



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MFM
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

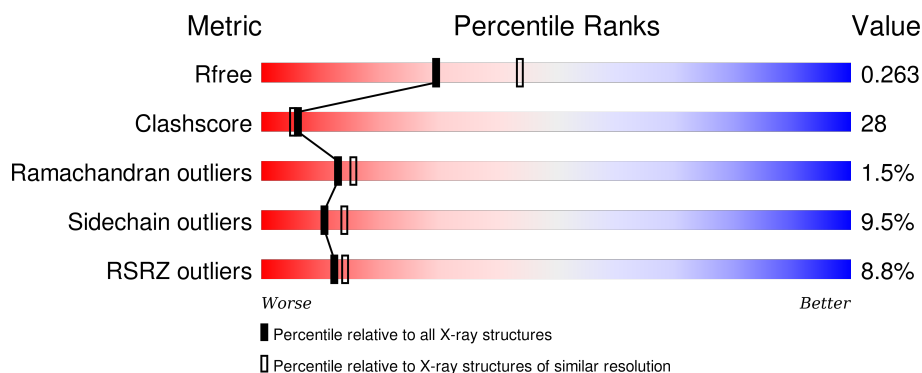
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (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 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	530	<div> <div>11%</div> <div>51% 40% 8%</div> </div>
1	B	530	<div> <div>11%</div> <div>50% 41% 7%</div> </div>
1	C	530	<div> <div>7%</div> <div>61% 32% 5%</div> </div>
1	D	530	<div> <div>8%</div> <div>55% 38% 5%</div> </div>
1	E	530	<div> <div>6%</div> <div>59% 33% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	530	<div> <div>9%</div> <div>58%</div> <div>35%</div> <div>5%</div> </div>

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			

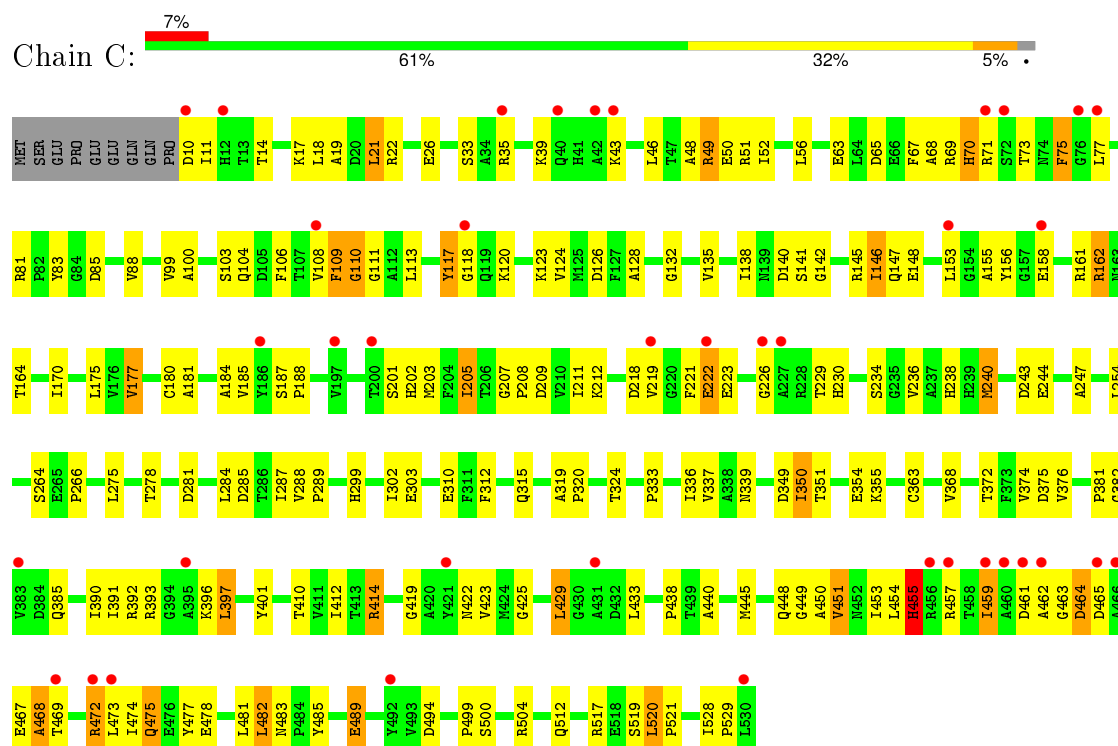
There are 6 discrepancies between the modelled and reference sequences:

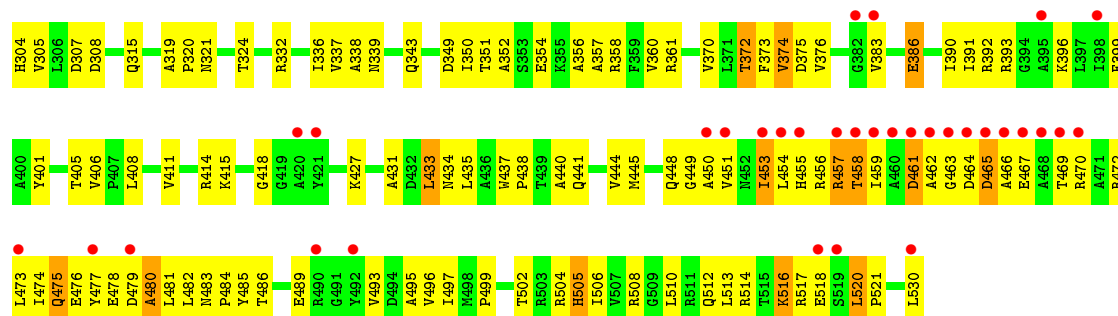
Chain	Residue	Modelled	Actual	Comment	Reference
C	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
F	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
A	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
B	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
D	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
E	422	ASN	ASP	ENGINEERED MUTATION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

3 Residue-property plots [i](#)

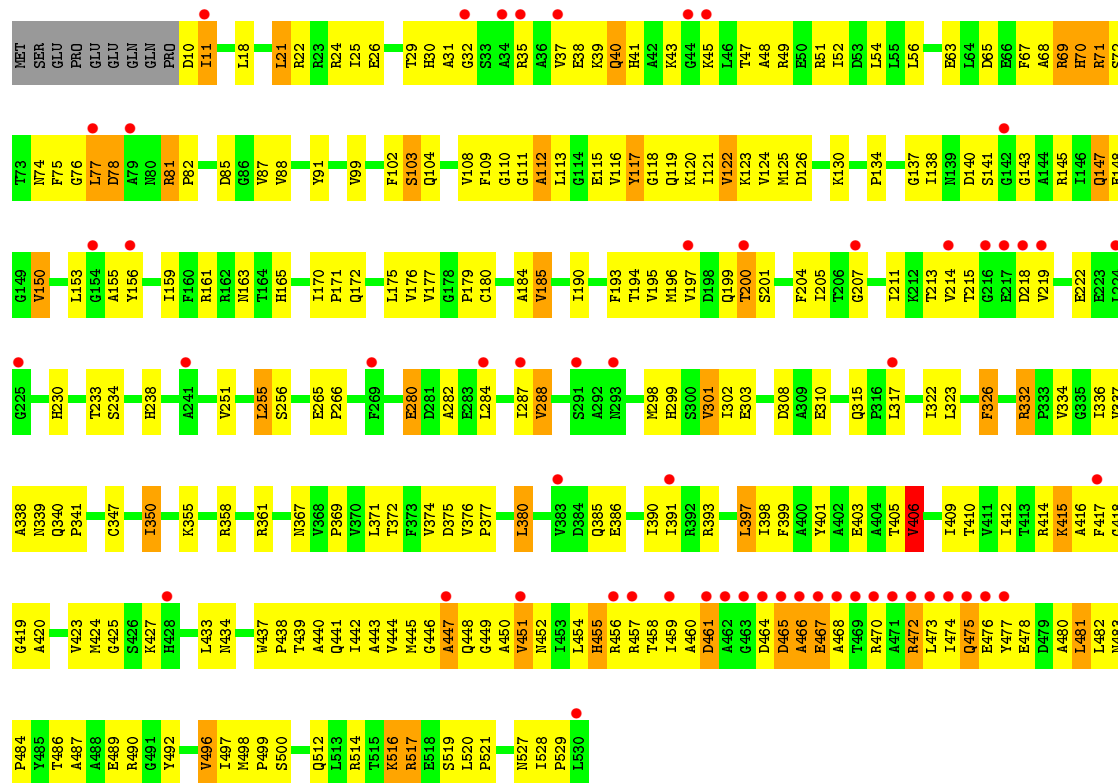
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Propionyl-CoA carboxylase complex B subunit

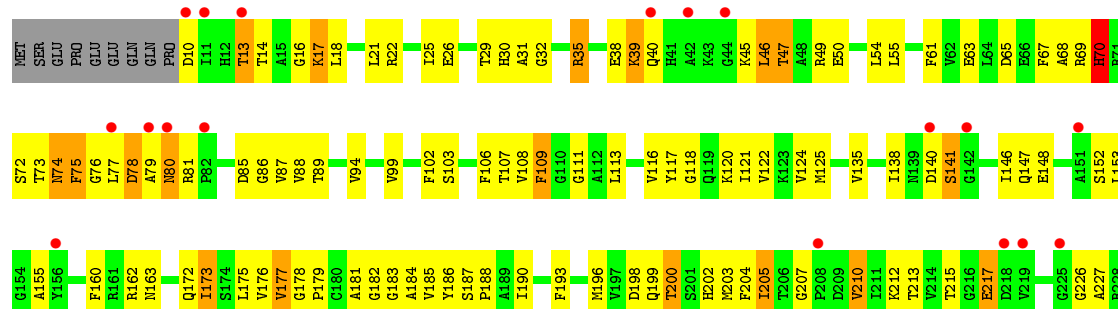


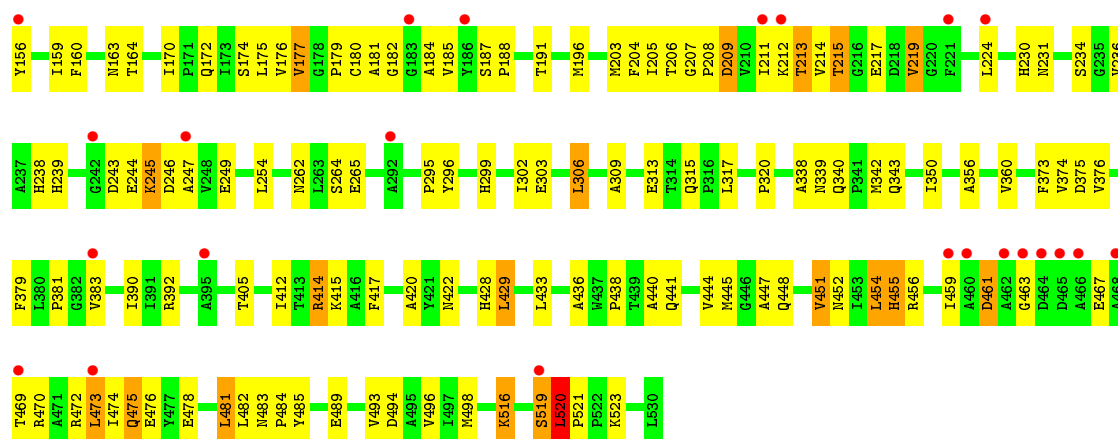


• Molecule 1: Propionyl-CoA carboxylase complex B subunit



• 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 45.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.82-2.38) 99.1 (45.00-2.38)	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 (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.224 , 0.268 0.213 , 0.263	Depositor DCC
R_{free} test set	9088 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	1.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 182382 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/4033	0.61	0/5478
1	B	0.44	0/4033	0.62	0/5478
1	C	0.41	0/4033	0.61	1/5478 (0.0%)
1	D	0.44	0/4033	0.62	1/5478 (0.0%)
1	E	0.41	0/4033	0.60	0/5478
1	F	0.41	0/4033	0.60	0/5478
All	All	0.42	0/24198	0.61	2/32868 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	GLY	N-CA-C	-5.39	99.61	113.10
1	C	109	PHE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3953	0	3882	310	0
1	B	3953	0	3882	299	0
1	C	3953	0	3882	192	0
1	D	3953	0	3882	218	0
1	E	3953	0	3882	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3953	0	3882	213	0
All	All	23718	0	23292	1319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HG21	1:B:401:TYR:OH	1.46	1.15
1:E:69:ARG:HH11	1:E:69:ARG:HG3	1.01	1.13
1:B:35:ARG:HH11	1:B:35:ARG:HG2	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:D:286:THR:O	1:D:288:VAL:HG12	1.55	1.04
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:HH11	1:A:69:ARG:HG2	1.27	1.00
1:A:350:ILE:HD11	1:A:393:ARG:HH11	1.24	0.99
1:B:35:ARG:HG2	1:B:35:ARG:NH1	1.69	0.98
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: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:NH1	1:E:69:ARG:HG3	1.80	0.92
1:D:32:GLY:HA3	1:D:107:THR:HG23	1.52	0.92
1:A:456:ARG:HD3	1:A:459:ILE:HG12	1.52	0.92
1:E:113:LEU:HD23	1:E:156:TYR:CE1	2.05	0.91
1:E:295:PRO:HB2	1:E:342:MET:CE	2.01	0.91
1:D:32:GLY:HA3	1:D:107:THR:CG2	2.01	0.90
1:B:35:ARG:CG	1:B:35:ARG:HH11	1.83	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:A:391:ILE:HD12	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:B:305:VAL:O	1:B:306:LEU:HG	1.76	0.85
1:D:472:ARG:HE	1:D:475:GLN:HB3	1.39	0.85
1:F:451:VAL:HA	1:F:454:LEU:HG	1.58	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:163:ASN:CB	1:A:190:ILE:HD11	2.08	0.83
1:A:138:ILE:HG22	1:A:175:LEU:HB3	1.59	0.83
1:A:380:LEU:HD11	1:A:385:GLN:CG	2.08	0.82
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:A:81:ARG:CG	1:A:81:ARG:HH11	1.86	0.82
1:E:520:LEU:HD22	1:E:521:PRO:HD2	1.60	0.82
1:C:187:SER:HB3	1:C:188:PRO:HD3	1.60	0.82
1:A:498:MET:HE2	1:A:500:SER:HB3	1.62	0.82
1:F:458:THR:HG21	1:F:469:THR:HG21	1.62	0.82
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:B:415:LYS:HD2	1:B:417:PHE:CE1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:ILE:HD12	1:D:175:LEU:HD23	1.63	0.80
1:D:49:ARG:O	1:D:50:GLU:HB2	1.79	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: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:386:GLU:OE2	1:D:391:ILE:HD11	1.83	0.78
1:E:69:ARG:HH11	1:E:69:ARG:CG	1.91	0.78
1:E:339:ASN:OD1	1:E:376:VAL:HG23	1.84	0.78
1:E:51:ARG:HG2	1:E:51:ARG:NH1	1.96	0.78
1:E:243:ASP:HB3	1:E:246:ASP:OD1	1.84	0.78
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:A:323:LEU:HD21	1:A:340:GLN:HB2	1.63	0.78
1:B:437:TRP:HE1	1:B:502:THR:HG21	1.49	0.78
1:F:18:LEU:HG	1:E:498:MET:CE	2.14	0.77
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PHE:C	1:C:111:GLY:H	1.88	0.76
1:A:211:ILE:HG21	1:B:383:VAL:HG23	1.67	0.75
1:A:498:MET:CE	1:A:500:SER:HB3	2.15	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:N	1:E:39:LYS:HD2	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:B:202:HIS:ND1	1:B:226:GLY:HA2	2.02	0.74
1:C:350:ILE:HB	1:C:393:ARG:HG2	1.67	0.74
1:A:69:ARG:NH1	1:A:69:ARG:HG2	1.94	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:D:286:THR:C	1:D:288:VAL:H	1.92	0.73
1:F:94:VAL:HG23	1:F:99:VAL:HG11	1.71	0.73
1:E:113:LEU:HD12	1:E:114:GLY:N	2.03	0.73
1:C:75:PHE:CE1	1:F:454:LEU:HD13	2.24	0.73
1:E:207:GLY:O	1:E:211:ILE:HG23	1.88	0.73
1:F:18:LEU:HG	1:E:498:MET:HE1	1.68	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: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:A:145:ARG:HD2	1:A:148:GLU:OE2	1.89	0.72
1:C:109:PHE:O	1:C:111:GLY:N	2.21	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: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:C:73:THR:HG21	1:B:73:THR:HG21	1.70	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:B:389:GLY:O	1:B:393:ARG:HG2	1.91	0.71
1:E:520:LEU:HD22	1:E:521:PRO:CD	2.20	0.71
1:A:40:GLN:NE2	1:A:41:HIS:H	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:HIS:HE2	1:A:148:GLU:CD	1.94	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:E:33:SER:O	1:E:37:VAL:HG13	1.91	0.70
1:C:208:PRO:CG	1:C:221:PHE:HE2	2.03	0.70
1:E:47:THR:HG22	1:E:50:GLU:CG	2.22	0.70
1:D:381:PRO:HB2	1:E:214:VAL:HG21	1.73	0.70
1:C:397:LEU:HG	1:C:423:VAL:CG1	2.21	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:B:348:LEU:HD21	1:B:424:MET:HE1	1.73	0.70
1:D:484:PRO:HD2	1:D:485:TYR:CD2	2.26	0.70
1:B:440:ALA:HB3	1:B:484:PRO:HB3	1.73	0.70
1:A:122:VAL:HG23	1:A:159:ILE:HG13	1.73	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:C:208:PRO:CD	1:C:221:PHE:HE2	2.03	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: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:E:295:PRO:HB2	1:E:342:MET:HE2	1.71	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:A:18:LEU:HD13	1:D:498:MET:CE	2.23	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:B:196:MET:CE	1:B:230:HIS:HB2	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:C:354:GLU:CD	1:C:393:ARG:HD2	2.13	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:E:295:PRO:HB2	1:E:342:MET:HE1	1.74	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:91:TYR:CD1	1:D:512:GLN:HG3	2.30	0.67
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:B:451:VAL:HG13	1:B:455:HIS:CD2	2.29	0.66
1:F:65:ASP:HB2	1:F:120:LYS:HE3	1.77	0.66
1:F:290:ASP:CG	1:B:13:THR:HG22	2.16	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:F:147:GLN:H	1:F:147:GLN:CD	1.98	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:B:74:ASN:HB2	1:B:77:LEU:CD1	2.27	0.65
1:A:103:SER:HA	1:A:138:ILE:HG13	1.77	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:E:47:THR:O	1:E:51:ARG:HG3	1.97	0.65
1:F:470:ARG:HH12	1:F:474:ILE:N	1.95	0.65
1:B:519:SER:O	1:B:520:LEU:HB2	1.97	0.65
1:C:339:ASN:HD22	1:C:374:VAL:HA	1.60	0.65
1:A:230:HIS:HA	1:A:234:SER:OG	1.96	0.65
1:E:209:ASP:O	1:E:212:LYS:HG2	1.97	0.65
1:B:446:GLY:HA3	1:B:448:GLN:HE21	1.61	0.65
1:B:22:ARG:O	1:B:26:GLU:HG2	1.96	0.65
1:E:467:GLU:C	1:E:469:THR:H	2.01	0.65
1:F:437:TRP:HE1	1:F:502:THR:CG2	2.09	0.65
1:C:21:LEU:O	1:C:21:LEU:HD12	1.97	0.65
1:F:520:LEU:HD12	1:F:521:PRO:HD2	1.79	0.65
1:C:75:PHE:N	1:C:75:PHE:HD2	1.95	0.65
1:D:324:THR:HA	1:D:336:ILE:O	1.97	0.64
1:D:280:GLU:O	1:D:283:GLU:HG2	1.96	0.64
1:F:479:ASP:O	1:F:480:ALA:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:51:ARG:CG	1:E:51:ARG:HH11	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:A:265:GLU:HB2	1:A:266:PRO:HD2	1.80	0.63
1:C:467:GLU:HA	1:C:467:GLU:OE1	1.98	0.63
1:A:69:ARG:HB2	1:D:489:GLU:HB2	1.81	0.63
1:D:288:VAL:HG21	1:D:439:THR:HG21	1.79	0.63
1:B:376:VAL:HG21	1:B:420:ALA:HB1	1.80	0.63
1:F:453:ILE:HG13	1:F:454:LEU:N	2.13	0.63
1:A:339:ASN:O	1:A:341:PRO:HD3	1.97	0.63
1:E:238:HIS:HA	1:E:315:GLN:HG2	1.79	0.63
1:A:399:PHE:O	1:A:403:GLU:HG2	1.98	0.63
1:F:386:GLU:HA	1:F:390:ILE:HG22	1.81	0.63
1:C:207:GLY:O	1:C:211:ILE:HG13	1.99	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:E:234:SER:HB2	1:E:236:VAL:HG23	1.80	0.63
1:F:504:ARG:O	1:F:508:ARG:HG3	1.97	0.63
1:A:450:ALA:O	1:A:454:LEU:HG	1.99	0.63
1:B:29:THR:HG22	1:B:49:ARG:HH12	1.64	0.63
1:A:194:THR:H	1:A:238:HIS:CD2	2.17	0.63
1:B:457:ARG:O	1:B:457:ARG:HG3	1.97	0.63
1:B:437:TRP:HB2	1:B:439:THR:HG23	1.81	0.63
1:B:118:GLY:HA3	1:B:155:ALA:HB1	1.81	0.63
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:A:43:LYS:HE3	1:A:45:LYS:HE2	1.80	0.62
1:B:414:ARG:O	1:B:440:ALA:HA	1.99	0.62
1:F:470:ARG:HH12	1:F:474:ILE:CA	2.12	0.62
1:C:120:LYS:O	1:C:123:LYS:HB3	1.99	0.62
1:F:207:GLY:O	1:F:211:ILE:HG12	1.99	0.62
1:D:69:ARG:HD3	1:D:81:ARG:O	1.99	0.62
1:D:391:ILE:HG21	1:E:185:VAL:CG2	2.30	0.62
1:A:24:ARG:HD2	1:D:485:TYR:CE1	2.34	0.62
1:B:69:ARG:HD3	1:B:81:ARG:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:300:SER:HA	1:B:303:GLU:CG	2.28	0.62
1:F:489:GLU:HG2	1:B:69:ARG:HB2	1.80	0.62
1:C:106:PHE:HD1	1:C:140:ASP:OD1	1.83	0.62
1:C:519:SER:O	1:C:520:LEU:CB	2.48	0.62
1:D:234:SER:O	1:E:392:ARG:NH1	2.33	0.62
1:B:94:VAL:HG23	1:B:99:VAL:HG11	1.80	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:138:ILE:CG2	1:B:175:LEU:HD23	2.27	0.62
1:C:49:ARG:O	1:C:50:GLU:CB	2.43	0.62
1:D:158:GLU:O	1:D:162:ARG:HG2	1.99	0.62
1:A:18:LEU:HD13	1:D:498:MET:HE1	1.81	0.61
1:F:230:HIS:HA	1:F:234:SER:OG	2.00	0.61
1:C:397:LEU:HD12	1:C:397:LEU:C	2.21	0.61
1:C:14:THR:HA	1:C:17:LYS:HE2	1.82	0.61
1:D:363:CYS:CB	1:D:368:VAL:HG22	2.29	0.61
1:F:45:LYS:HD3	1:F:200:THR:CB	2.30	0.61
1:A:299:HIS:O	1:A:303:GLU:HG3	2.00	0.61
1:F:448:GLN:HG2	1:F:449:GLY:N	2.16	0.61
1:D:94:VAL:HG23	1:D:99:VAL:HG11	1.81	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:F:56:LEU:HD12	1:F:61:PHE:HB2	1.82	0.61
1:C:397:LEU:HD12	1:C:397:LEU:O	2.01	0.61
1:E:47:THR:HG22	1:E:50:GLU:H	1.64	0.61
1:B:350:ILE:HD13	1:B:390:ILE:HD13	1.81	0.61
1:A:414:ARG:O	1:A:440:ALA:HA	2.00	0.61
1:D:472:ARG:NE	1:D:475:GLN:HB3	2.14	0.61
1:D:391:ILE:CG2	1:E:185:VAL:CG2	2.78	0.61
1:C:354:GLU:OE2	1:C:393:ARG:HD2	2.01	0.61
1:E:203:MET:HB2	1:E:230:HIS:HE1	1.62	0.61
1:C:374:VAL:HG23	1:C:412:ILE:HG23	1.83	0.61
1:E:219:VAL:HG11	1:E:224:LEU:HD13	1.83	0.61
1:D:451:VAL:HG13	1:D:455:HIS:HB2	1.83	0.61
1:B:121:ILE:O	1:B:125:MET:HG3	2.01	0.61
1:B:339:ASN:HD21	1:B:424:MET:CE	2.14	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:A:69:ARG:NH1	1:A:81:ARG:HB3	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HG13	1:A:460:ALA:H	1.65	0.60
1:F:337:VAL:O	1:F:372:THR:HA	2.01	0.60
1:E:474:ILE:HG22	1:E:475:GLN:N	2.15	0.60
1:A:520:LEU:HG	1:A:521:PRO:HD2	1.82	0.60
1:A:26:GLU:OE1	1:A:26:GLU:N	2.34	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:D:75:PHE:HD2	1:D:147:GLN:HB3	1.66	0.60
1:E:230:HIS:HA	1:E:234:SER:OG	2.01	0.60
1:D:483:ASN:ND2	1:D:485:TYR:HB2	2.15	0.60
1:C:483:ASN:ND2	1:C:485:TYR:HB2	2.17	0.60
1:D:470:ARG:HG2	1:D:471:ALA:N	2.17	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:374:VAL:HG22	1:C:412:ILE:HA	1.83	0.60
1:A:391:ILE:CD1	1:A:391:ILE:H	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:E:203:MET:O	1:E:230:HIS:CE1	2.55	0.60
1:B:40:GLN:OE1	1:B:45:LYS:HB2	2.01	0.60
1:D:466:ALA:HB1	1:D:470:ARG:HD2	1.84	0.59
1:C:158:GLU:HG3	1:C:162:ARG:NH2	2.15	0.59
1:F:485:TYR:HE2	1:B:17:LYS:HZ1	1.50	0.59
1:A:445:MET:HG3	1:A:450:ALA:HB2	1.84	0.59
1:E:451:VAL:HB	1:E:455:HIS:HE1	1.66	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: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:F:45:LYS:HD2	1:F:244:GLU:OE2	2.03	0.59
1:B:29:THR:HG22	1:B:49:ARG:NH1	2.17	0.59
1:C:350:ILE:HG13	1:C:351:THR:N	2.16	0.59
1:B:496:VAL:HG13	1:E:67:PHE:CE2	2.38	0.59
1:A:35:ARG:NH1	1:A:38:GLU:OE1	2.34	0.59
1:F:457:ARG:HH11	1:F:457:ARG:HG3	1.67	0.59
1:C:451:VAL:O	1:C:454:LEU:O	2.20	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:F:497:ILE:HD12	1:F:497:ILE:O	2.03	0.59
1:C:77:LEU:HD11	1:C:147:GLN:HG2	1.85	0.59
1:E:74:ASN:HB3	1:E:75:PHE:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:286:THR:OG1	1:D:287:ILE:N	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:F:158:GLU:OE1	1:F:161:ARG:NH2	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:A:380:LEU:HD12	1:A:380:LEU:C	2.24	0.58
1:B:402:ALA:HA	1:B:429:LEU:O	2.03	0.58
1:B:334:VAL:HG21	1:B:371:LEU:HD11	1.84	0.58
1:A:350:ILE:HG22	1:A:385:GLN:NE2	2.17	0.58
1:F:456:ARG:O	1:F:459:ILE:HG13	2.03	0.58
1:D:454:LEU:HD21	1:E:75:PHE:CE2	2.39	0.58
1:C:464:ASP:CG	1:C:465:ASP:H	2.07	0.58
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:CD2	1:C:75:PHE:N	2.68	0.58
1:B:140:ASP:O	1:B:141:SER:C	2.41	0.58
1:B:74:ASN:HB2	1:B:77:LEU:HD11	1.84	0.58
1:A:52:ILE:HD11	1:A:103:SER:HB2	1.86	0.58
1:A:51:ARG:HH11	1:A:138:ILE:CD1	2.16	0.58
1:F:437:TRP:HE1	1:F:502:THR:HG22	1.68	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:A:10:ASP:CG	1:A:11:ILE:H	2.07	0.58
1:B:77:LEU:HD21	1:B:147:GLN:HG2	1.86	0.58
1:F:470:ARG:NH1	1:F:474:ILE:N	2.51	0.58
1:E:243:ASP:OD1	1:E:244:GLU:N	2.37	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:F:69:ARG:HG2	1:E:489:GLU:HG2	1.85	0.57
1:E:340:GLN:CD	1:E:342:MET:HB2	2.25	0.57
1:A:288:VAL:CG2	1:A:439:THR:HG21	2.32	0.57
1:F:470:ARG:HH12	1:F:474:ILE:HA	1.69	0.57
1:F:176:VAL:CG2	1:F:196:MET:HG2	2.35	0.57
1:D:196:MET:CE	1:D:230:HIS:HB2	2.34	0.57
1:B:176:VAL:HB	1:B:196:MET:HG2	1.85	0.57
1:A:104:GLN:HE21	1:A:140:ASP:N	2.02	0.57
1:A:77:LEU:HD11	1:A:147:GLN:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:196:MET:HE1	1:B:230:HIS:HB2	1.85	0.57
1:B:203:MET:O	1:B:230:HIS:HE1	1.88	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: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:D:138:ILE:HD13	1:D:175:LEU:HB3	1.86	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:C:477:TYR:CE2	1:C:481:LEU:HD12	2.38	0.57
1:A:194:THR:H	1:A:238:HIS:HD2	1.52	0.57
1:E:63:GLU:OE1	1:E:88:VAL:HG13	2.04	0.57
1:B:54:LEU:HG	1:B:248:VAL:HG11	1.87	0.57
1:C:103:SER:HB2	1:C:138:ILE:HD12	1.85	0.57
1:A:185:VAL:HG11	1:A:205:ILE:HG23	1.85	0.57
1:B:72:SER:HB2	1:B:148:GLU:OE1	2.05	0.57
1:A:391:ILE:N	1:A:391:ILE:HD12	2.15	0.57
1:F:451:VAL:HG13	1:F:455:HIS:CD2	2.40	0.57
1:B:196:MET:CE	1:B:227:ALA:HA	2.35	0.57
1:C:46:LEU:HD12	1:C:50:GLU:OE2	2.05	0.57
1:B:203:MET:HB2	1:B:230:HIS:CE1	2.40	0.57
1:F:40:GLN:HG3	1:F:45:LYS:HB2	1.86	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:A:454:LEU:HD21	1:B:146:ILE:CG2	2.35	0.57
1:A:150:VAL:HG12	1:A:153:LEU:HD12	1.85	0.57
1:E:451:VAL:HB	1:E:455:HIS:CE1	2.40	0.57
1:A:517:ARG:HG3	1:A:517:ARG:HH11	1.70	0.56
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: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:E:177:VAL:O	1:E:177:VAL:HG23	2.06	0.56
1:E:47:THR:CG2	1:E:50:GLU:H	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:LEU:O	1:E:145:ARG:HB2	2.05	0.56
1:F:475:GLN:HA	1:F:478:GLU:CG	2.33	0.56
1:E:245:LYS:CG	1:E:246:ASP:N	2.68	0.56
1:F:18:LEU:HG	1:E:498:MET:HE3	1.86	0.56
1:C:472:ARG:HD3	1:C:475:GLN:HE21	1.69	0.56
1:C:208:PRO:CG	1:C:221:PHE:CE2	2.87	0.56
1:A:134:PRO:HB3	1:A:171:PRO:HB2	1.86	0.56
1:E:181:ALA:HA	1:E:204:PHE:O	2.05	0.56
1:E:155:ALA:O	1:E:159:ILE:HG12	2.05	0.56
1:D:509:GLY:O	1:D:513:LEU:HB2	2.04	0.56
1:B:520:LEU:HG	1:B:521:PRO:CD	2.34	0.56
1:D:440:ALA:HB3	1:D:484:PRO:HB3	1.86	0.56
1:D:313:GLU:OE2	1:D:316:PRO:HA	2.04	0.56
1:C:118:GLY:HA3	1:C:155:ALA:HB1	1.87	0.56
1:C:475:GLN:HA	1:C:478:GLU:HB2	1.88	0.56
1:C:397:LEU:HD11	1:C:401:TYR:CE2	2.41	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: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:HG13	1:C:376:VAL:O	2.05	0.56
1:B:410:THR:OG1	1:B:434:ASN:ND2	2.39	0.56
1:A:69:ARG:CG	1:A:69:ARG:HH11	2.07	0.56
1:A:71:ARG:NH2	1:D:490:ARG:HE	2.04	0.56
1:C:70:HIS:C	1:C:70:HIS:HD1	2.09	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:C:10:ASP:O	1:C:11:ILE:HD13	2.06	0.56
1:D:356:ALA:O	1:D:360:VAL:HG23	2.05	0.56
1:A:88:VAL:O	1:A:103:SER:N	2.39	0.56
1:F:462:ALA:HB1	1:F:465:ASP:OD2	2.05	0.56
1:C:109:PHE:C	1:C:111:GLY:N	2.55	0.56
1:D:69:ARG:CD	1:D:81:ARG:O	2.54	0.56
1:A:113:LEU:HD13	1:A:156:TYR:CE1	2.41	0.56
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:D:196:MET:HE1	1:D:230:HIS:HB2	1.89	0.55
1:D:323:LEU:O	1:D:337:VAL:HA	2.06	0.55
1:D:77:LEU:HD11	1:D:147:GLN:CG	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:438:PRO:HG3	1:B:21:LEU:HD22	1.88	0.55
1:D:297:ASP:OD1	1:D:299:HIS:HD2	1.88	0.55
1:A:284:LEU:O	1:A:287:ILE:HG22	2.06	0.55
1:B:485:TYR:O	1:B:489:GLU:HG3	2.07	0.55
1:A:464:ASP:O	1:A:465:ASP:HB3	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: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:D:82:PRO:O	1:D:84:GLY:O	2.24	0.55
1:B:456:ARG:HG2	1:B:459:ILE:HG12	1.87	0.55
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:C:22:ARG:O	1:C:26:GLU:HG2	2.07	0.55
1:B:456:ARG:C	1:B:458:THR:H	2.10	0.55
1:B:459:ILE:HG13	1:B:460:ALA:N	2.22	0.55
1:A:298:MET:HE3	1:A:301:VAL:HG11	1.89	0.55
1:E:379:PHE:O	1:E:381:PRO:HD3	2.07	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:E:376:VAL:O	1:E:376:VAL:HG12	2.06	0.54
1:F:434:ASN:O	1:F:493:VAL:HG13	2.07	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: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:F:477:TYR:O	1:F:481:LEU:HB2	2.07	0.54
1:A:88:VAL:HB	1:A:103:SER:HB3	1.90	0.54
1:B:339:ASN:HD21	1:B:424:MET:HE2	1.72	0.54
1:C:414:ARG:O	1:C:440:ALA:HA	2.08	0.54
1:E:433:LEU:HA	1:E:494:ASP:OD2	2.07	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:B:70:HIS:ND1	1:B:70:HIS:C	2.60	0.54
1:D:499:PRO:O	1:D:502:THR:HG23	2.08	0.54
1:F:437:TRP:CZ2	1:F:502:THR:HG21	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:68:ALA:HA	1:A:489:GLU:HA	1.90	0.54
1:B:489:GLU:CB	1:E:69:ARG:HB2	2.38	0.54
1:D:514:ARG:HH11	1:D:514:ARG:HG3	1.72	0.54
1:C:205:ILE:HD11	1:F:390:ILE:HG21	1.90	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:F:206:THR:OG1	1:F:211:ILE:HD11	2.08	0.54
1:D:422:ASN:O	1:D:429:LEU:HD22	2.07	0.54
1:F:375:ASP:OD1	1:F:415:LYS:HG2	2.08	0.54
1:B:456:ARG:HG2	1:B:459:ILE:CD1	2.38	0.54
1:F:441:GLN:CG	1:F:482:LEU:HB3	2.38	0.53
1:B:343:GLN:OE1	1:B:344:PHE:CE2	2.61	0.53
1:B:140:ASP:OD1	1:B:141:SER:N	2.37	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:B:196:MET:HE2	1:B:230:HIS:HB2	1.89	0.53
1:F:35:ARG:NH2	1:F:38:GLU:OE1	2.41	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:C:474:ILE:O	1:C:475:GLN:CB	2.55	0.53
1:B:456:ARG:HD2	1:B:456:ARG:O	2.09	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: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:B:61:PHE:CZ	1:B:63:GLU:HG3	2.43	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: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:D:514:ARG:HG3	1:D:514:ARG:NH1	2.23	0.53
1:C:146:ILE:HD12	1:F:445:MET:CE	2.38	0.53
1:E:70:HIS:O	1:E:81:ARG:HD2	2.09	0.53
1:E:444:VAL:HG23	1:E:445:MET:HG2	1.88	0.53
1:E:231:ASN:HD21	1:E:239:HIS:CA	2.22	0.53
1:A:451:VAL:HA	1:A:454:LEU:HD12	1.90	0.53
1:F:486:THR:HA	1:F:489:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:ALA:HB2	1:D:482:LEU:HD11	1.90	0.53
1:F:26:GLU:O	1:F:30:HIS:HD2	1.91	0.53
1:B:380:LEU:HD23	1:B:385:GLN:CD	2.29	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:350:ILE:HD12	1:F:390:ILE:HD13	1.90	0.53
1:F:284:LEU:HD22	1:F:437:TRP:CH2	2.44	0.53
1:D:295:PRO:HB2	1:D:342:MET:HE3	1.90	0.53
1:F:285:ASP:HB3	1:B:18:LEU:CD1	2.39	0.53
1:D:196:MET:CE	1:D:237:ALA:HB2	2.38	0.53
1:F:89:THR:HB	1:F:124:VAL:HG11	1.91	0.53
1:D:319:ALA:HB2	1:D:351:THR:HB	1.91	0.53
1:D:47:THR:O	1:D:51:ARG:HG3	2.09	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:47:THR:HG22	1:B:50:GLU:CD	2.29	0.53
1:D:275:LEU:HD22	1:D:508:ARG:NH1	2.24	0.53
1:B:284:LEU:O	1:B:287:ILE:HG22	2.09	0.53
1:E:33:SER:HB3	1:E:36:ALA:HB3	1.91	0.52
1:A:528:ILE:C	1:B:358:ARG:HH12	2.12	0.52
1:C:467:GLU:O	1:C:468:ALA:C	2.48	0.52
1:D:399:PHE:CD2	1:E:164:THR:HG23	2.43	0.52
1:A:361:ARG:HH21	1:B:528:ILE:HG12	1.74	0.52
1:A:234:SER:O	1:B:392:ARG:HD3	2.08	0.52
1:C:164:THR:HG23	1:F:399:PHE:CD2	2.44	0.52
1:D:417:PHE:O	1:D:420:ALA:HB3	2.08	0.52
1:E:339:ASN:CG	1:E:376:VAL:HG23	2.29	0.52
1:A:380:LEU:HD11	1:A:385:GLN:CD	2.30	0.52
1:A:350:ILE:CD1	1:A:393:ARG:HH11	2.11	0.52
1:E:39:LYS:CD	1:E:39:LYS:N	2.71	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:C:315:GLN:OE1	1:C:355:LYS:HG3	2.09	0.52
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.90	0.52
1:F:406:VAL:C	1:F:516:LYS:HE3	2.30	0.52
1:E:156:TYR:CE1	1:E:184:ALA:HB2	2.44	0.52
1:B:72:SER:CB	1:B:148:GLU:OE1	2.57	0.52
1:F:291:SER:HB3	1:F:294:GLN:CD	2.30	0.52
1:D:297:ASP:OD1	1:D:299:HIS:CD2	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:HG23	1:C:56:LEU:HD22	1.91	0.52
1:F:470:ARG:NH1	1:F:474:ILE:HG13	2.25	0.52
1:E:375:ASP:OD2	1:E:414:ARG:HD2	2.10	0.52
1:E:70:HIS:HA	1:E:116:VAL:HG11	1.90	0.52
1:D:443:ALA:HB2	1:D:482:LEU:HD23	1.92	0.52
1:F:445:MET:HE3	1:F:450:ALA:HA	1.91	0.52
1:C:212:LYS:HE2	1:C:218:ASP:HB3	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:B:456:ARG:HG2	1:B:459:ILE:HD11	1.91	0.52
1:F:411:VAL:HG12	1:F:435:LEU:HB2	1.91	0.52
1:E:520:LEU:CD2	1:E:521:PRO:HD2	2.36	0.52
1:A:153:LEU:HD21	1:B:444:VAL:HA	1.92	0.52
1:C:396:LYS:HE2	1:C:529:PRO:O	2.10	0.52
1:A:112:ALA:HB1	1:A:145:ARG:CA	2.41	0.51
1:F:489:GLU:HA	1:B:68:ALA:HA	1.93	0.51
1:D:196:MET:HE3	1:D:237:ALA:HB2	1.91	0.51
1:C:153:LEU:HD11	1:F:444:VAL:HA	1.91	0.51
1:A:70:HIS:HB2	1:A:85:ASP:OD1	2.10	0.51
1:E:456:ARG:HA	1:E:459:ILE:HG22	1.92	0.51
1:B:140:ASP:O	1:B:179:PRO:HG2	2.11	0.51
1:C:175:LEU:HD11	1:C:247:ALA:HB1	1.92	0.51
1:D:35:ARG:N	1:D:35:ARG:CD	2.72	0.51
1:E:39:LYS:H	1:E:39:LYS:HD2	1.73	0.51
1:D:497:ILE:HD12	1:D:498:MET:H	1.75	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:C:104:GLN:HB3	1:C:117:TYR:OH	2.11	0.51
1:D:520:LEU:HD12	1:D:521:PRO:HD2	1.92	0.51
1:B:344:PHE:N	1:B:344:PHE:CD2	2.77	0.51
1:A:336:ILE:N	1:A:336:ILE:HD12	2.24	0.51
1:C:177:VAL:HA	1:C:201:SER:OG	2.11	0.51
1:B:483:ASN:HB2	1:B:485:TYR:CD1	2.46	0.51
1:F:451:VAL:CG1	1:F:455:HIS:HB2	2.39	0.51
1:C:454:LEU:HD21	1:F:75:PHE:CE2	2.46	0.51
1:C:218:ASP:O	1:C:219:VAL:HG13	2.10	0.51
1:F:356:ALA:O	1:F:360:VAL:HG23	2.11	0.51
1:A:418:GLY:HA2	1:B:153:LEU:HD21	1.91	0.51
1:D:486:THR:O	1:D:489:GLU:HG2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:CD1	1:D:285:ASP:HB3	2.40	0.51
1:D:321:ASN:HD21	1:D:352:ALA:HB2	1.74	0.51
1:E:48:ALA:HA	1:E:51:ARG:HD2	1.93	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:A:391:ILE:HG23	1:B:185:VAL:CG2	2.41	0.51
1:A:112:ALA:HB1	1:A:145:ARG:HA	1.93	0.51
1:D:49:ARG:HH22	1:D:63:GLU:CD	2.14	0.51
1:A:332:ARG:NE	1:A:514:ARG:HH12	2.08	0.51
1:D:45:LYS:HB2	1:D:244:GLU:OE2	2.10	0.51
1:F:213:THR:HG22	1:F:213:THR:O	2.10	0.51
1:E:39:LYS:H	1:E:39:LYS:CD	2.22	0.51
1:B:45:LYS:HD2	1:B:200:THR:HG22	1.93	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:E:374:VAL:HB	1:E:412:ILE:HD13	1.93	0.51
1:E:51:ARG:HD3	1:E:138:ILE:HG21	1.92	0.51
1:F:475:GLN:O	1:F:479:ASP:HB2	2.11	0.51
1:C:475:GLN:H	1:C:477:TYR:H	1.59	0.51
1:E:456:ARG:O	1:E:459:ILE:HG22	2.11	0.51
1:F:45:LYS:HD3	1:F:200:THR:HG21	1.93	0.51
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:C:519:SER:O	1:C:520:LEU:HB2	2.11	0.50
1:A:207:GLY:O	1:A:211:ILE:HD12	2.10	0.50
1:C:397:LEU:CD1	1:C:401:TYR:CD2	2.93	0.50
1:D:280:GLU:HG3	1:D:281:ASP:H	1.76	0.50
1:A:118:GLY:HA3	1:A:155:ALA:HB1	1.92	0.50
1:D:194:THR:N	1:D:238:HIS:HD2	1.99	0.50
1:C:14:THR:O	1:C:18:LEU:HD13	2.12	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:F:238:HIS:HA	1:F:315:GLN:HG2	1.93	0.50
1:A:153:LEU:HD22	1:B:418:GLY:O	2.12	0.50
1:F:105:ASP:C	1:F:107:THR:H	2.13	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:B:196:MET:HE1	1:B:227:ALA:HA	1.93	0.50
1:E:461:ASP:C	1:E:463:GLY:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:GLY:C	1:A:448:GLN:H	2.14	0.50
1:F:441:GLN:HG2	1:F:482:LEU:HB3	1.94	0.50
1:A:341:PRO:HG3	1:A:375:ASP:HB3	1.93	0.50
1:B:457:ARG:CG	1:B:457:ARG:O	2.59	0.50
1:A:22:ARG:O	1:A:26:GLU:OE1	2.30	0.50
1:C:71:ARG:NH2	1:A:490:ARG:HG2	2.26	0.50
1:A:82:PRO:HG2	1:A:109:PHE:HE2	1.77	0.50
1:B:353:SER:HB3	1:B:394:GLY:HA2	1.94	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: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:D:353:SER:OG	1:D:394:GLY:HA2	2.12	0.50
1:B:377:PRO:O	1:B:417:PHE:HD1	1.95	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: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:456:ARG:HG2	1:B:459:ILE:CG1	2.42	0.50
1:B:419:GLY:O	1:B:423:VAL:HG23	2.12	0.50
1:A:69:ARG:HH12	1:A:81:ARG:HB3	1.76	0.49
1:F:45:LYS:HE2	1:F:200:THR:HB	1.92	0.49
1:B:496:VAL:CG1	1:E:67:PHE:HD2	2.24	0.49
1:A:251:VAL:O	1:A:255:LEU:HD22	2.12	0.49
1:D:507:VAL:O	1:D:511:ARG:HG3	2.12	0.49
1:B:410:THR:HG21	1:B:425:GLY:O	2.12	0.49
1:A:205:ILE:HD13	1:B:390:ILE:HG12	1.94	0.49
1:D:104:GLN:HG3	1:D:138:ILE:O	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:F:285:ASP:HB3	1:B:18:LEU:HD11	1.94	0.49
1:C:48:ALA:C	1:C:49:ARG:O	2.48	0.49
1:C:396:LYS:HD3	1:F:530:LEU:HG	1.94	0.49
1:E:376:VAL:CG1	1:E:420:ALA:HB1	2.25	0.49
1:F:163:ASN:HA	1:F:172:GLN:HE22	1.75	0.49
1:A:75:PHE:CE2	1:B:454:LEU:HD13	2.47	0.49
1:F:321:ASN:HA	1:F:343:GLN:HB2	1.94	0.49
1:F:281:ASP:O	1:F:284:LEU:HB2	2.13	0.49
1:D:146:ILE:HG23	1:E:444:VAL:HG21	1.94	0.49
1:A:326:PHE:HB3	1:A:334:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:GLU:HG2	1:E:69:ARG:HB2	1.95	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:B:517:ARG:HG3	1:B:517:ARG:NH1	2.27	0.49
1:A:163:ASN:HB3	1:A:190:ILE:CG1	2.43	0.49
1:F:290:ASP:OD1	1:B:13:THR:HG22	2.13	0.49
1:A:49:ARG:HG3	1:A:88:VAL:HG21	1.94	0.49
1:C:350:ILE:HD13	1:C:393:ARG:NH1	2.27	0.49
1:C:208:PRO:HG3	1:C:221:PHE:CE2	2.47	0.49
1:A:393:ARG:HH22	1:B:393:ARG:NH1	2.11	0.49
1:E:520:LEU:HD13	1:E:521:PRO:HD2	1.94	0.49
1:B:397:LEU:HD23	1:B:423:VAL:CG1	2.43	0.49
1:B:89:THR:HB	1:B:124:VAL:HG11	1.95	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:B:498:MET:CE	1:E:18:LEU:HG	2.43	0.49
1:D:410:THR:HB	1:D:434:ASN:ND2	2.27	0.49
1:A:377:PRO:HA	1:A:417:PHE:HD2	1.78	0.49
1:F:496:VAL:HB	1:B:67:PHE:HE2	1.76	0.49
1:E:214:VAL:HG23	1:E:215:THR:N	2.28	0.49
1:D:337:VAL:O	1:D:372:THR:HA	2.12	0.49
1:A:40:GLN:NE2	1:A:41:HIS:N	2.59	0.49
1:C:208:PRO:HD3	1:C:221:PHE:CE2	2.47	0.49
1:B:46:LEU:HB3	1:B:50:GLU:HB2	1.94	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:E:356:ALA:O	1:E:360:VAL:HG23	2.12	0.48
1:D:121:ILE:O	1:D:125:MET:HG3	2.13	0.48
1:C:482:LEU:HD23	1:C:482:LEU:N	2.28	0.48
1:B:343:GLN:C	1:B:344:PHE:HD2	2.16	0.48
1:D:302:ILE:HD13	1:D:336:ILE:HG21	1.95	0.48
1:F:21:LEU:HD22	1:E:438:PRO:HG3	1.95	0.48
1:B:350:ILE:HG21	1:B:393:ARG:NH1	2.29	0.48
1:F:18:LEU:CG	1:E:498:MET:HE1	2.41	0.48
1:B:455:HIS:CD2	1:B:455:HIS:N	2.81	0.48
1:C:391:ILE:HG23	1:F:185:VAL:HG22	1.96	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:E:51:ARG:CG	1:E:51:ARG:NH1	2.66	0.48
1:C:208:PRO:CD	1:C:221:PHE:CE2	2.93	0.48
1:A:457:ARG:HH22	1:A:461:ASP:CG	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:234:SER:CB	1:E:236:VAL:HG23	2.43	0.48
1:F:289:PRO:HB2	1:F:294:GLN:HG3	1.96	0.48
1:F:77:LEU:HD13	1:F:147:GLN:HG3	1.94	0.48
1:E:21:LEU:O	1:E:25:ILE:HG13	2.13	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: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: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:HD2	1:C:106:PHE:O	1.97	0.48
1:D:65:ASP:HB2	1:D:120:LYS:HE3	1.94	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
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:243:ASP:OD2	1:C:244:GLU:N	2.47	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:A:391:ILE:HG23	1:B:185:VAL:HG23	1.95	0.48
1:F:458:THR:HA	1:F:461:ASP:HB2	1.96	0.48
1:D:104:GLN:HE21	1:D:140:ASP:H	1.62	0.48
1:C:126:ASP:OD1	1:C:162:ARG:HD3	2.14	0.48
1:F:357:ALA:O	1:F:361:ARG:HG3	2.14	0.48
1:B:370:VAL:HB	1:B:408:LEU:HD23	1.95	0.48
1:C:469:THR:O	1:C:473:LEU:HG	2.13	0.48
1:E:245:LYS:HG2	1:E:246:ASP:H	1.77	0.47
1:C:51:ARG:HH12	1:C:140:ASP:HB2	1.78	0.47
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.77	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:F:10:ASP:O	1:F:16:GLY:HA3	2.14	0.47
1:E:103:SER:HB2	1:E:138:ILE:HD12	1.95	0.47
1:A:454:LEU:HD21	1:B:146:ILE:HG21	1.95	0.47
1:A:369:PRO:HA	1:A:406:VAL:CG1	2.40	0.47
1:C:158:GLU:OE2	1:C:161:ARG:NH2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:110:GLY:O	1:C:142:GLY:N	2.40	0.47
1:B:77:LEU:HD21	1:B:147:GLN:HB3	1.97	0.47
1:A:527:ASN:O	1:B:358:ARG:NH1	2.47	0.47
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:E:112:ALA:HA	1:E:143:GLY:O	2.15	0.47
1:C:517:ARG:O	1:C:517:ARG:HG3	2.14	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:B:375:ASP:OD2	1:B:414:ARG:HD2	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:E:14:THR:O	1:E:18:LEU:HD13	2.14	0.47
1:D:161:ARG:HD3	1:E:428:HIS:O	2.14	0.47
1:B:530:LEU:HA	1:B:530:LEU:HD23	1.58	0.47
1:A:393:ARG:NH2	1:B:393:ARG:NH1	2.62	0.47
1:A:459:ILE:HG13	1:A:460:ALA:N	2.30	0.47
1:B:527:ASN:O	1:B:528:ILE:C	2.53	0.47
1:C:381:PRO:HG2	1:F:214:VAL:HG21	1.95	0.47
1:E:470:ARG:O	1:E:474:ILE:HG13	2.14	0.47
1:F:177:VAL:HA	1:F:201:SER:OG	2.14	0.47
1:A:401:TYR:CD1	1:A:425:GLY:HA2	2.49	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:D:350:ILE:HD13	1:D:390:ILE:HD13	1.96	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:C:99:VAL:HG12	1:C:100:ALA:N	2.30	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:E:299:HIS:HE1	1:E:313:GLU:OE1	1.97	0.47
1:A:447:ALA:O	1:A:474:ILE:HG23	2.15	0.47
1:D:319:ALA:N	1:D:320:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:ARG:CD	1:A:403:GLU:OE2	2.61	0.47
1:E:472:ARG:O	1:E:476:GLU:HB2	2.15	0.47
1:A:18:LEU:HD13	1:D:498:MET:HE3	1.96	0.47
1:B:451:VAL:C	1:B:453:ILE:H	2.18	0.47
1:A:35:ARG:NH2	1:A:39:LYS:NZ	2.63	0.47
1:D:296:TYR:O	1:D:342:MET:HG2	2.15	0.47
1:C:202:HIS:ND1	1:C:226:GLY:HA2	2.29	0.47
1:D:262:ASN:ND2	1:E:523:LYS:HA	2.29	0.47
1:E:87:VAL:HG23	1:E:104:GLN:HA	1.97	0.47
1:A:386:GLU:OE2	1:B:204:PHE:HA	2.15	0.47
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:F:25:ILE:O	1:F:29:THR:HG23	2.14	0.46
1:E:320:PRO:HB2	1:E:343:GLN:HG3	1.96	0.46
1:D:51:ARG:HH11	1:D:51:ARG:HG2	1.80	0.46
1:B:337:VAL:CG2	1:B:372:THR:HG22	2.45	0.46
1:F:457:ARG:NH1	1:F:458:THR:OG1	2.45	0.46
1:B:86:GLY:HA2	1:B:108:VAL:HB	1.96	0.46
1:C:10:ASP:CG	1:C:11:ILE:H	2.19	0.46
1:D:21:LEU:HD12	1:D:21:LEU:O	2.15	0.46
1:A:47:THR:O	1:A:48:ALA:HB3	2.15	0.46
1:B:281:ASP:O	1:B:500:SER:HA	2.16	0.46
1:D:286:THR:O	1:D:287:ILE:CG2	2.56	0.46
1:A:153:LEU:HG	1:B:444:VAL:HG12	1.97	0.46
1:A:70:HIS:NE2	1:A:148:GLU:CD	2.67	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:B:490:ARG:HD3	1:B:492:TYR:CZ	2.50	0.46
1:D:107:THR:O	1:D:107:THR:CG2	2.62	0.46
1:B:77:LEU:O	1:B:79:ALA:N	2.49	0.46
1:B:455:HIS:HE1	1:B:477:TYR:CE2	2.33	0.46
1:D:441:GLN:HG2	1:D:482:LEU:O	2.16	0.46
1:B:80:ASN:O	1:B:80:ASN:ND2	2.49	0.46
1:C:209:ASP:N	1:C:209:ASP:OD1	2.47	0.46
1:D:350:ILE:HG21	1:D:393:ARG:NH1	2.31	0.46
1:B:496:VAL:HG13	1:E:67:PHE:HE2	1.80	0.46
1:B:111:GLY:C	1:B:141:SER:HB2	2.35	0.46
1:D:513:LEU:HD12	1:D:513:LEU:HA	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:CG2	1:A:371:LEU:HG	2.45	0.46
1:C:285:ASP:OD1	1:C:499:PRO:HD2	2.16	0.46
1:D:458:THR:HG22	1:D:458:THR:O	2.16	0.46
1:E:51:ARG:NH2	1:E:177:VAL:HG21	2.31	0.46
1:B:305:VAL:O	1:B:306:LEU:CB	2.63	0.46
1:A:442:ILE:CD1	1:A:487:ALA:H	2.28	0.46
1:D:354:GLU:OE2	1:D:393:ARG:CD	2.59	0.46
1:A:47:THR:HG22	1:A:47:THR:O	2.16	0.46
1:C:382:GLY:O	1:C:385:GLN:HB2	2.15	0.46
1:E:47:THR:HG22	1:E:50:GLU:N	2.29	0.46
1:E:36:ALA:HA	1:E:39:LYS:CD	2.41	0.46
1:A:175:LEU:HA	1:A:195:VAL:HG13	1.98	0.46
1:C:145:ARG:HG3	1:C:148:GLU:HG3	1.98	0.46
1:D:197:VAL:HG12	1:D:247:ALA:HB2	1.96	0.46
1:B:280:GLU:O	1:B:283:GLU:HG3	2.16	0.46
1:F:517:ARG:O	1:F:518:GLU:HB3	2.15	0.46
1:A:350:ILE:HG13	1:A:393:ARG:HD2	1.96	0.46
1:D:381:PRO:HB2	1:E:214:VAL:CG2	2.45	0.46
1:B:69:ARG:NE	1:B:81:ARG:O	2.48	0.46
1:A:372:THR:HG21	1:A:401:TYR:HE1	1.79	0.46
1:C:146:ILE:HD12	1:F:445:MET:HE1	1.97	0.46
1:D:211:ILE:HG21	1:E:383:VAL:HG23	1.97	0.46
1:C:363:CYS:HB3	1:C:368:VAL:HG22	1.98	0.46
1:E:69:ARG:NH1	1:E:69:ARG:CG	2.60	0.46
1:B:350:ILE:HG21	1:B:393:ARG:HH12	1.81	0.46
1:F:458:THR:CG2	1:F:469:THR:HG21	2.41	0.46
1:F:493:VAL:HG12	1:F:495:ALA:H	1.80	0.46
1:A:443:ALA:O	1:B:153:LEU:HD11	2.16	0.46
1:A:376:VAL:HG21	1:A:420:ALA:HB1	1.98	0.46
1:A:393:ARG:HH12	1:B:393:ARG:NH2	2.14	0.45
1:A:459:ILE:HD12	1:A:460:ALA:N	2.32	0.45
1:D:47:THR:O	1:D:49:ARG:O	2.34	0.45
1:E:459:ILE:HD11	1:E:470:ARG:HB2	1.98	0.45
1:B:108:VAL:HG12	1:B:109:PHE:CD1	2.50	0.45
1:A:113:LEU:HD23	1:A:113:LEU:O	2.15	0.45
1:A:437:TRP:CE2	1:A:499:PRO:HA	2.50	0.45
1:D:480:ALA:O	1:D:481:LEU:HD23	2.16	0.45
1:E:156:TYR:HE1	1:E:184:ALA:HB2	1.81	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:36:ALA:CA	1:E:39:LYS:HD3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:ILE:O	1:C:474:ILE:HG22	2.16	0.45
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:A:288:VAL:HG22	1:A:288:VAL:O	2.16	0.45
1:A:138:ILE:HG22	1:A:175:LEU:CB	2.39	0.45
1:A:516:LYS:HB2	1:A:516:LYS:HE2	1.78	0.45
1:B:184:ALA:C	1:B:186:TYR:H	2.20	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:D:10:ASP:CG	1:D:11:ILE:H	2.20	0.45
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.68	0.45
1:E:461:ASP:C	1:E:463:GLY:H	2.20	0.45
1:F:187:SER:HB3	1:F:188:PRO:CD	2.45	0.45
1:B:296:TYR:O	1:B:342:MET:HG2	2.17	0.45
1:A:475:GLN:HA	1:A:475:GLN:NE2	2.31	0.45
1:D:286:THR:C	1:D:288:VAL:N	2.64	0.45
1:A:116:VAL:HA	1:A:119:GLN:OE1	2.16	0.45
1:A:104:GLN:HB3	1:A:117:TYR:OH	2.16	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:A:77:LEU:HD21	1:A:147:GLN:HG3	1.98	0.45
1:F:70:HIS:O	1:F:81:ARG:NH1	2.49	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:D:414:ARG:HA	1:D:439:THR:O	2.17	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:A:372:THR:CG2	1:A:401:TYR:OH	2.64	0.45
1:E:87:VAL:O	1:E:120:LYS:NZ	2.43	0.45
1:F:298:MET:O	1:F:301:VAL:HG13	2.17	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:B:451:VAL:HG13	1:B:455:HIS:NE2	2.32	0.45
1:B:31:ALA:HB1	1:B:108:VAL:HG22	1.99	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:F:180:CYS:SG	1:F:185:VAL:HA	2.57	0.45
1:B:322:ILE:HD13	1:B:356:ALA:HB2	1.98	0.45
1:E:472:ARG:O	1:E:474:ILE:O	2.35	0.45
1:B:87:VAL:HG13	1:B:120:LYS:CD	2.45	0.45
1:C:67:PHE:CD2	1:A:496:VAL:CG2	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:ASN:O	1:E:429:LEU:HD22	2.17	0.45
1:D:520:LEU:CB	1:D:521:PRO:CD	2.92	0.44
1:A:43:LYS:HE3	1:A:45:LYS:CE	2.45	0.44
1:B:238:HIS:HA	1:B:315:GLN:HG3	1.99	0.44
1:C:319:ALA:N	1:C:320:PRO:HD3	2.33	0.44
1:D:447:ALA:HB2	1:D:478:GLU:HG3	2.00	0.44
1:F:476:GLU:OE1	1:F:476:GLU:HA	2.17	0.44
1:F:141:SER:O	1:F:179:PRO:HG2	2.18	0.44
1:D:108:VAL:HG12	1:D:109:PHE:CD1	2.52	0.44
1:B:32:GLY:H	1:B:107:THR:CG2	2.29	0.44
1:F:478:GLU:HB3	1:F:482:LEU:HD22	1.99	0.44
1:B:14:THR:O	1:B:18:LEU:HG	2.17	0.44
1:A:70:HIS:ND1	1:A:71:ARG:N	2.59	0.44
1:E:455:HIS:ND1	1:E:455:HIS:N	2.64	0.44
1:A:196:MET:HB3	1:A:201:SER:OG	2.17	0.44
1:D:298:MET:SD	1:D:301:VAL:HG11	2.57	0.44
1:D:107:THR:O	1:D:107:THR:HG23	2.16	0.44
1:A:115:GLU:HG3	1:A:116:VAL:N	2.33	0.44
1:E:467:GLU:C	1:E:469:THR:N	2.68	0.44
1:D:422:ASN:HA	1:D:426:SER:CB	2.46	0.44
1:D:321:ASN:ND2	1:D:352:ALA:HB2	2.33	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:347:CYS:SG	1:A:380:LEU:HB3	2.58	0.44
1:B:77:LEU:HD21	1:B:147:GLN:CB	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:D:483:ASN:HB2	1:D:484:PRO:CD	2.47	0.44
1:B:230:HIS:CD2	1:B:234:SER:OG	2.63	0.44
1:F:45:LYS:CE	1:F:200:THR:HB	2.48	0.44
1:B:109:PHE:C	1:B:111:GLY:H	2.21	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:E:473:LEU:HD13	1:E:473:LEU:HA	1.87	0.44
1:D:51:ARG:HG2	1:D:51:ARG:NH1	2.33	0.44
1:C:438:PRO:HG3	1:D:21:LEU:HD22	1.99	0.44
1:D:398:ILE:HG21	1:E:160:PHE:HB3	1.99	0.44
1:A:40:GLN:CD	1:A:41:HIS:H	2.20	0.44
1:B:196:MET:HE2	1:B:230:HIS:CB	2.47	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:PHE:C	1:E:111:GLY:H	2.21	0.44
1:E:187:SER:O	1:E:191:THR:HG23	2.18	0.44
1:C:70:HIS:C	1:C:70:HIS:ND1	2.68	0.44
1:D:447:ALA:HB1	1:D:474:ILE:HG23	1.99	0.44
1:B:113:LEU:HD21	1:B:155:ALA:HB3	2.00	0.44
1:F:370:VAL:HB	1:F:408:LEU:HD23	1.99	0.44
1:E:414:ARG:O	1:E:441:GLN:N	2.39	0.44
1:D:506:ILE:O	1:D:510:LEU:HG	2.18	0.44
1:F:106:PHE:O	1:F:106:PHE:CD2	2.70	0.44
1:B:417:PHE:HA	1:B:443:ALA:O	2.18	0.44
1:B:75:PHE:HD1	1:B:76:GLY:N	2.16	0.44
1:C:397:LEU:HD11	1:C:401:TYR:HE2	1.82	0.44
1:F:375:ASP:CG	1:F:414:ARG:HB3	2.38	0.44
1:D:342:MET:HA	1:D:342:MET:CE	2.47	0.44
1:A:302:ILE:HD13	1:A:336:ILE:HG21	1.99	0.44
1:F:319:ALA:N	1:F:320:PRO:HD3	2.32	0.44
1:C:181:ALA:O	1:C:184:ALA:HB3	2.18	0.44
1:E:78:ASP:N	1:E:78:ASP:OD1	2.50	0.44
1:B:377:PRO:HB3	1:B:415:LYS:HE3	1.99	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:C:482:LEU:N	1:C:482:LEU:CD2	2.81	0.43
1:D:24:ARG:NH1	1:D:83:TYR:OH	2.43	0.43
1:C:254:LEU:HD13	1:C:312:PHE:HE2	1.82	0.43
1:A:459:ILE:HG21	1:A:470:ARG:HE	1.83	0.43
1:A:51:ARG:NH1	1:A:138:ILE:HD12	2.33	0.43
1:D:196:MET:HE3	1:D:237:ALA:CB	2.48	0.43
1:A:529:PRO:HG3	1:B:190:ILE:HA	1.99	0.43
1:D:440:ALA:HB3	1:D:484:PRO:HG3	2.00	0.43
1:F:163:ASN:ND2	1:F:187:SER:OG	2.46	0.43
1:A:238:HIS:HA	1:A:315:GLN:HG3	2.00	0.43
1:A:102:PHE:CE2	1:A:137:GLY:HA3	2.53	0.43
1:F:11:ILE:HD12	1:F:11:ILE:N	2.33	0.43
1:C:449:GLY:O	1:C:453:ILE:HD13	2.19	0.43
1:A:350:ILE:HG13	1:A:393:ARG:CD	2.49	0.43
1:A:449:GLY:HA2	1:A:452:ASN:HD21	1.83	0.43
1:F:483:ASN:HB2	1:F:485:TYR:HD2	1.83	0.43
1:F:46:LEU:HB2	1:F:244:GLU:OE1	2.18	0.43
1:A:35:ARG:NH2	1:A:39:LYS:HE2	2.33	0.43
1:D:294:GLN:OE1	1:D:295:PRO:HD2	2.18	0.43
1:A:419:GLY:O	1:A:423:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:SER:O	1:D:179:PRO:HG2	2.17	0.43
1:C:288:VAL:HG12	1:C:289:PRO:O	2.19	0.43
1:A:51:ARG:HH11	1:A:138:ILE:HD13	1.82	0.43
1:B:405:THR:HA	1:B:518:GLU:OE1	2.17	0.43
1:C:230:HIS:HA	1:C:234:SER:OG	2.19	0.43
1:A:374:VAL:CG1	1:A:376:VAL:HG12	2.48	0.43
1:E:86:GLY:HA2	1:E:108:VAL:HB	1.99	0.43
1:E:47:THR:HG22	1:E:50:GLU:CB	2.48	0.43
1:A:153:LEU:CD2	1:B:444:VAL:HG12	2.49	0.43
1:F:485:TYR:HE2	1:B:17:LYS:NZ	2.16	0.43
1:B:448:GLN:O	1:B:452:ASN:OD1	2.36	0.43
1:C:392:ARG:NH1	1:F:234:SER:O	2.52	0.43
1:A:126:ASP:O	1:A:130:LYS:HB3	2.18	0.43
1:F:445:MET:CE	1:F:450:ALA:HA	2.48	0.43
1:B:372:THR:OG1	1:B:410:THR:HG22	2.18	0.43
1:F:105:ASP:C	1:F:107:THR:N	2.72	0.43
1:C:63:GLU:OE2	1:C:88:VAL:HG23	2.17	0.43
1:C:472:ARG:HA	1:C:472:ARG:HD3	1.61	0.43
1:F:210:VAL:O	1:F:214:VAL:HG23	2.18	0.43
1:A:10:ASP:CG	1:A:11:ILE:N	2.70	0.43
1:C:324:THR:HA	1:C:336:ILE:O	2.18	0.43
1:F:338:ALA:HB1	1:F:373:PHE:HB2	2.00	0.43
1:C:135:VAL:HG23	1:C:170:ILE:HD12	2.00	0.43
1:C:461:ASP:C	1:C:463:GLY:N	2.71	0.43
1:D:286:THR:O	1:D:288:VAL:N	2.47	0.43
1:A:205:ILE:CD1	1:B:390:ILE:HG12	2.49	0.43
1:E:340:GLN:O	1:E:340:GLN:HG3	2.18	0.43
1:A:465:ASP:O	1:A:466:ALA:C	2.57	0.43
1:A:478:GLU:O	1:A:482:LEU:HB2	2.18	0.43
1:E:474:ILE:O	1:E:476:GLU:N	2.46	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:B:177:VAL:HG23	1:B:178:GLY:H	1.83	0.43
1:A:156:TYR:CE1	1:A:184:ALA:HB2	2.54	0.43
1:B:498:MET:HE1	1:E:18:LEU:HG	1.98	0.43
1:C:461:ASP:O	1:C:462:ALA:C	2.57	0.43
1:B:135:VAL:HG12	1:B:172:GLN:HA	2.00	0.43
1:B:78:ASP:OD1	1:B:78:ASP:N	2.51	0.43
1:B:212:LYS:HG3	1:B:213:THR:N	2.34	0.43
1:D:193:PHE:HA	1:D:238:HIS:CD2	2.54	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:45:LYS:CD	1:F:200:THR:HB	2.49	0.43
1:E:483:ASN:HB2	1:E:484:PRO:CD	2.49	0.43
1:C:146:ILE:H	1:C:146:ILE:HG12	1.30	0.43
1:B:275:LEU:HD11	1:B:508:ARG:NH2	2.33	0.43
1:B:290:ASP:N	1:B:290:ASP:OD2	2.51	0.43
1:D:288:VAL:O	1:D:288:VAL:HG22	2.18	0.43
1:A:52:ILE:HG23	1:A:56:LEU:HD12	2.01	0.43
1:E:185:VAL:C	1:E:188:PRO:HD2	2.40	0.43
1:C:350:ILE:HG22	1:C:390:ILE:CD1	2.48	0.43
1:E:451:VAL:HA	1:E:454:LEU:HB2	2.00	0.43
1:A:451:VAL:HG13	1:A:477:TYR:CD1	2.54	0.43
1:B:437:TRP:NE1	1:B:502:THR:CG2	2.76	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:E:118:GLY:HA3	1:E:155:ALA:HB1	2.01	0.43
1:C:238:HIS:HA	1:C:315:GLN:HG2	2.00	0.43
1:C:113:LEU:HD12	1:C:117:TYR:CE2	2.53	0.43
1:B:74:ASN:H	1:B:77:LEU:HD12	1.84	0.42
1:F:451:VAL:HG13	1:F:455:HIS:CB	2.47	0.42
1:E:141:SER:O	1:E:179:PRO:O	2.36	0.42
1:A:374:VAL:HG22	1:A:424:MET:HB3	2.01	0.42
1:F:141:SER:O	1:F:179:PRO:O	2.37	0.42
1:E:129:LEU:HA	1:E:170:ILE:HD13	2.00	0.42
1:A:121:ILE:O	1:A:125:MET:HG3	2.20	0.42
1:E:246:ASP:O	1:E:249:GLU:N	2.51	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: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:B:77:LEU:HD21	1:B:147:GLN:CG	2.48	0.42
1:F:456:ARG:HG3	1:F:457:ARG:N	2.34	0.42
1:D:437:TRP:CE2	1:D:499:PRO:HA	2.54	0.42
1:F:45:LYS:HE3	1:F:177:VAL:O	2.19	0.42
1:B:290:ASP:HB3	1:E:13:THR:HA	2.00	0.42
1:C:180:CYS:HB3	1:C:203:MET:HG2	2.01	0.42
1:A:398:ILE:HD13	1:B:160:PHE:CD2	2.54	0.42
1:E:98:PRO:O	1:E:134:PRO:HD2	2.19	0.42
1:D:523:LYS:HA	1:E:262:ASN:ND2	2.33	0.42
1:A:438:PRO:HD3	1:A:497:ILE:O	2.19	0.42
1:B:483:ASN:HB2	1:B:485:TYR:HD1	1.83	0.42
1:A:459:ILE:CG1	1:A:460:ALA:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:GLN:HG2	1:F:475:GLN:O	2.18	0.42
1:A:238:HIS:CE1	1:A:315:GLN:NE2	2.87	0.42
1:D:262:ASN:HD21	1:E:523:LYS:HA	1.85	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:E:113:LEU:CD1	1:E:117:TYR:CD2	2.95	0.42
1:D:391:ILE:HG21	1:E:185:VAL:HG21	2.01	0.42
1:C:108:VAL:O	1:C:109:PHE:CG	2.73	0.42
1:A:40:GLN:H	1:A:40:GLN:CD	2.22	0.42
1:C:414:ARG:HA	1:C:440:ALA:HA	2.02	0.42
1:C:164:THR:HG23	1:F:399:PHE:CE2	2.54	0.42
1:D:35:ARG:N	1:D:35:ARG:HD2	2.33	0.42
1:A:176:VAL:HG12	1:A:201:SER:HB2	2.02	0.42
1:A:76:GLY:O	1:A:78:ASP:N	2.52	0.42
1:C:83:TYR:C	1:C:85:ASP:H	2.23	0.42
1:F:305:VAL:HG11	1:F:506:ILE:CD1	2.49	0.42
1:B:489:GLU:CG	1:E:69:ARG:HB2	2.49	0.42
1:B:148:GLU:HB2	1:B:152:SER:OG	2.19	0.42
1:F:451:VAL:HG13	1:F:455:HIS:HD2	1.83	0.42
1:D:520:LEU:CB	1:D:521:PRO:HD2	2.42	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:D:342:MET:HA	1:D:342:MET:HE2	2.01	0.42
1:C:170:ILE:O	1:C:170:ILE:HG13	2.18	0.42
1:E:447:ALA:HB2	1:E:478:GLU:HG3	2.01	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:D:454:LEU:HD21	1:E:75:PHE:CZ	2.53	0.42
1:A:337:VAL:O	1:A:372:THR:HA	2.19	0.42
1:F:472:ARG:O	1:F:476:GLU:HG2	2.19	0.42
1:B:32:GLY:H	1:B:107:THR:HG21	1.85	0.42
1:E:121:ILE:O	1:E:125:MET:HG3	2.20	0.42
1:B:372:THR:CG2	1:B:410:THR:HG22	2.49	0.42
1:C:519:SER:O	1:C:520:LEU:HB3	2.20	0.42
1:A:108:VAL:O	1:A:110:GLY:O	2.38	0.42
1:F:89:THR:HG22	1:F:102:PHE:HB2	2.02	0.42
1:B:488:ALA:O	1:E:68:ALA:HA	2.19	0.42
1:B:163:ASN:HD22	1:B:172:GLN:HE22	1.68	0.42
1:E:254:LEU:HD12	1:E:254:LEU:HA	1.74	0.42
1:D:287:ILE:O	1:D:289:PRO:HD3	2.19	0.42
1:A:193:PHE:HA	1:A:238:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:CD2	1:B:482:LEU:N	2.83	0.42
1:C:372:THR:HB	1:C:410:THR:HB	2.02	0.42
1:B:315:GLN:N	1:B:316:PRO:HD3	2.34	0.42
1:F:427:LYS:CD	1:F:431:ALA:O	2.68	0.42
1:B:324:THR:HA	1:B:336:ILE:O	2.20	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:A:21:LEU:O	1:A:21:LEU:HD12	2.20	0.42
1:A:65:ASP:OD2	1:A:123:LYS:HD3	2.20	0.42
1:F:458:THR:HA	1:F:461:ASP:CB	2.50	0.42
1:C:397:LEU:HG	1:C:423:VAL:HG12	1.97	0.42
1:A:405:THR:O	1:A:516:LYS:CD	2.68	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:C:240:MET:O	1:C:240:MET:HG3	2.18	0.42
1:C:459:ILE:HD13	1:C:459:ILE:C	2.41	0.42
1:A:340:GLN:O	1:A:340:GLN:HG3	2.19	0.41
1:E:66:GLU:HG2	1:E:67:PHE:CE1	2.55	0.41
1:B:265:GLU:HB2	1:B:266:PRO:CD	2.50	0.41
1:C:33:SER:OG	1:C:35:ARG:HG3	2.20	0.41
1:C:397:LEU:HD11	1:C:401:TYR:CD2	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:E:146:ILE:H	1:E:146:ILE:HG13	1.50	0.41
1:D:346:GLY:O	1:D:377:PRO:HD2	2.20	0.41
1:A:466:ALA:O	1:A:467:GLU:C	2.59	0.41
1:A:529:PRO:N	1:B:358:ARG:HH12	2.19	0.41
1:C:397:LEU:CD1	1:C:401:TYR:CE2	3.03	0.41
1:A:87:VAL:HG23	1:A:104:GLN:HA	2.02	0.41
1:D:478:GLU:HG3	1:D:482:LEU:HD12	2.02	0.41
1:A:177:VAL:HG12	1:A:197:VAL:CG2	2.51	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:C:299:HIS:O	1:C:303:GLU:HG3	2.21	0.41
1:F:433:LEU:HA	1:F:433:LEU:HD12	1.89	0.41
1:A:455:HIS:ND1	1:A:455:HIS:N	2.67	0.41
1:D:182:GLY:C	1:D:205:ILE:HD12	2.40	0.41
1:B:35:ARG:CZ	1:B:39:LYS:HZ2	2.33	0.41
1:D:193:PHE:CB	1:D:254:LEU:HD21	2.50	0.41
1:E:214:VAL:CG2	1:E:215:THR:N	2.84	0.41
1:A:442:ILE:CD1	1:A:487:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:O	1:A:75:PHE:CD1	2.74	0.41
1:F:319:ALA:HB2	1:F:351:THR:HB	2.02	0.41
1:B:238:HIS:HA	1:B:315:GLN:CG	2.50	0.41
1:B:215:THR:OG1	1:B:217:GLU:OE1	2.38	0.41
1:E:103:SER:HA	1:E:138:ILE:HB	2.03	0.41
1:A:153:LEU:HD21	1:B:418:GLY:HA2	2.02	0.41
1:F:438:PRO:O	1:B:17:LYS:HG3	2.20	0.41
1:D:196:MET:HE2	1:D:230:HIS:HB2	2.01	0.41
1:C:106:PHE:O	1:C:109:PHE:O	2.39	0.41
1:F:203:MET:HE3	1:F:236:VAL:HG11	2.02	0.41
1:F:300:SER:O	1:F:304:HIS:ND1	2.53	0.41
1:D:70:HIS:HA	1:D:116:VAL:HG21	2.01	0.41
1:A:442:ILE:HG13	1:A:442:ILE:O	2.19	0.41
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.51	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:F:102:PHE:CD1	1:F:102:PHE:C	2.93	0.41
1:B:181:ALA:HA	1:B:204:PHE:O	2.21	0.41
1:D:180:CYS:SG	1:D:185:VAL:HA	2.60	0.41
1:B:442:ILE:HG21	1:B:487:ALA:HB2	2.03	0.41
1:A:440:ALA:HB3	1:A:484:PRO:HB3	2.02	0.41
1:A:70:HIS:HA	1:A:116:VAL:HG21	2.02	0.41
1:B:29:THR:HA	1:B:49:ARG:CZ	2.51	0.41
1:B:70:HIS:O	1:B:81:ARG:HD2	2.21	0.41
1:F:45:LYS:NZ	1:F:244:GLU:OE2	2.49	0.41
1:B:241:ALA:HB1	1:B:246:ASP:CB	2.49	0.41
1:F:473:LEU:HA	1:F:476:GLU:HB2	2.01	0.41
1:B:354:GLU:OE2	1:B:393:ARG:HD2	2.20	0.41
1:C:156:TYR:CE1	1:C:184:ALA:HB2	2.56	0.41
1:F:427:LYS:HD3	1:F:427:LYS:HA	1.66	0.41
1:E:32:GLY:HA3	1:E:107:THR:OG1	2.20	0.41
1:F:464:ASP:C	1:F:466:ALA:H	2.24	0.41
1:B:122:VAL:HG13	1:B:162:ARG:NE	2.36	0.41
1:B:35:ARG:HB3	1:B:39:LYS:NZ	2.35	0.41
1:A:180:CYS:SG	1:A:185:VAL:HA	2.60	0.41
1:B:414:ARG:HH11	1:B:414:ARG:HD2	1.72	0.41
1:A:103:SER:HA	1:A:138:ILE:CG1	2.47	0.41
1:F:461:ASP:O	1:F:462:ALA:C	2.58	0.41
1:B:348:LEU:HD11	1:B:424:MET:HE2	2.02	0.41
1:E:414:ARG:HA	1:E:440:ALA:HA	2.02	0.41
1:A:372:THR:HG21	1:A:401:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:VAL:CG1	1:B:103:SER:HB3	2.51	0.41
1:D:20:ASP:O	1:D:24:ARG:HG2	2.21	0.41
1:C:266:PRO:HB2	1:C:333:PRO:HG2	2.02	0.41
1:B:513:LEU:HD21	1:E:127:PHE:HE1	1.86	0.41
1:A:205:ILE:CD1	1:B:390:ILE:HG21	2.51	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:F:451:VAL:C	1:F:453:ILE:N	2.73	0.41
1:C:397:LEU:CD1	1:C:397:LEU:C	2.89	0.41
1:F:70:HIS:ND1	1:F:71:ARG:N	2.69	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:C:393:ARG:HA	1:C:393:ARG:HD3	1.82	0.40
1:F:77:LEU:CD1	1:F:147:GLN:HG3	2.50	0.40
1:A:298:MET:CE	1:A:301:VAL:HG11	2.51	0.40
1:C:275:LEU:O	1:C:504:ARG:HD2	2.20	0.40
1:A:170:ILE:HG13	1:A:170:ILE:O	2.20	0.40
1:A:390:ILE:HG13	1:A:390:ILE:O	2.21	0.40
1:B:35:ARG:NH1	1:B:38:GLU:OE1	2.54	0.40
1:E:208:PRO:CA	1:E:211:ILE:HG12	2.35	0.40
1:E:516:LYS:O	1:E:516:LYS:HG3	2.20	0.40
1:A:70:HIS:CD2	1:A:72:SER:HB3	2.57	0.40
1:D:49:ARG:NH2	1:D:63:GLU:OE1	2.51	0.40
1:F:74:ASN:HB3	1:F:75:PHE:CD1	2.57	0.40
1:D:278:THR:OG1	1:D:280:GLU:HG3	2.22	0.40
1:A:457:ARG:HG3	1:A:457:ARG:O	2.20	0.40
1:F:10:ASP:OD1	1:F:11:ILE:N	2.43	0.40
1:E:87:VAL:CG1	1:E:120:LYS:HD3	2.51	0.40
1:D:197:VAL:CG1	1:D:247:ALA:HB2	2.50	0.40
1:D:108:VAL:HG12	1:D:109:PHE:N	2.35	0.40
1:E:338:ALA:HA	1:E:373:PHE:O	2.21	0.40
1:A:280:GLU:HG3	1:A:280:GLU:H	1.50	0.40
1:B:35:ARG:HB3	1:B:39:LYS:HZ1	1.86	0.40
1:A:65:ASP:HB3	1:A:68:ALA:HB2	2.03	0.40
1:E:47:THR:H	1:E:50:GLU:CD	2.25	0.40
1:A:91:TYR:CE1	1:D:512:GLN:HG3	2.55	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:B:458:THR:O	1:B:458:THR:HG22	2.21	0.40
1:A:108:VAL:HG12	1:A:109:PHE:HD2	1.87	0.40
1:D:113:LEU:HD13	1:D:156:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:GLY:C	1:E:86:GLY:H	2.24	0.40
1:B:350:ILE:HD13	1:B:390:ILE:CD1	2.50	0.40
1:B:75:PHE:CD1	1:B:76:GLY:N	2.89	0.40
1:F:68:ALA:HA	1:E:489:GLU:HA	2.02	0.40
1:E:481:LEU:C	1:E:483:ASN:H	2.24	0.40
1:A:397:LEU:HD22	1:A:401:TYR:CE2	2.56	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:E:65:ASP:OD2	1:E:123:LYS:HD2	2.21	0.40
1:A:282:ALA:HA	1:A:500:SER:OG	2.21	0.40
1:C:111:GLY:O	1:C:141:SER:HB2	2.20	0.40
1:B:344:PHE:C	1:B:346:GLY:H	2.23	0.40
1:C:464:ASP:CG	1:C:465:ASP:N	2.74	0.40
1:B:140:ASP:O	1:B:179:PRO:CD	2.69	0.40
1:A:457:ARG:CZ	1:A:461:ASP:HB2	2.51	0.40
1:F:193:PHE:HA	1:F:238:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/530 (98%)	470 (91%)	38 (7%)	11 (2%)	9	9
1	B	519/530 (98%)	455 (88%)	52 (10%)	12 (2%)	8	8
1	C	519/530 (98%)	475 (92%)	37 (7%)	7 (1%)	15	19
1	D	519/530 (98%)	472 (91%)	41 (8%)	6 (1%)	16	21
1	E	519/530 (98%)	476 (92%)	39 (8%)	4 (1%)	24	33
1	F	519/530 (98%)	479 (92%)	33 (6%)	7 (1%)	15	19
All	All	3114/3180 (98%)	2827 (91%)	240 (8%)	47 (2%)	13	15

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
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

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Mol	Chain	Res	Type
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%)	361 (88%)	51 (12%)	6	6
1	B	412/421 (98%)	371 (90%)	41 (10%)	9	12
1	C	412/421 (98%)	383 (93%)	29 (7%)	19	27
1	D	412/421 (98%)	377 (92%)	35 (8%)	13	18
1	E	412/421 (98%)	370 (90%)	42 (10%)	9	12
1	F	412/421 (98%)	376 (91%)	36 (9%)	13	17
All	All	2472/2526 (98%)	2238 (90%)	234 (10%)	11	14

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	LEU
1	C	49	ARG
1	C	70	HIS
1	C	75	PHE
1	C	117	TYR
1	C	124	VAL
1	C	146	ILE
1	C	162	ARG
1	C	177	VAL
1	C	205	ILE
1	C	222	GLU
1	C	223	GLU
1	C	229	THR

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Mol	Chain	Res	Type
1	C	236	VAL
1	C	240	MET
1	C	264	SER
1	C	310	GLU
1	C	349	ASP
1	C	350	ILE
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	F	11	ILE
1	F	35	ARG
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
1	F	209	ASP
1	F	215	THR
1	F	217	GLU
1	F	219	VAL
1	F	246	ASP
1	F	251	VAL
1	F	264	SER
1	F	294	GLN
1	F	301	VAL
1	F	332	ARG
1	F	358	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

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Mol	Chain	Res	Type
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	A	21	LEU
1	A	40	GLN
1	A	54	LEU
1	A	63	GLU
1	A	69	ARG
1	A	70	HIS
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	147	GLN
1	A	150	VAL
1	A	185	VAL
1	A	200	THR
1	A	215	THR
1	A	233	THR
1	A	255	LEU
1	A	256	SER
1	A	280	GLU
1	A	288	VAL
1	A	301	VAL
1	A	308	ASP
1	A	310	GLU
1	A	317	LEU
1	A	326	PHE
1	A	332	ARG
1	A	350	ILE
1	A	358	ARG
1	A	380	LEU

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Mol	Chain	Res	Type
1	A	397	LEU
1	A	406	VAL
1	A	415	LYS
1	A	427	LYS
1	A	433	LEU
1	A	444	VAL
1	A	455	HIS
1	A	458	THR
1	A	461	ASP
1	A	472	ARG
1	A	473	LEU
1	A	475	GLN
1	A	481	LEU
1	A	486	THR
1	A	496	VAL
1	A	512	GLN
1	A	516	LYS
1	A	517	ARG
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	70	HIS
1	B	80	ASN
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	304	HIS

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Mol	Chain	Res	Type
1	B	310	GLU
1	B	334	VAL
1	B	374	VAL
1	B	387	HIS
1	B	392	ARG
1	B	414	ARG
1	B	433	LEU
1	B	439	THR
1	B	448	GLN
1	B	455	HIS
1	B	457	ARG
1	B	469	THR
1	B	472	ARG
1	B	481	LEU
1	B	482	LEU
1	B	490	ARG
1	B	493	VAL
1	B	496	VAL
1	D	35	ARG
1	D	40	GLN
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	236	VAL
1	D	265	GLU
1	D	280	GLU
1	D	286	THR
1	D	301	VAL
1	D	310	GLU
1	D	337	VAL
1	D	342	MET
1	D	358	ARG
1	D	372	THR
1	D	384	ASP
1	D	387	HIS
1	D	392	ARG
1	D	403	GLU
1	D	427	LYS
1	D	429	LEU

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Mol	Chain	Res	Type
1	D	433	LEU
1	D	439	THR
1	D	470	ARG
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	517	ARG
1	D	520	LEU
1	E	39	LYS
1	E	40	GLN
1	E	43	LYS
1	E	47	THR
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	152	SER
1	E	153	LEU
1	E	174	SER
1	E	177	VAL
1	E	180	CYS
1	E	209	ASP
1	E	213	THR
1	E	215	THR
1	E	219	VAL
1	E	245	LYS
1	E	264	SER
1	E	265	GLU
1	E	306	LEU
1	E	317	LEU
1	E	429	LEU
1	E	448	GLN
1	E	451	VAL

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Mol	Chain	Res	Type
1	E	452	ASN
1	E	454	LEU
1	E	455	HIS
1	E	461	ASP
1	E	473	LEU
1	E	475	GLN
1	E	481	LEU
1	E	493	VAL
1	E	516	LYS
1	E	519	SER
1	E	520	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	HIS
1	C	239	HIS
1	C	293	ASN
1	C	299	HIS
1	C	339	ASN
1	C	448	GLN
1	C	455	HIS
1	C	475	GLN
1	F	30	HIS
1	F	172	GLN
1	F	199	GLN
1	F	253	GLN
1	F	299	HIS
1	F	339	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	422	ASN
1	A	475	GLN
1	A	512	GLN
1	B	30	HIS
1	B	80	ASN
1	B	172	GLN

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Mol	Chain	Res	Type
1	B	230	HIS
1	B	299	HIS
1	B	339	ASN
1	B	422	ASN
1	B	434	ASN
1	B	448	GLN
1	B	455	HIS
1	B	475	GLN
1	B	512	GLN
1	D	104	GLN
1	D	172	GLN
1	D	238	HIS
1	D	253	GLN
1	D	299	HIS
1	D	343	GLN
1	D	527	ASN
1	E	80	ASN
1	E	172	GLN
1	E	199	GLN
1	E	230	HIS
1	E	231	ASN
1	E	239	HIS
1	E	299	HIS
1	E	343	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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%)	0.68	56 (10%) 8 9	39, 81, 153, 270	0
1	B	521/530 (98%)	0.70	57 (10%) 7 9	35, 81, 154, 242	0
1	C	521/530 (98%)	0.50	38 (7%) 18 20	25, 64, 134, 204	0
1	D	521/530 (98%)	0.57	44 (8%) 14 16	23, 63, 139, 258	0
1	E	521/530 (98%)	0.54	33 (6%) 23 27	26, 65, 137, 192	0
1	F	521/530 (98%)	0.59	47 (9%) 12 13	25, 64, 138, 266	0
All	All	3126/3180 (98%)	0.60	275 (8%) 12 14	23, 70, 143, 270	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	459	ILE	8.5
1	F	460	ALA	8.0
1	D	459	ILE	7.6
1	F	383	VAL	7.5
1	E	466	ALA	7.5
1	B	466	ALA	7.2
1	F	470	ARG	6.9
1	D	462	ALA	6.2
1	E	462	ALA	6.1
1	E	44	GLY	6.0
1	B	462	ALA	5.9
1	B	477	TYR	5.9
1	C	466	ALA	5.7
1	A	447	ALA	5.6
1	A	462	ALA	5.6
1	F	469	THR	5.5
1	C	459	ILE	5.3
1	F	451	VAL	5.1
1	D	472	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	468	ALA	5.1
1	F	466	ALA	5.0
1	A	142	GLY	5.0
1	E	383	VAL	5.0
1	D	455	HIS	5.0
1	B	208	PRO	4.9
1	F	462	ALA	4.9
1	B	469	THR	4.9
1	B	77	LEU	4.9
1	E	468	ALA	4.9
1	D	460	ALA	4.8
1	B	473	LEU	4.6
1	F	453	ILE	4.6
1	B	456	ARG	4.6
1	A	417	PHE	4.6
1	A	473	LEU	4.6
1	F	477	TYR	4.5
1	E	460	ALA	4.5
1	C	465	ASP	4.5
1	D	465	ASP	4.5
1	D	469	THR	4.5
1	D	519	SER	4.4
1	F	464	ASP	4.3
1	D	466	ALA	4.3
1	A	317	LEU	4.2
1	A	477	TYR	4.2
1	F	463	GLY	4.2
1	A	225	GLY	4.2
1	B	519	SER	4.2
1	A	451	VAL	4.1
1	A	468	ALA	4.1
1	F	465	ASP	4.1
1	B	465	ASP	4.1
1	F	219	VAL	4.0
1	B	470	ARG	3.9
1	B	291	SER	3.9
1	F	519	SER	3.8
1	F	473	LEU	3.8
1	E	35	ARG	3.8
1	E	36	ALA	3.8
1	D	457	ARG	3.7
1	C	76	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	454	LEU	3.7
1	B	218	ASP	3.7
1	C	462	ALA	3.7
1	A	459	ILE	3.6
1	D	490	ARG	3.6
1	B	468	ALA	3.6
1	A	463	GLY	3.6
1	A	224	LEU	3.5
1	C	77	LEU	3.5
1	A	200	THR	3.4
1	F	282	ALA	3.4
1	F	10	ASP	3.4
1	D	461	ASP	3.4
1	C	469	THR	3.3
1	B	142	GLY	3.3
1	D	287	ILE	3.3
1	B	40	GLN	3.3
1	E	76	GLY	3.2
1	A	218	ASP	3.2
1	B	460	ALA	3.2
1	B	459	ILE	3.2
1	B	11	ILE	3.1
1	E	242	GLY	3.1
1	A	37	VAL	3.1
1	A	284	LEU	3.1
1	F	467	GLU	3.1
1	F	35	ARG	3.1
1	D	456	ARG	3.1
1	A	469	THR	3.1
1	B	518	GLU	3.1
1	A	530	LEU	3.1
1	D	451	VAL	3.1
1	B	464	ASP	3.0
1	A	461	ASP	3.0
1	A	207	GLY	3.0
1	E	183	GLY	3.0
1	C	460	ALA	3.0
1	A	35	ARG	3.0
1	A	241	ALA	3.0
1	A	474	ILE	3.0
1	A	44	GLY	2.9
1	F	33	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	233	THR	2.9
1	A	475	GLN	2.9
1	A	456	ARG	2.9
1	A	457	ARG	2.9
1	A	466	ALA	2.9
1	B	467	GLU	2.9
1	D	473	LEU	2.9
1	E	463	GLY	2.9
1	A	293	ASN	2.9
1	D	471	ALA	2.9
1	C	461	ASP	2.9
1	F	457	ARG	2.9
1	A	154	GLY	2.9
1	D	421	TYR	2.9
1	D	474	ILE	2.9
1	B	452	ASN	2.9
1	E	142	GLY	2.8
1	D	159	ILE	2.8
1	B	140	ASP	2.8
1	B	281	ASP	2.8
1	A	45	LYS	2.8
1	E	155	ALA	2.8
1	A	470	ARG	2.8
1	E	473	LEU	2.8
1	B	448	GLN	2.8
1	A	197	VAL	2.8
1	B	293	ASN	2.8
1	A	471	ALA	2.8
1	E	519	SER	2.7
1	D	383	VAL	2.7
1	A	464	ASP	2.7
1	A	32	GLY	2.7
1	A	287	ILE	2.7
1	F	454	LEU	2.7
1	B	530	LEU	2.7
1	E	459	ILE	2.7
1	D	44	GLY	2.7
1	E	211	ILE	2.6
1	F	44	GLY	2.6
1	D	218	ASP	2.6
1	F	398	ILE	2.6
1	C	108	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	44	GLY	2.6
1	F	450	ALA	2.6
1	B	79	ALA	2.6
1	B	219	VAL	2.6
1	E	212	LYS	2.6
1	B	296	TYR	2.6
1	F	420	ALA	2.6
1	D	31	ALA	2.6
1	F	154	GLY	2.5
1	B	395	ALA	2.5
1	A	34	ALA	2.5
1	C	227	ALA	2.5
1	B	13	THR	2.5
1	B	418	GLY	2.5
1	B	446	GLY	2.5
1	D	491	GLY	2.5
1	C	12	HIS	2.5
1	D	470	ARG	2.5
1	A	79	ALA	2.5
1	E	154	GLY	2.5
1	A	476	GLU	2.5
1	F	421	TYR	2.4
1	C	219	VAL	2.4
1	A	219	VAL	2.4
1	A	216	GLY	2.4
1	D	37	VAL	2.4
1	F	518	GLU	2.4
1	F	492	TYR	2.4
1	B	304	HIS	2.4
1	F	288	VAL	2.4
1	B	269	PHE	2.4
1	F	395	ALA	2.4
1	B	292	ALA	2.4
1	E	469	THR	2.4
1	C	492	TYR	2.4
1	D	151	ALA	2.4
1	C	35	ARG	2.4
1	A	465	ASP	2.3
1	B	461	ASP	2.3
1	C	473	LEU	2.3
1	C	383	VAL	2.3
1	A	11	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	10	ASP	2.3
1	E	80	ASN	2.3
1	C	226	GLY	2.3
1	C	457	ARG	2.3
1	C	472	ARG	2.3
1	F	458	THR	2.3
1	B	311	PHE	2.3
1	E	221	PHE	2.3
1	F	76	GLY	2.3
1	B	225	GLY	2.3
1	D	76	GLY	2.3
1	C	197	VAL	2.3
1	E	156	TYR	2.3
1	A	467	GLU	2.3
1	A	77	LEU	2.3
1	F	461	ASP	2.3
1	F	479	ASP	2.3
1	B	80	ASN	2.3
1	B	286	THR	2.3
1	D	492	TYR	2.3
1	C	456	ARG	2.3
1	C	530	LEU	2.3
1	B	383	VAL	2.3
1	D	395	ALA	2.3
1	E	186	TYR	2.3
1	D	417	PHE	2.3
1	E	465	ASP	2.3
1	D	419	GLY	2.2
1	B	450	ALA	2.2
1	C	40	GLN	2.2
1	D	284	LEU	2.2
1	C	431	ALA	2.2
1	B	447	ALA	2.2
1	E	464	ASP	2.2
1	A	383	VAL	2.2
1	D	475	GLN	2.2
1	F	468	ALA	2.2
1	B	42	ALA	2.2
1	E	292	ALA	2.2
1	C	421	TYR	2.2
1	D	463	GLY	2.2
1	C	153	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	472	ARG	2.2
1	D	282	ALA	2.2
1	A	428	HIS	2.2
1	C	200	THR	2.2
1	F	293	ASN	2.1
1	C	72	SER	2.1
1	B	282	ALA	2.1
1	B	431	ALA	2.1
1	B	82	PRO	2.1
1	A	269	PHE	2.1
1	E	247	ALA	2.1
1	F	382	GLY	2.1
1	D	391	ILE	2.1
1	A	214	VAL	2.1
1	C	10	ASP	2.1
1	F	490	ARG	2.1
1	C	395	ALA	2.1
1	F	155	ALA	2.1
1	C	43	LYS	2.1
1	A	391	ILE	2.1
1	A	291	SER	2.1
1	F	75	PHE	2.1
1	D	35	ARG	2.1
1	D	118	GLY	2.1
1	A	217	GLU	2.1
1	E	395	ALA	2.1
1	B	151	ALA	2.0
1	C	222	GLU	2.0
1	C	118	GLY	2.0
1	E	32	GLY	2.0
1	C	42	ALA	2.0
1	B	397	LEU	2.0
1	E	153	LEU	2.0
1	E	224	LEU	2.0
1	A	156	TYR	2.0
1	F	291	SER	2.0
1	F	455	HIS	2.0
1	C	71	ARG	2.0
1	B	457	ARG	2.0
1	F	159	ILE	2.0
1	D	216	GLY	2.0
1	C	158	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	530	LEU	2.0
1	D	46	LEU	2.0
1	C	186	TYR	2.0
1	B	156	TYR	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.