3	4
1	B	412/421 (98%)	367 (89%)	45 (11%)	6	8
1	C	412/421 (98%)	378 (92%)	34 (8%)	10	15
1	D	412/421 (98%)	374 (91%)	38 (9%)	8	12
1	E	412/421 (98%)	363 (88%)	49 (12%)	5	6
1	F	412/421 (98%)	374 (91%)	38 (9%)	8	12
All	All	2472/2526 (98%)	2212 (90%)	260 (10%)	6	9

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	17	LYS
1	C	21	LEU
1	C	56	LEU
1	C	70	HIS
1	C	75	PHE
1	C	88	VAL
1	C	124	VAL
1	C	146	ILE
1	C	162	ARG
1	C	173	ILE
1	C	177	VAL
1	C	205	ILE
1	C	222	GLU
1	C	223	GLU
1	C	229	THR
1	C	236	VAL
1	C	240	MET
1	C	264	SER
1	C	310	GLU
1	C	350	ILE
1	C	368	VAL
1	C	374	VAL
1	C	397	LEU
1	C	429	LEU
1	C	448	GLN
1	C	451	VAL
1	C	455	HIS
1	C	457	ARG
1	C	459	ILE
1	C	472	ARG
1	C	482	LEU
1	C	489	GLU
1	C	493	VAL
1	C	506	ILE
1	F	11	ILE
1	F	40	GLN
1	F	77	LEU
1	F	107	THR
1	F	113	LEU
1	F	117	TYR
1	F	147	GLN
1	F	177	VAL
1	F	199	GLN

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Mol	Chain	Res	Type
1	F	209	ASP
1	F	215	THR
1	F	217	GLU
1	F	219	VAL
1	F	251	VAL
1	F	264	SER
1	F	277	VAL
1	F	284	LEU
1	F	294	GLN
1	F	301	VAL
1	F	321	ASN
1	F	332	ARG
1	F	372	THR
1	F	374	VAL
1	F	383	VAL
1	F	386	GLU
1	F	433	LEU
1	F	453	ILE
1	F	457	ARG
1	F	458	THR
1	F	461	ASP
1	F	467	GLU
1	F	475	GLN
1	F	505	HIS
1	F	512	GLN
1	F	513	LEU
1	F	516	LYS
1	F	520	LEU
1	F	530	LEU
1	A	21	LEU
1	A	40	GLN
1	A	54	LEU
1	A	63	GLU
1	A	69	ARG
1	A	71	ARG
1	A	81	ARG
1	A	99	VAL
1	A	103	SER
1	A	117	TYR
1	A	122	VAL
1	A	124	VAL
1	A	138	ILE

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Mol	Chain	Res	Type
1	A	147	GLN
1	A	150	VAL
1	A	185	VAL
1	A	195	VAL
1	A	200	THR
1	A	210	VAL
1	A	215	THR
1	A	233	THR
1	A	255	LEU
1	A	256	SER
1	A	264	SER
1	A	280	GLU
1	A	288	VAL
1	A	301	VAL
1	A	310	GLU
1	A	317	LEU
1	A	326	PHE
1	A	332	ARG
1	A	350	ILE
1	A	380	LEU
1	A	386	GLU
1	A	391	ILE
1	A	406	VAL
1	A	415	LYS
1	A	427	LYS
1	A	433	LEU
1	A	444	VAL
1	A	453	ILE
1	A	455	HIS
1	A	458	THR
1	A	461	ASP
1	A	472	ARG
1	A	473	LEU
1	A	474	ILE
1	A	475	GLN
1	A	481	LEU
1	A	486	THR
1	A	493	VAL
1	A	496	VAL
1	A	512	GLN
1	A	516	LYS
1	A	517	ARG

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Mol	Chain	Res	Type
1	A	519	SER
1	B	13	THR
1	B	17	LYS
1	B	35	ARG
1	B	39	LYS
1	B	46	LEU
1	B	47	THR
1	B	64	LEU
1	B	70	HIS
1	B	80	ASN
1	B	88	VAL
1	B	108	VAL
1	B	116	VAL
1	B	117	TYR
1	B	173	ILE
1	B	177	VAL
1	B	200	THR
1	B	205	ILE
1	B	210	VAL
1	B	217	GLU
1	B	229	THR
1	B	244	GLU
1	B	245	LYS
1	B	260	SER
1	B	275	LEU
1	B	290	ASP
1	B	303	GLU
1	B	310	GLU
1	B	334	VAL
1	B	368	VAL
1	B	372	THR
1	B	374	VAL
1	B	414	ARG
1	B	433	LEU
1	B	439	THR
1	B	448	GLN
1	B	455	HIS
1	B	456	ARG
1	B	457	ARG
1	B	469	THR
1	B	481	LEU
1	B	482	LEU

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Mol	Chain	Res	Type
1	B	490	ARG
1	B	493	VAL
1	B	496	VAL
1	B	522	PRO
1	D	35	ARG
1	D	40	GLN
1	D	49	ARG
1	D	107	THR
1	D	115	GLU
1	D	117	TYR
1	D	147	GLN
1	D	218	ASP
1	D	219	VAL
1	D	229	THR
1	D	236	VAL
1	D	253	GLN
1	D	265	GLU
1	D	280	GLU
1	D	286	THR
1	D	288	VAL
1	D	301	VAL
1	D	310	GLU
1	D	337	VAL
1	D	342	MET
1	D	368	VAL
1	D	372	THR
1	D	391	ILE
1	D	392	ARG
1	D	427	LYS
1	D	429	LEU
1	D	433	LEU
1	D	439	THR
1	D	470	ARG
1	D	473	LEU
1	D	493	VAL
1	D	494	ASP
1	D	496	VAL
1	D	502	THR
1	D	505	HIS
1	D	513	LEU
1	D	514	ARG
1	D	517	ARG

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Mol	Chain	Res	Type
1	E	37	VAL
1	E	40	GLN
1	E	43	LYS
1	E	47	THR
1	E	51	ARG
1	E	58	GLU
1	E	64	LEU
1	E	69	ARG
1	E	70	HIS
1	E	71	ARG
1	E	78	ASP
1	E	116	VAL
1	E	117	TYR
1	E	124	VAL
1	E	145	ARG
1	E	146	ILE
1	E	148	GLU
1	E	152	SER
1	E	153	LEU
1	E	174	SER
1	E	177	VAL
1	E	209	ASP
1	E	211	ILE
1	E	213	THR
1	E	215	THR
1	E	219	VAL
1	E	231	ASN
1	E	245	LYS
1	E	264	SER
1	E	265	GLU
1	E	290	ASP
1	E	306	LEU
1	E	317	LEU
1	E	393	ARG
1	E	429	LEU
1	E	451	VAL
1	E	452	ASN
1	E	454	LEU
1	E	455	HIS
1	E	461	ASP
1	E	473	LEU
1	E	475	GLN

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Mol	Chain	Res	Type
1	E	481	LEU
1	E	493	VAL
1	E	496	VAL
1	E	506	ILE
1	E	516	LYS
1	E	519	SER
1	E	520	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	80	ASN
1	C	230	HIS
1	C	239	HIS
1	C	293	ASN
1	C	299	HIS
1	C	339	ASN
1	C	422	ASN
1	C	448	GLN
1	C	455	HIS
1	C	475	GLN
1	F	30	HIS
1	F	163	ASN
1	F	172	GLN
1	F	199	GLN
1	F	253	GLN
1	F	262	ASN
1	F	299	HIS
1	F	339	ASN
1	F	367	ASN
1	F	505	HIS
1	F	512	GLN
1	A	30	HIS
1	A	104	GLN
1	A	172	GLN
1	A	238	HIS
1	A	315	GLN
1	A	385	GLN
1	A	475	GLN
1	A	512	GLN
1	B	12	HIS
1	B	30	HIS

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Mol	Chain	Res	Type
1	B	74	ASN
1	B	80	ASN
1	B	139	ASN
1	B	147	GLN
1	B	163	ASN
1	B	172	GLN
1	B	230	HIS
1	B	299	HIS
1	B	339	ASN
1	B	340	GLN
1	B	367	ASN
1	B	422	ASN
1	B	434	ASN
1	B	441	GLN
1	B	448	GLN
1	B	455	HIS
1	B	475	GLN
1	B	512	GLN
1	B	527	ASN
1	D	104	GLN
1	D	172	GLN
1	D	238	HIS
1	D	239	HIS
1	D	253	GLN
1	D	262	ASN
1	D	299	HIS
1	D	343	GLN
1	D	387	HIS
1	D	422	ASN
1	D	527	ASN
1	E	163	ASN
1	E	172	GLN
1	E	230	HIS
1	E	231	ASN
1	E	239	HIS
1	E	262	ASN
1	E	294	GLN
1	E	299	HIS
1	E	343	GLN
1	E	455	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	521/530 (98%)	0.83	58 (11%) 10 9	39, 81, 153, 270	0
1	B	521/530 (98%)	0.86	60 (11%) 9 8	35, 81, 154, 242	0
1	C	521/530 (98%)	0.53	39 (7%) 20 19	25, 64, 134, 204	0
1	D	521/530 (98%)	0.54	41 (7%) 18 17	23, 63, 140, 258	0
1	E	521/530 (98%)	0.61	39 (7%) 20 19	26, 65, 137, 192	0
1	F	521/530 (98%)	0.54	36 (6%) 23 21	25, 64, 138, 266	0
All	All	3126/3180 (98%)	0.65	273 (8%) 16 15	23, 70, 143, 270	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	466	ALA	7.2
1	F	470	ARG	6.3
1	A	44	GLY	6.0
1	B	77	LEU	5.2
1	F	383	VAL	5.1
1	F	459	ILE	5.0
1	B	468	ALA	4.9
1	B	140	ASP	4.9
1	D	466	ALA	4.8
1	C	462	ALA	4.6
1	A	77	LEU	4.5
1	C	44	GLY	4.5
1	B	466	ALA	4.5
1	F	460	ALA	4.4
1	F	466	ALA	4.4
1	F	468	ALA	4.3
1	A	288	VAL	4.2
1	B	470	ARG	4.1
1	D	469	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	454	LEU	4.1
1	C	466	ALA	4.0
1	C	383	VAL	4.0
1	F	475	GLN	4.0
1	D	465	ASP	4.0
1	E	383	VAL	3.9
1	D	286	THR	3.9
1	C	106	PHE	3.8
1	A	468	ALA	3.8
1	B	471	ALA	3.8
1	A	520	LEU	3.8
1	B	462	ALA	3.7
1	F	441	GLN	3.7
1	D	455	HIS	3.7
1	A	417	PHE	3.6
1	A	447	ALA	3.6
1	B	460	ALA	3.6
1	D	383	VAL	3.6
1	A	142	GLY	3.5
1	B	142	GLY	3.5
1	A	462	ALA	3.5
1	D	382	GLY	3.5
1	E	465	ASP	3.5
1	B	210	VAL	3.5
1	E	468	ALA	3.5
1	A	130	LYS	3.5
1	F	477	TYR	3.5
1	B	75	PHE	3.4
1	A	498	MET	3.4
1	D	462	ALA	3.4
1	B	465	ASP	3.4
1	A	225	GLY	3.3
1	C	108	VAL	3.3
1	E	460	ALA	3.3
1	B	463	GLY	3.3
1	E	463	GLY	3.3
1	C	71	ARG	3.3
1	B	477	TYR	3.3
1	E	462	ALA	3.2
1	D	459	ILE	3.2
1	B	469	THR	3.2
1	C	520	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	229	THR	3.2
1	D	468	ALA	3.1
1	E	84	GLY	3.1
1	A	391	ILE	3.1
1	F	458	THR	3.1
1	D	109	PHE	3.1
1	E	140	ASP	3.1
1	E	452	ASN	3.1
1	D	464	ASP	3.1
1	E	346	GLY	3.1
1	C	72	SER	3.0
1	C	77	LEU	3.0
1	A	430	GLY	3.0
1	B	80	ASN	3.0
1	C	459	ILE	3.0
1	E	79	ALA	3.0
1	F	483	ASN	3.0
1	A	466	ALA	2.9
1	B	520	LEU	2.9
1	A	317	LEU	2.9
1	A	40	GLN	2.9
1	C	388	ASP	2.9
1	F	109	PHE	2.9
1	B	40	GLN	2.9
1	B	47	THR	2.9
1	D	458	THR	2.9
1	D	497	ILE	2.9
1	B	461	ASP	2.9
1	F	45	LYS	2.8
1	B	448	GLN	2.8
1	A	464	ASP	2.8
1	B	207	GLY	2.8
1	A	68	ALA	2.8
1	B	456	ARG	2.8
1	C	384	ASP	2.8
1	F	452	ASN	2.8
1	D	72	SER	2.8
1	C	31	ALA	2.8
1	C	76	GLY	2.8
1	E	67	PHE	2.8
1	C	455	HIS	2.7
1	F	469	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	449	GLY	2.7
1	A	23	ARG	2.7
1	C	269	PHE	2.7
1	C	464	ASP	2.7
1	C	46	LEU	2.7
1	F	453	ILE	2.7
1	A	463	GLY	2.7
1	D	417	PHE	2.7
1	C	10	ASP	2.7
1	F	464	ASP	2.7
1	D	391	ILE	2.7
1	A	71	ARG	2.7
1	C	109	PHE	2.6
1	F	108	VAL	2.6
1	E	177	VAL	2.6
1	E	384	ASP	2.6
1	B	13	THR	2.6
1	E	35	ARG	2.6
1	B	320	PRO	2.6
1	A	461	ASP	2.6
1	B	453	ILE	2.6
1	D	519	SER	2.6
1	A	70	HIS	2.6
1	B	518	GLU	2.6
1	B	213	THR	2.6
1	A	383	VAL	2.5
1	A	455	HIS	2.5
1	B	23	ARG	2.5
1	A	48	ALA	2.5
1	E	86	GLY	2.5
1	C	176	VAL	2.5
1	A	451	VAL	2.5
1	C	483	ASN	2.5
1	A	465	ASP	2.5
1	B	365	ALA	2.5
1	E	28	ALA	2.5
1	A	30	HIS	2.5
1	B	186	TYR	2.5
1	A	10	ASP	2.5
1	F	471	ALA	2.5
1	D	460	ALA	2.5
1	C	521	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	220	GLY	2.5
1	C	469	THR	2.4
1	F	518	GLU	2.4
1	F	451	VAL	2.4
1	D	454	LEU	2.4
1	B	212	LYS	2.4
1	F	450	ALA	2.4
1	C	463	GLY	2.4
1	A	457	ARG	2.4
1	E	242	GLY	2.4
1	C	70	HIS	2.4
1	A	483	ASN	2.4
1	B	293	ASN	2.4
1	B	452	ASN	2.4
1	D	456	ARG	2.4
1	D	518	GLU	2.4
1	B	276	ALA	2.4
1	E	34	ALA	2.4
1	E	469	THR	2.4
1	F	519	SER	2.4
1	F	347	CYS	2.4
1	A	459	ILE	2.4
1	E	210	VAL	2.4
1	D	281	ASP	2.4
1	A	200	THR	2.4
1	D	46	LEU	2.4
1	D	520	LEU	2.4
1	A	517	ARG	2.4
1	B	478	GLU	2.4
1	E	10	ASP	2.3
1	F	382	GLY	2.3
1	B	76	GLY	2.3
1	A	284	LEU	2.3
1	C	50	GLU	2.3
1	D	217	GLU	2.3
1	E	461	ASP	2.3
1	A	477	TYR	2.3
1	C	152	SER	2.3
1	A	11	ILE	2.3
1	B	148	GLU	2.3
1	E	520	LEU	2.3
1	A	218	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	295	PRO	2.3
1	A	76	GLY	2.3
1	E	44	GLY	2.3
1	A	436	ALA	2.3
1	B	459	ILE	2.3
1	E	211	ILE	2.3
1	E	85	ASP	2.3
1	C	216	GLY	2.3
1	B	206	THR	2.3
1	B	233	THR	2.3
1	F	476	GLU	2.3
1	E	40	GLN	2.3
1	B	383	VAL	2.3
1	D	473	LEU	2.2
1	B	464	ASP	2.2
1	D	377	PRO	2.2
1	C	393	ARG	2.2
1	A	456	ARG	2.2
1	A	470	ARG	2.2
1	B	71	ARG	2.2
1	E	216	GLY	2.2
1	E	225	GLY	2.2
1	A	215	THR	2.2
1	B	27	GLU	2.2
1	C	45	LYS	2.2
1	D	287	ILE	2.2
1	B	444	VAL	2.2
1	E	454	LEU	2.2
1	E	221	PHE	2.2
1	D	44	GLY	2.2
1	B	33	SER	2.2
1	B	109	PHE	2.2
1	E	456	ARG	2.2
1	E	483	ASN	2.2
1	C	389	GLY	2.2
1	B	110	GLY	2.2
1	B	382	GLY	2.2
1	D	226	GLY	2.2
1	B	304	HIS	2.2
1	C	215	THR	2.2
1	F	439	THR	2.2
1	B	474	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	37	VAL	2.2
1	D	218	ASP	2.2
1	D	461	ASP	2.2
1	A	45	LYS	2.2
1	D	84	GLY	2.2
1	F	462	ALA	2.2
1	C	222	GLU	2.1
1	A	217	GLU	2.1
1	B	202	HIS	2.1
1	F	227	ALA	2.1
1	F	198	ASP	2.1
1	D	483	ASN	2.1
1	D	277	VAL	2.1
1	C	221	PHE	2.1
1	A	109	PHE	2.1
1	B	418	GLY	2.1
1	A	458	THR	2.1
1	A	460	ALA	2.1
1	A	485	TYR	2.1
1	E	116	VAL	2.1
1	F	517	ARG	2.1
1	D	472	ARG	2.1
1	C	39	LYS	2.1
1	B	442	ILE	2.1
1	A	150	VAL	2.1
1	B	220	GLY	2.1
1	E	183	GLY	2.1
1	F	502	THR	2.0
1	A	276	ALA	2.0
1	C	12	HIS	2.0
1	F	473	LEU	2.0
1	A	530	LEU	2.0
1	B	10	ASP	2.0
1	D	10	ASP	2.0
1	B	205	ILE	2.0
1	D	474	ILE	2.0
1	C	472	ARG	2.0
1	D	374	VAL	2.0
1	A	75	PHE	2.0
1	B	269	PHE	2.0
1	E	106	PHE	2.0
1	F	520	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	211	ILE	2.0
1	D	490	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.