Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 07:57 PM EST

PDB ID	:	4JK1
Title	:	X-ray crystal structure of Escherichia coli sigma70 holoenzyme in complex with Guanosine tetraphosphate (ppGpp)
Authors	:	Murakami, K.S.
Deposited on	:	2013-03-09
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

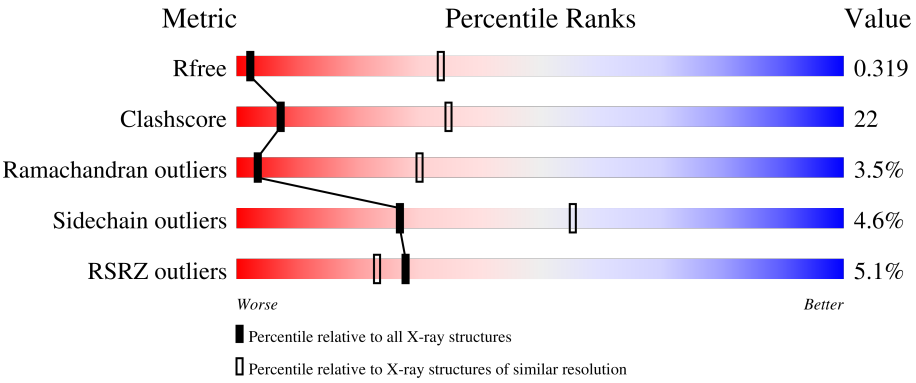
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 <=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	329	4% 64% 31%
1	B	329	4% 39% 26% 33%
1	F	329	5% 48% 20% 30%
1	G	329	4% 39% 26% 34%
2	C	1342	3% 55% 39% 5%

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Mol	Chain	Length	Quality of chain
2	H	1342	6% 57% 38% 5%
3	D	1407	3% 43% 35% 5% 18%
3	I	1407	5% 44% 34% 18%
4	E	91	% 56% 38%
4	J	91	5% 45% 36% 16%
5	X	613	7% 51% 30% 16%
5	Y	613	5% 44% 28% 25%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 56126 atoms, of which 11 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 Escherichia coli RNA polymerase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called Escherichia coli RNA polymerase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called Escherichia coli RNA polymerase beta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

- Molecule 4 is a protein called Escherichia coli RNA polymerase omega subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

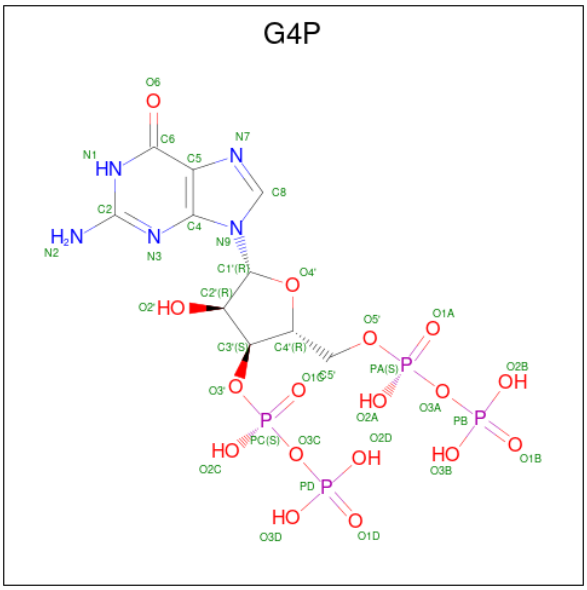
- Molecule 5 is a protein called Escherichia coli RNA polymerase sigma70 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	I	2	Total	Zn	0	0
			2	2		

- Molecule 7 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



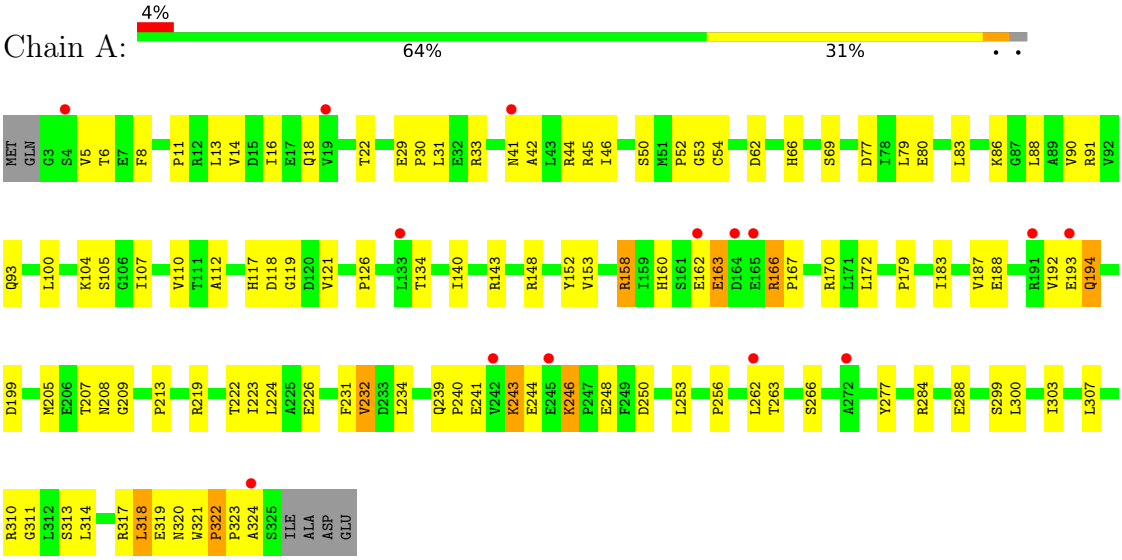
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	D	1	Total	C	H	N	O	P	0	0
			47	10	11	5	17	4		

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.

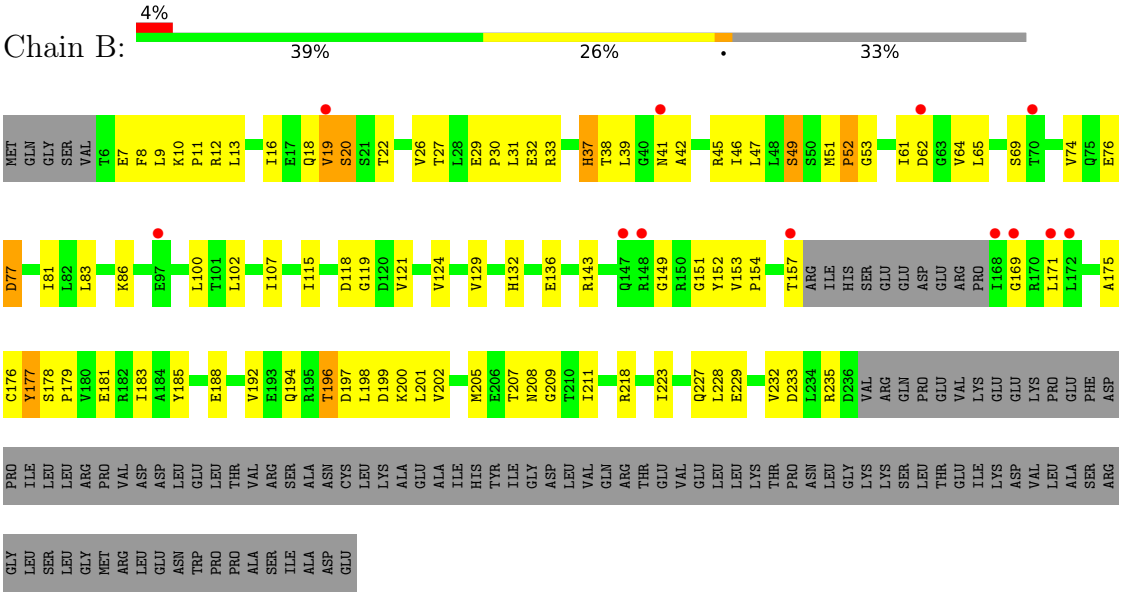
• Molecule 1: Escherichia coli RNA polymerase alpha subunit

Chain A:

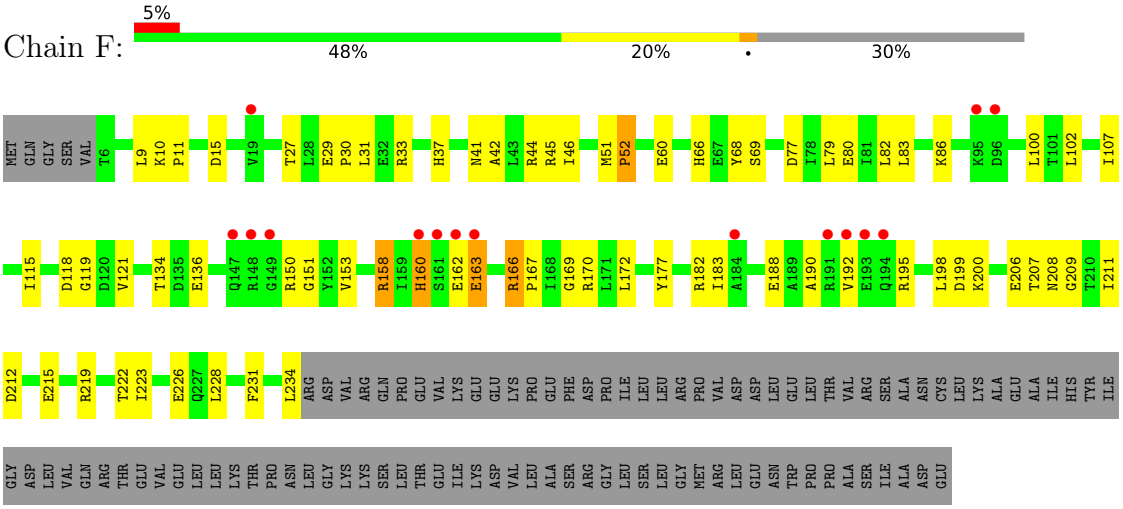


• Molecule 1: Escherichia coli RNA polymerase alpha subunit

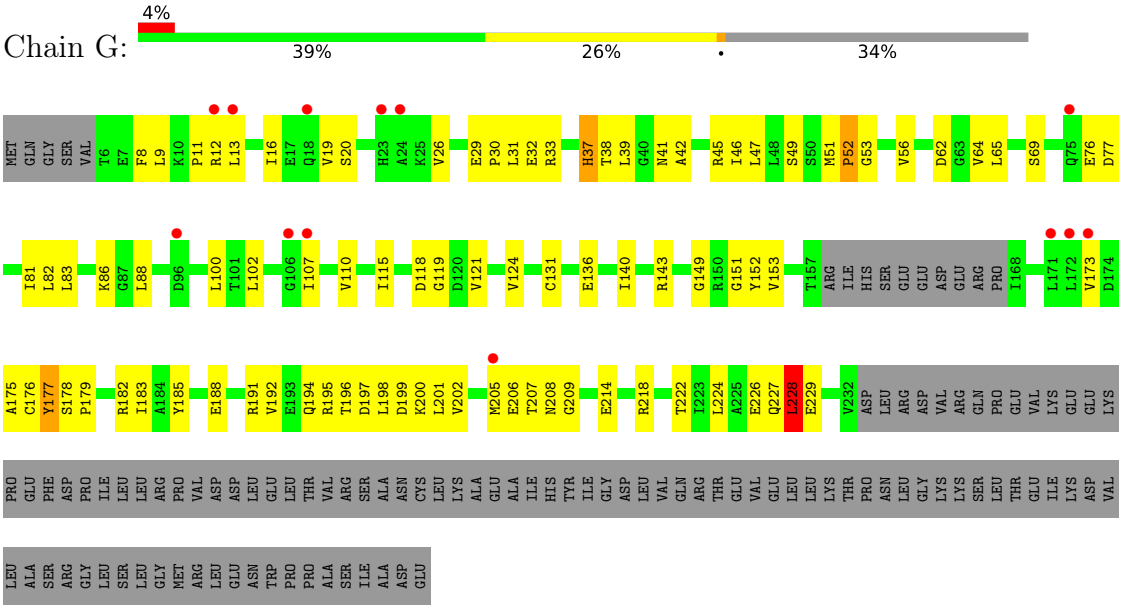
Chain B:



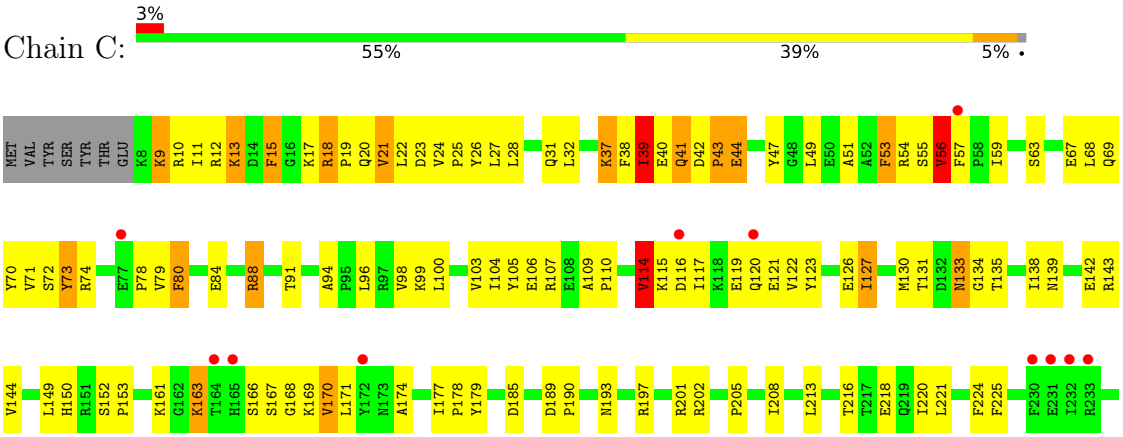
• Molecule 1: Escherichia coli RNA polymerase alpha subunit

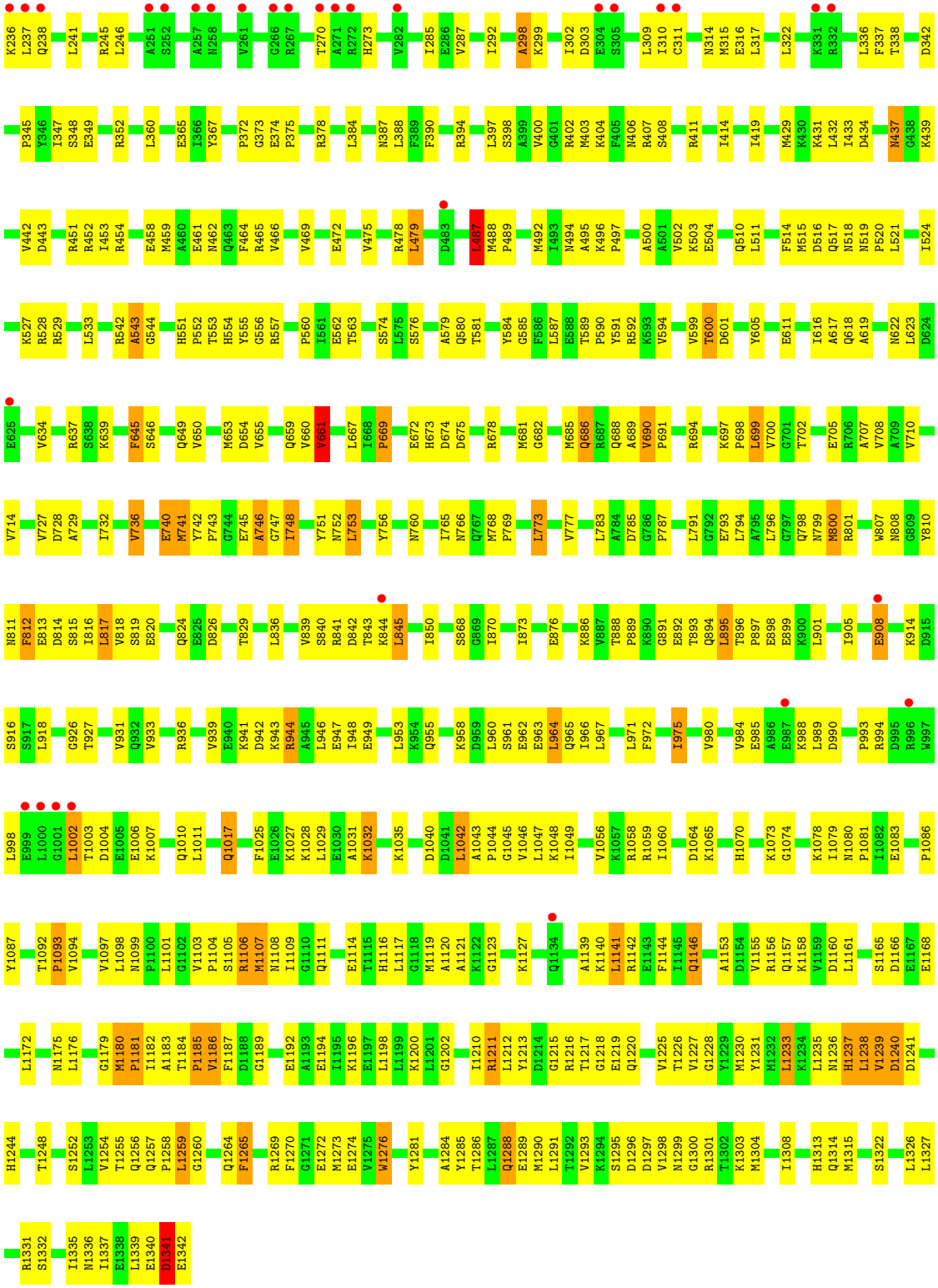


• Molecule 1: Escherichia coli RNA polymerase alpha subunit



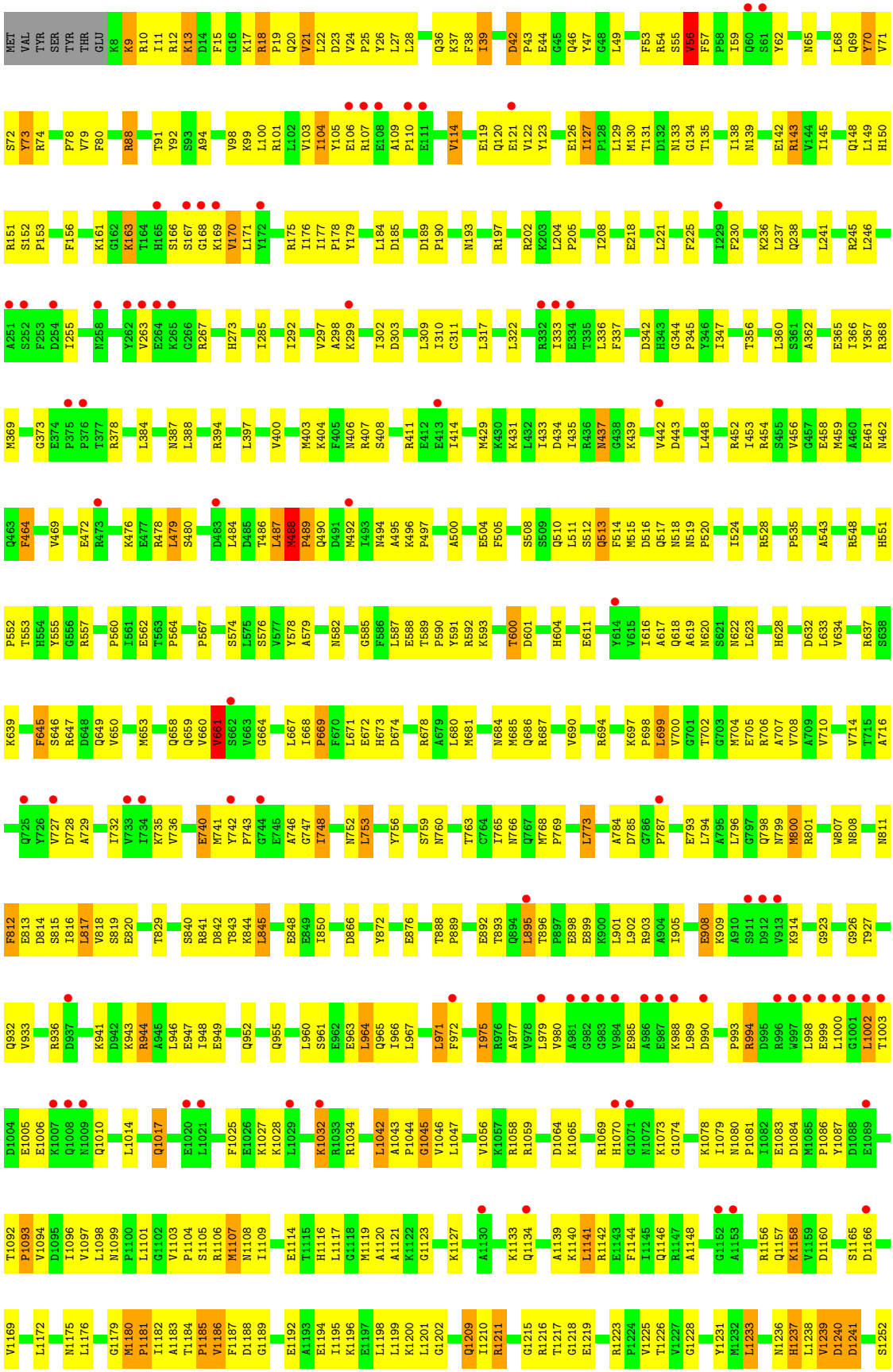
• Molecule 2: Escherichia coli RNA polymerase beta subunit





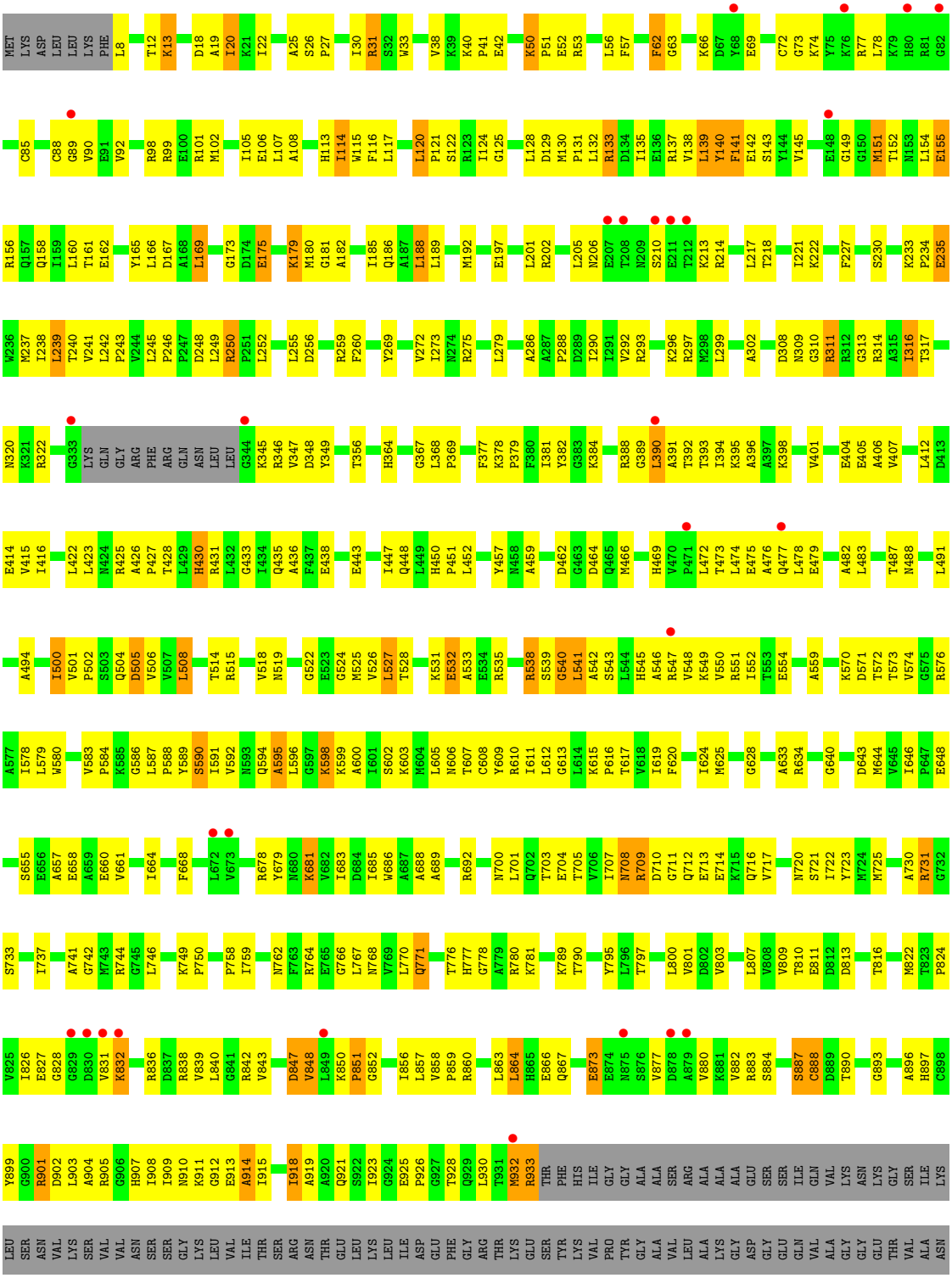
• Molecule 2: Escherichia coli RNA polymerase beta subunit

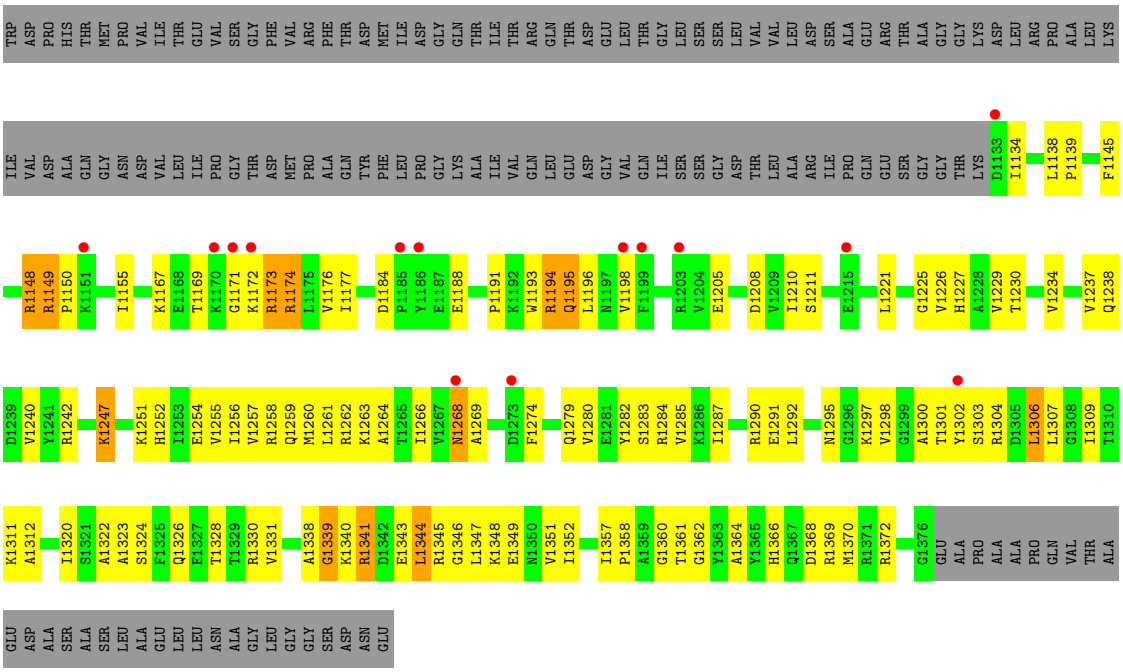
Chain H:



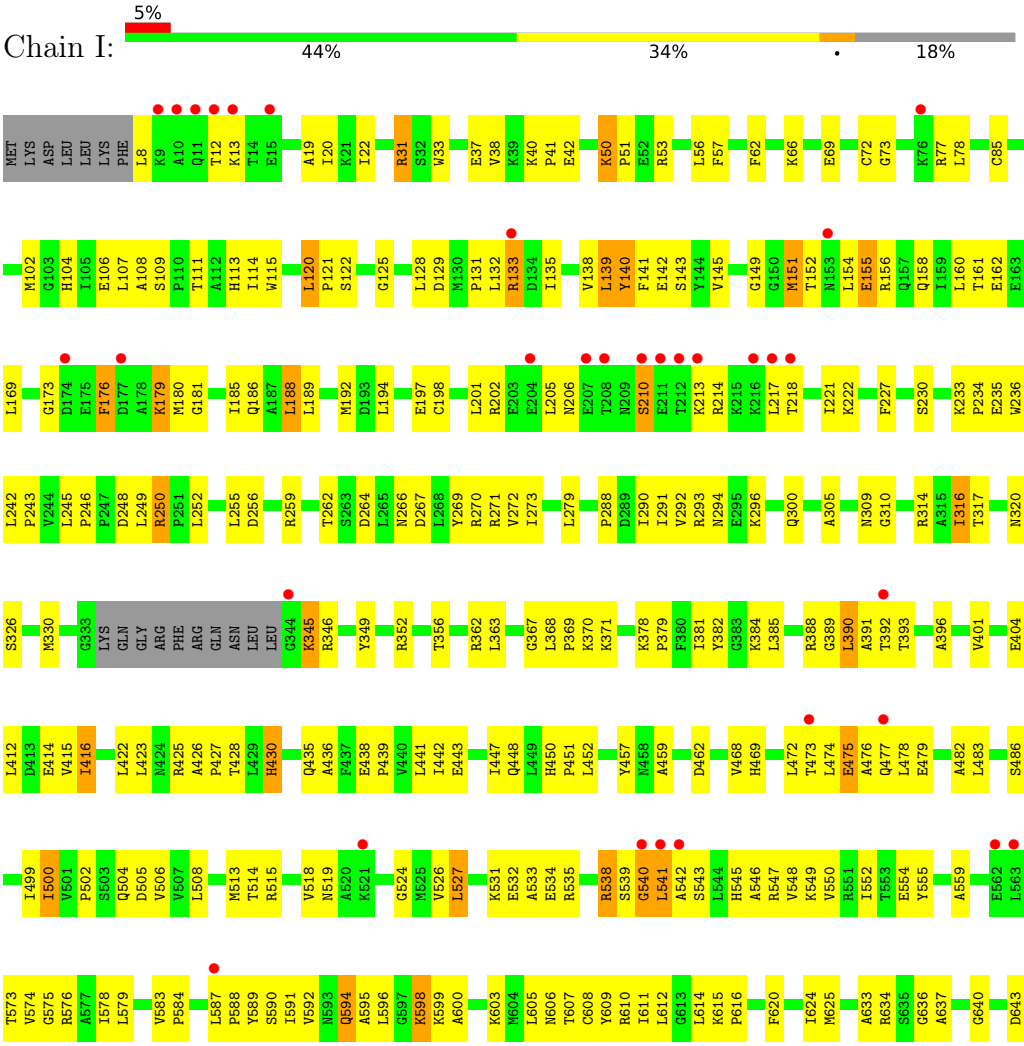
• Molecule 3: Escherichia coli RNA polymerase beta' subunit

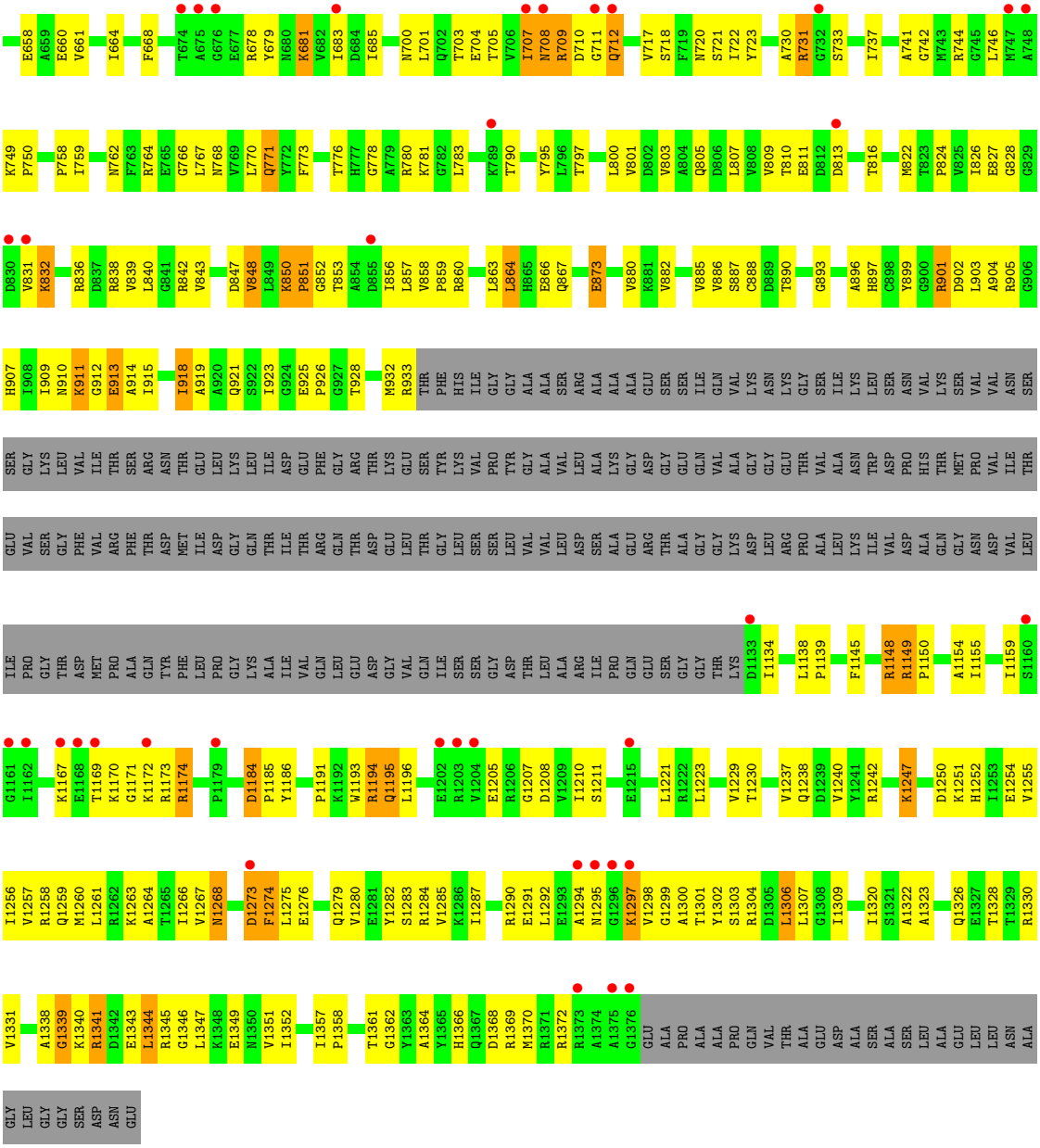
Chain D:





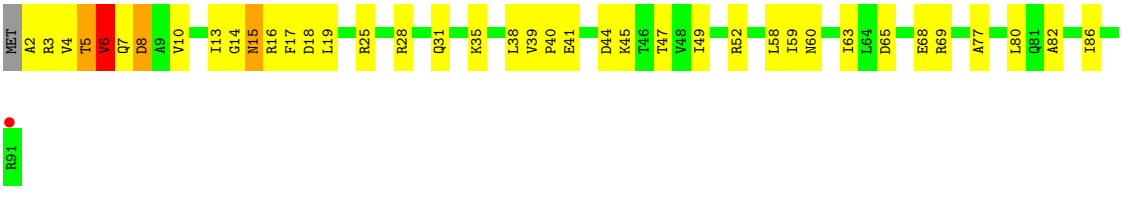
• Molecule 3: Escherichia coli RNA polymerase beta' subunit





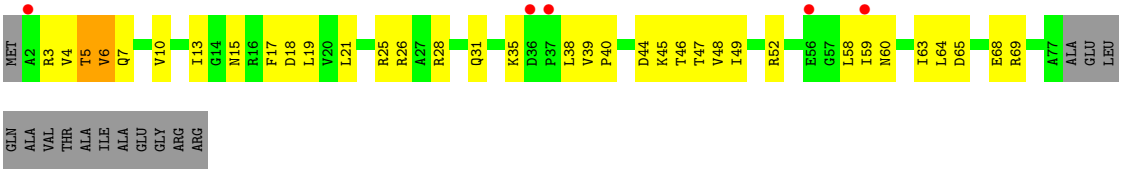
• Molecule 4: Escherichia coli RNA polymerase omega subunit

Chain E:



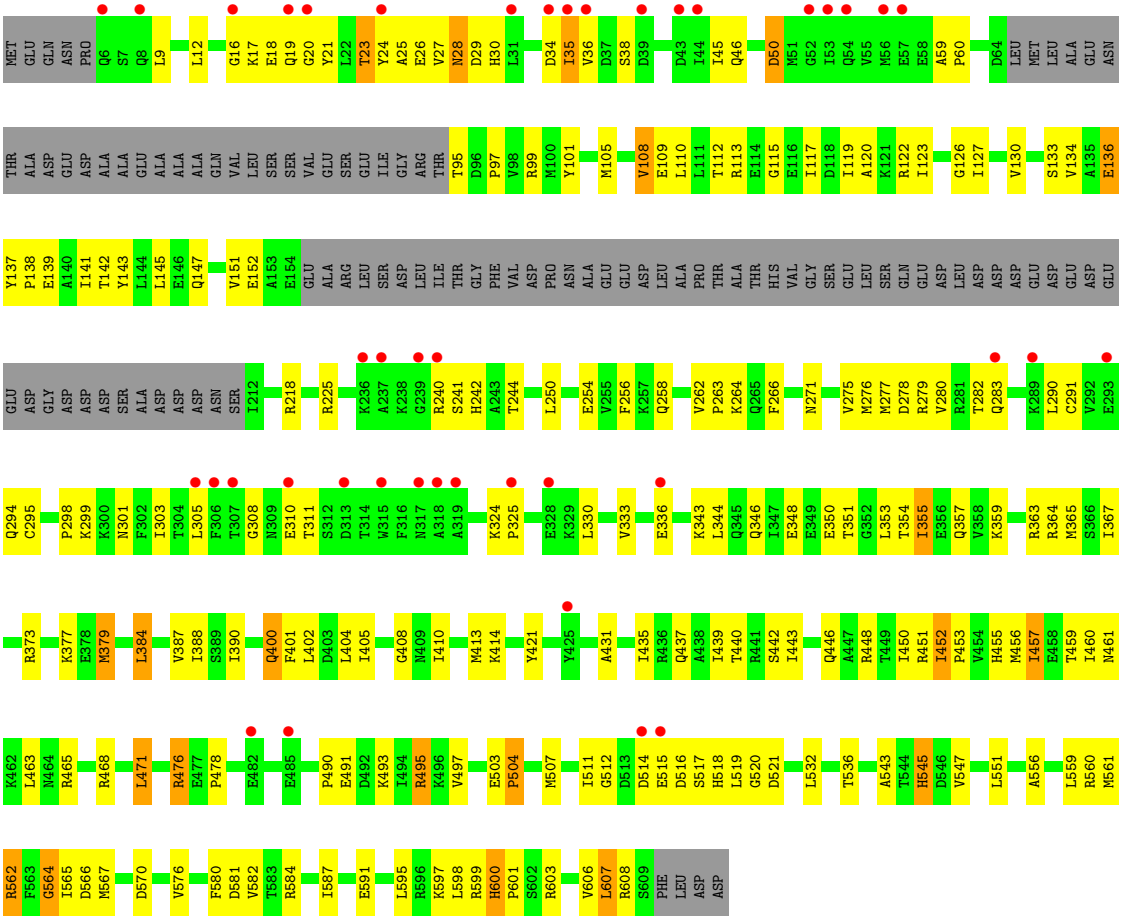
• Molecule 4: Escherichia coli RNA polymerase omega subunit

Chain J:



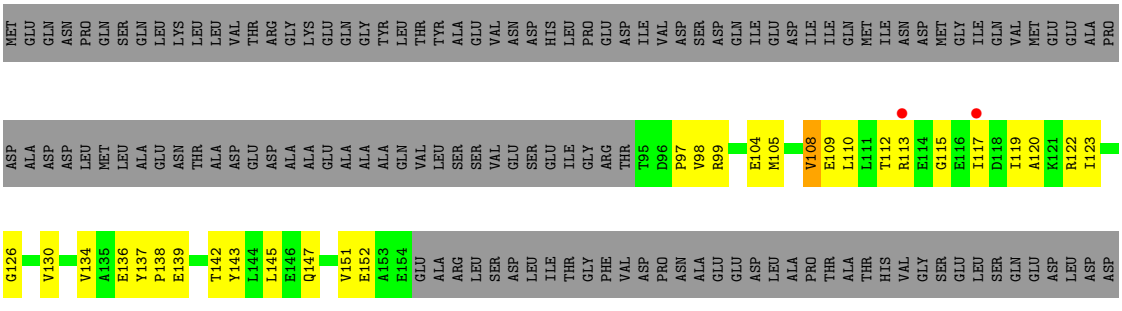
• Molecule 5: Escherichia coli RNA polymerase sigma70 subunit

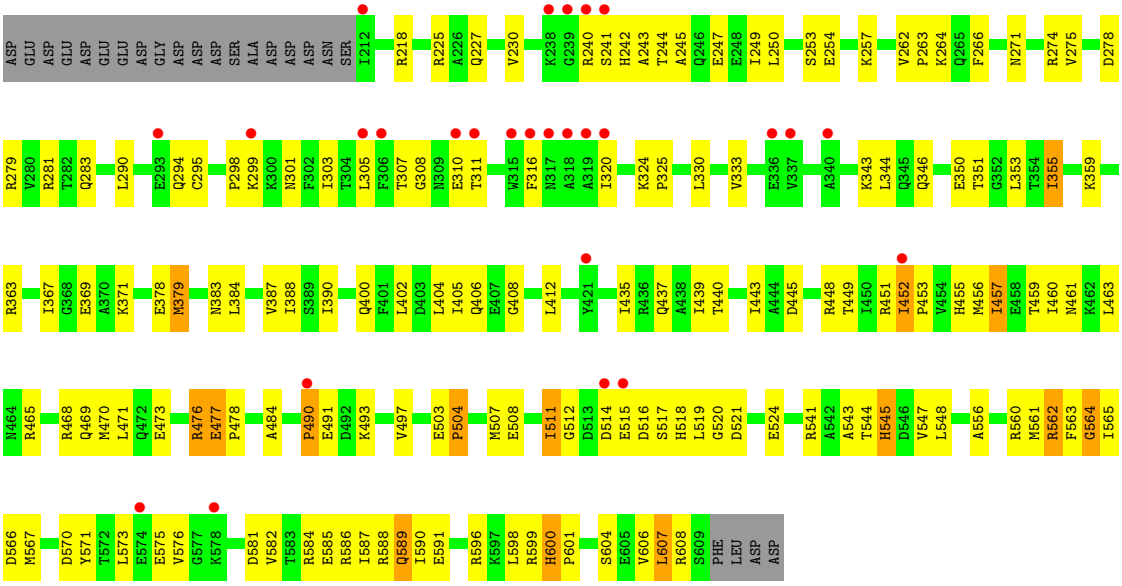
Chain X:



• Molecule 5: Escherichia coli RNA polymerase sigma70 subunit

Chain Y:




ASP GLU ASP GLU ASP GLU GLU ASP GLY ASP ASP ASP SER ALA ASP ASP ASP ASN SER I212 R218 R225 A226 Q227 V230 K238 G239 R240 S241 H242 A243 T244 A245 Q246 E247 E248 I249 L250 S253 E254 K257 V262 P263 K264 Q265 F266 N271 R274 V275 D278
R279 V280 R281 T282 Q283 L290 E293 Q294 C295 P298 K299 K300 N301 F302 I303 T304 L305 F306 T307 G308 N309 E310 T311 W315 F316 N317 A318 A319 I320 K324 P325 L330 V333 E336 V337 A340 K343 L344 Q345 Q346 E350 T351 G352 L353 T354 I355 K359
R363 I367 G368 E369 A370 K371 E378 M379 N383 L384 V387 I388 S389 I390 Q400 F401 L402 D403 L404 I405 Q406 E407 G408 L412 Y421 I435 R436 Q437 A438 I439 T440 I443 A444 D445 R448 T449 I450 R451 I452 P453 V454 H455 M456 I457 E458 T459 I460 N461 K462 L463
N464 R465 R468 Q469 M470 L471 Q472 E473 R476 E477 P478 A484 P490 E491 D492 K493 V497 E503 P504 M507 E508 I511 G512 D513 D514 E515 D516 S517 H518 L519 G520 D521 E524 R541 A542 A543 T544 H545 D546 V547 L548 A556 R560 M561 R562 F563 G564 I565
D566 M567 D570 Y571 T572 L573 E574 E575 V576 G577 K578 D581 V582 T583 R584 E585 R586 I587 R588 Q589 I590 E591 R596 K597 L598 R599 H600 P601 S604 E605 V606 L607 R608 S609 PHE LEU ASP ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	184.57Å 203.82Å 307.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.90 29.84 – 3.85	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.84-3.90) 82.4 (29.84-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.252 , 0.320 0.253 , 0.319	Depositor DCC
R_{free} test set	4799 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	124.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	56126	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, G4P

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	0.19	0/2548	0.37	0/3454
1	B	0.19	0/1725	0.38	0/2337
1	F	0.19	0/1797	0.38	0/2436
1	G	0.19	0/1690	0.37	0/2290
2	C	0.20	0/10690	0.37	0/14423
2	H	0.20	0/10690	0.37	0/14423
3	D	0.20	0/9198	0.38	0/12413
3	I	0.20	0/9198	0.38	0/12413
4	E	0.19	0/710	0.38	0/956
4	J	0.19	0/607	0.37	0/817
5	X	0.20	0/4253	0.36	0/5719
5	Y	0.20	0/3783	0.35	0/5083
All	All	0.20	0/56889	0.37	0/76764

There are no bond length outliers.

There are no bond angle outliers.

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	2514	0	2566	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1738	89	0
1	F	1775	0	1800	62	0
1	G	1671	0	1706	84	0
2	C	10523	0	10546	517	0
2	H	10523	0	10546	501	0
3	D	9060	0	9257	530	0
3	I	9060	0	9257	511	0
4	E	708	0	719	40	0
4	J	605	0	612	32	0
5	X	4198	0	4250	169	0
5	Y	3732	0	3809	137	0
6	D	2	0	0	0	0
6	I	2	0	0	0	0
7	D	36	11	11	2	0
All	All	56115	11	56817	2538	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 22.

All (2538) 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)
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.28	1.14
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.29	1.11
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.23	1.11
2:H:488:MET:HB2	2:H:490:GLN:H	1.14	1.05
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.38	1.02
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.42	1.01
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.41	1.01
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.43	1.00
1:B:12:ARG:H	1:B:30:PRO:HG2	1.27	0.99
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.42	0.98
2:C:54:ARG:H	2:C:55:SER:HB2	1.26	0.97
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.44	0.97
2:H:54:ARG:H	2:H:55:SER:HB2	1.25	0.97
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.44	0.96
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.47	0.94
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.50	0.94
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.47	0.94
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.48	0.93
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.50	0.92
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.50	0.92
2:H:488:MET:HB2	2:H:490:GLN:N	1.85	0.92
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.52	0.91
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.52	0.91
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.53	0.91
2:C:163:LYS:H	2:C:163:LYS:HD3	1.33	0.91
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.51	0.91
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	1.52	0.90
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.52	0.89
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.52	0.89
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.39	0.88
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.55	0.88
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.51	0.88
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.56	0.88
3:D:546:ALA:H	3:D:547:ARG:HA	1.37	0.88
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.57	0.87
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.55	0.87
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.04	0.87
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.55	0.86
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.58	0.86
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.04	0.86
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.57	0.86
3:I:546:ALA:H	3:I:547:ARG:HA	1.40	0.86
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.40	0.86
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.58	0.85
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.56	0.85
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.58	0.85
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.56	0.85
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.05	0.85
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.56	0.85
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.59	0.84
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.59	0.84
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.41	0.84
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.59	0.83
2:H:1101:LEU:HD21	3:I:508:LEU:HD12	1.60	0.83
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.60	0.83
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.58	0.83
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.60	0.82
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.60	0.82
3:D:643:ASP:O	3:D:720:ASN:ND2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:908:GLU:HG2	2:H:909:LYS:H	1.44	0.81
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.59	0.81
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.46	0.81
2:C:1101:LEU:HD21	3:D:508:LEU:HD12	1.62	0.81
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.45	0.81
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.62	0.81
2:C:131:THR:HG21	2:C:135:THR:HG22	1.62	0.81
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.62	0.81
4:E:5:THR:HA	4:E:6:VAL:CB	2.09	0.81
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.43	0.81
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.61	0.81
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.61	0.81
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.63	0.81
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.62	0.81
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.63	0.80
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.61	0.80
3:D:541:LEU:HD23	3:D:541:LEU:H	1.46	0.80
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.62	0.80
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.64	0.80
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.06	0.80
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.64	0.80
2:H:163:LYS:H	2:H:163:LYS:HD3	1.46	0.80
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.64	0.79
5:X:240:ARG:HD3	5:X:244:THR:HB	1.64	0.79
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.64	0.79
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.62	0.79
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.65	0.79
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.47	0.78
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.65	0.78
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.46	0.78
3:I:541:LEU:HD23	3:I:541:LEU:H	1.48	0.78
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.64	0.78
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.66	0.78
3:D:828:GLY:HA2	3:D:832:LYS:H	1.47	0.78
3:D:316:ILE:HG23	3:D:317:THR:H	1.49	0.78
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.48	0.78
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.66	0.77
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.19	0.77
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.66	0.77
5:X:35:ILE:HG13	5:X:36:VAL:H	1.47	0.77
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.66	0.77
2:C:800:MET:HE2	2:C:800:MET:HA	1.66	0.77
3:I:643:ASP:O	3:I:720:ASN:ND2	2.14	0.77
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.66	0.77
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	1.65	0.77
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.67	0.77
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.67	0.76
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.68	0.76
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.19	0.76
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.68	0.76
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.66	0.76
2:H:54:ARG:N	2:H:55:SER:HB2	2.00	0.76
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.66	0.76
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.65	0.76
3:D:230:SER:HB2	3:D:1339:GLY:H	1.51	0.76
2:C:131:THR:CG2	2:C:135:THR:HG22	2.16	0.75
4:J:5:THR:HA	4:J:6:VAL:CB	2.16	0.75
2:C:54:ARG:N	2:C:55:SER:HB2	2.01	0.75
3:D:1149:ARG:HD3	3:D:1149:ARG:H	1.50	0.75
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.67	0.75
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.69	0.75
2:H:800:MET:HE2	2:H:800:MET:HA	1.68	0.75
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.69	0.74
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.69	0.74
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.69	0.74
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.68	0.74
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.70	0.74
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.69	0.74
2:H:131:THR:HG21	2:H:135:THR:HG22	1.70	0.74
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.69	0.74
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.71	0.73
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.53	0.73
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.70	0.73
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.70	0.73
2:H:131:THR:CG2	2:H:135:THR:HG22	2.18	0.73
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.70	0.73
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.71	0.73
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.69	0.73
2:C:403:MET:HG3	2:C:414:ILE:HB	1.71	0.73
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.70	0.73
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.51	0.73
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.69	0.73
3:I:850:LYS:O	3:I:852:GLY:N	2.21	0.73
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.71	0.73
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.23	0.73
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.70	0.72
5:Y:448:ARG:HD2	5:Y:452:ILE:HD12	1.70	0.72
3:I:230:SER:HB2	3:I:1339:GLY:H	1.52	0.72
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.71	0.72
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.54	0.72
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.70	0.72
4:E:5:THR:HA	4:E:6:VAL:HB	1.71	0.72
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.24	0.72
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.25	0.72
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.70	0.72
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.53	0.72
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.71	0.71
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.20	0.71
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.72	0.71
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.73	0.71
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.71	0.71
2:C:309:LEU:HD23	2:C:309:LEU:H	1.55	0.71
3:D:546:ALA:H	3:D:547:ARG:CA	2.04	0.71
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.54	0.71
1:B:49:SER:HA	1:B:151:GLY:HA2	1.73	0.71
1:G:45:ARG:O	3:I:538:ARG:NH2	2.23	0.71
2:H:660:VAL:HG22	2:H:661:VAL:H	1.54	0.71
3:I:828:GLY:HA2	3:I:832:LYS:H	1.56	0.71
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.71	0.71
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.72	0.71
1:G:12:ARG:H	1:G:30:PRO:HG2	1.55	0.71
2:C:660:VAL:HG22	2:C:661:VAL:H	1.56	0.71
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.73	0.71
3:D:546:ALA:N	3:D:547:ARG:HA	2.05	0.71
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.71	0.71
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.55	0.71
3:D:828:GLY:HA2	3:D:832:LYS:N	2.06	0.70
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.24	0.70
4:E:5:THR:HA	4:E:6:VAL:HG12	1.72	0.70
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.24	0.70
2:H:142:GLU:HG2	2:H:515:MET:SD	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:690:VAL:HG22	2:C:691:PRO:HD2	1.73	0.70
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.73	0.70
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.56	0.70
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.72	0.70
3:D:850:LYS:O	3:D:852:GLY:N	2.25	0.70
2:C:37:LYS:HA	2:C:37:LYS:HE3	1.74	0.70
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.74	0.70
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.74	0.70
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.56	0.70
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.73	0.70
5:X:511:ILE:HG23	5:X:512:GLY:H	1.57	0.70
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.27	0.70
3:I:546:ALA:N	3:I:547:ARG:HA	2.06	0.70
2:C:127:ILE:H	2:C:127:ILE:HD13	1.55	0.69
1:G:65:LEU:HD23	1:G:65:LEU:H	1.56	0.69
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.73	0.69
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.20	0.69
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.73	0.69
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.75	0.69
2:H:127:ILE:H	2:H:127:ILE:HD13	1.56	0.69
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.73	0.69
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.73	0.69
2:H:600:THR:HG22	2:H:601:ASP:H	1.56	0.69
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.57	0.69
2:C:54:ARG:H	2:C:55:SER:CB	2.04	0.69
2:C:1042:LEU:HD13	2:C:1042:LEU:H	1.58	0.69
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.73	0.69
5:X:108:VAL:HG23	5:X:109:GLU:H	1.58	0.69
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.73	0.69
2:H:309:LEU:HD23	2:H:309:LEU:H	1.55	0.69
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.75	0.69
2:H:1042:LEU:HD13	2:H:1042:LEU:H	1.58	0.69
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.75	0.69
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.27	0.69
2:C:170:VAL:HG23	2:C:171:LEU:H	1.57	0.69
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.22	0.69
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.92	0.69
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.72	0.68
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.24	0.68
3:I:128:LEU:HD11	3:I:188:LEU:HD22	1.75	0.68
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.75	0.68
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.58	0.68
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.56	0.68
2:H:487:LEU:CB	2:H:488:MET:HA	2.23	0.68
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.23	0.68
3:I:828:GLY:HA2	3:I:832:LYS:N	2.08	0.68
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.09	0.68
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.76	0.68
5:X:139:GLU:HA	5:X:142:THR:HG22	1.76	0.68
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.76	0.68
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.76	0.68
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.76	0.68
2:H:403:MET:HG3	2:H:414:ILE:HB	1.75	0.68
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.23	0.68
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.58	0.68
3:D:422:LEU:HA	3:D:436:ALA:HA	1.75	0.68
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.94	0.68
4:E:5:THR:HA	4:E:6:VAL:CG1	2.23	0.68
3:I:546:ALA:H	3:I:547:ARG:CA	2.06	0.68
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.42	0.67
2:H:54:ARG:H	2:H:55:SER:CB	2.02	0.67
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.77	0.67
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.27	0.67
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.77	0.67
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.76	0.67
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.25	0.67
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.77	0.67
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.29	0.67
2:H:487:LEU:HB3	2:H:488:MET:HA	1.76	0.67
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.75	0.67
2:C:845:LEU:HD13	2:C:845:LEU:H	1.58	0.67
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.59	0.67
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.24	0.67
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.76	0.67
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.58	0.67
1:B:45:ARG:O	3:D:538:ARG:NH2	2.28	0.67
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.76	0.67
5:X:112:THR:HG22	5:X:113:ARG:H	1.59	0.67
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.77	0.67
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:5:THR:HB	4:E:7:GLN:HB2	1.76	0.67
5:X:476:ARG:H	5:X:476:ARG:HD2	1.60	0.67
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.25	0.67
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.77	0.67
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.28	0.67
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.77	0.67
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.75	0.67
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.28	0.66
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.77	0.66
2:H:845:LEU:HD13	2:H:845:LEU:H	1.58	0.66
2:H:55:SER:CB	2:H:56:VAL:HG22	2.26	0.66
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.77	0.66
2:C:600:THR:HG22	2:C:601:ASP:H	1.60	0.66
3:D:259:ARG:HH21	5:X:504:PRO:HB2	1.60	0.66
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.77	0.66
2:H:131:THR:HG23	2:H:133:ASN:H	1.59	0.66
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.24	0.66
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.78	0.66
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.75	0.66
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.78	0.66
2:H:170:VAL:HG23	2:H:171:LEU:H	1.61	0.66
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.31	0.66
5:X:457:ILE:O	5:X:461:ASN:ND2	2.28	0.66
2:H:484:LEU:H	2:H:484:LEU:HD22	1.60	0.66
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.24	0.66
3:D:836:ARG:HH12	3:D:839:VAL:HB	1.60	0.66
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.78	0.66
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.78	0.66
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.77	0.66
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.78	0.66
3:D:822:MET:SD	3:D:838:ARG:NH1	2.69	0.66
3:I:133:ARG:O	3:I:133:ARG:NH2	2.27	0.66
1:B:29:GLU:HA	1:B:200:LYS:CB	2.26	0.66
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.78	0.66
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.78	0.66
2:H:1252:SER:OG	2:H:1255:THR:O	2.14	0.66
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.78	0.65
2:H:241:LEU:HD22	2:H:285:ILE:HD13	1.79	0.65
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.78	0.65
2:C:55:SER:CB	2:C:56:VAL:HG22	2.26	0.65
2:H:488:MET:HE3	2:H:489:PRO:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:488:MET:H	2:H:489:PRO:HA	1.60	0.65
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.28	0.65
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.77	0.65
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.79	0.65
3:I:422:LEU:HA	3:I:436:ALA:HA	1.79	0.65
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.61	0.65
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.29	0.65
2:C:1288:GLN:HA	2:C:1288:GLN:HE21	1.61	0.65
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.77	0.65
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.78	0.65
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.27	0.65
3:I:145:VAL:HG22	3:I:180:MET:SD	2.37	0.65
4:J:5:THR:CA	4:J:6:VAL:HB	2.27	0.65
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.77	0.65
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.62	0.65
1:G:49:SER:OG	3:I:538:ARG:NH2	2.30	0.65
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.78	0.65
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.79	0.65
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.12	0.65
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.79	0.65
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.78	0.64
2:C:106:GLU:N	2:C:107:ARG:HA	2.11	0.64
2:C:699:LEU:H	2:C:799:ASN:HD21	1.45	0.64
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.63	0.64
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.79	0.64
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.79	0.64
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.62	0.64
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.62	0.64
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.12	0.64
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.61	0.64
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.63	0.64
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.31	0.64
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.79	0.64
3:D:590:SER:O	3:D:594:GLN:N	2.31	0.64
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.61	0.64
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.29	0.64
2:C:488:MET:N	2:C:489:PRO:HD3	2.13	0.64
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.80	0.64
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.33	0.64
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.32	0.64
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.80	0.64
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.80	0.64
2:C:20:GLN:O	2:C:22:LEU:N	2.31	0.64
2:C:131:THR:HG23	2:C:133:ASN:H	1.63	0.64
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.78	0.63
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.81	0.63
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.13	0.63
5:Y:476:ARG:H	5:Y:476:ARG:HD2	1.63	0.63
2:C:714:VAL:HG23	2:C:787:PRO:HD2	1.78	0.63
3:D:438:GLU:OE1	4:E:3:ARG:NH1	2.32	0.63
1:F:68:TYR:HB3	2:H:756:TYR:CD1	2.33	0.63
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.79	0.63
3:D:128:LEU:HA	3:D:192:MET:HE1	1.79	0.63
1:G:191:ARG:HH12	3:I:443:GLU:HG2	1.64	0.63
4:J:5:THR:HA	4:J:6:VAL:HB	1.78	0.63
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.31	0.63
2:H:1288:GLN:HA	2:H:1288:GLN:HE21	1.61	0.63
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.31	0.63
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.81	0.63
3:D:932:MET:O	3:D:933:ARG:HG3	1.97	0.63
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.13	0.63
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.80	0.63
2:H:21:VAL:HG13	2:H:22:LEU:H	1.64	0.63
3:I:151:MET:SD	3:I:151:MET:N	2.71	0.63
2:C:189:ASP:OD1	2:C:193:ASN:N	2.25	0.63
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.29	0.63
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.80	0.63
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.46	0.63
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.81	0.63
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.31	0.63
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.80	0.63
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.80	0.62
2:C:1239:VAL:O	2:C:1241:ASP:N	2.31	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.31	0.62
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.81	0.62
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.81	0.62
3:I:644:MET:O	3:I:764:ARG:NH1	2.32	0.62
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.34	0.62
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.14	0.62
2:H:528:ARG:NH2	2:H:576:SER:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.81	0.62
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.29	0.62
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.62
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.63	0.62
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.80	0.62
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.81	0.62
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.81	0.62
3:I:720:ASN:O	3:I:722:ILE:N	2.32	0.62
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.81	0.62
2:H:106:GLU:N	2:H:107:ARG:HA	2.13	0.62
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.14	0.62
3:I:1287:ILE:HG22	3:I:1290:ARG:HE	1.64	0.62
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.29	0.62
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.81	0.62
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.82	0.62
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.81	0.62
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.29	0.62
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.64	0.62
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.81	0.62
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.64	0.62
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.82	0.62
4:J:5:THR:HA	4:J:6:VAL:HG12	1.82	0.62
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.24	0.62
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.64	0.62
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.24	0.62
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.32	0.62
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.64	0.61
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.82	0.61
2:H:487:LEU:HB3	2:H:488:MET:CA	2.29	0.61
3:D:252:LEU:HD23	3:D:252:LEU:H	1.66	0.61
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.30	0.61
3:D:588:PRO:HG2	3:D:591:ILE:HD11	1.82	0.61
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.80	0.61
2:H:800:MET:HA	2:H:800:MET:CE	2.30	0.61
3:I:139:LEU:HD13	3:I:140:TYR:N	2.15	0.61
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.65	0.61
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.30	0.61
3:D:151:MET:SD	3:D:151:MET:N	2.73	0.61
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.64	0.61
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.33	0.61
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.81	0.61
2:H:1237:HIS:O	2:H:1238:LEU:HG	2.00	0.61
3:I:213:LYS:O	3:I:217:LEU:HG	2.00	0.61
3:I:827:GLU:O	3:I:831:VAL:HG12	1.99	0.61
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.81	0.61
1:B:227:GLN:O	1:B:228:LEU:HG	1.99	0.61
2:C:699:LEU:HD12	2:C:1121:ALA:HB1	1.83	0.61
3:D:77:ARG:HG3	3:D:78:LEU:H	1.64	0.61
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.81	0.61
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.65	0.61
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.66	0.61
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.82	0.61
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.65	0.61
3:I:1341:ARG:NH2	3:I:1343:GLU:OE1	2.34	0.61
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.66	0.61
5:X:503:GLU:N	5:X:504:PRO:HA	2.15	0.61
2:H:91:THR:HG22	2:H:139:ASN:H	1.65	0.61
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.16	0.61
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.36	0.61
2:C:1237:HIS:O	2:C:1238:LEU:HG	2.00	0.61
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.82	0.61
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.83	0.61
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.83	0.61
3:D:1297:LYS:HA	3:D:1297:LYS:HZ2	1.64	0.61
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.31	0.61
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.83	0.61
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.31	0.61
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.83	0.61
5:X:517:SER:O	5:X:518:HIS:ND1	2.34	0.61
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.83	0.61
3:I:252:LEU:H	3:I:252:LEU:HD23	1.65	0.61
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.83	0.60
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.01	0.60
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.83	0.60
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.16	0.60
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.82	0.60
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.83	0.60
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.30	0.60
2:H:94:ALA:N	2:H:126:GLU:OE2	2.25	0.60
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.83	0.60
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:487:LEU:HB3	2:H:488:MET:CG	2.32	0.60
2:C:562:GLU:HG2	2:C:574:SER:CB	2.32	0.60
3:D:711:GLY:O	3:D:712:GLN:HG2	2.00	0.60
3:D:720:ASN:O	3:D:722:ILE:N	2.34	0.60
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.36	0.60
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.83	0.60
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.30	0.60
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.35	0.60
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.82	0.60
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.17	0.60
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.82	0.60
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.83	0.60
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.82	0.60
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.17	0.60
3:I:514:THR:HG23	3:I:576:ARG:HE	1.66	0.60
5:Y:585:GLU:HB3	5:Y:589:GLN:NE2	2.15	0.60
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.82	0.60
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.82	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.66	0.60
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.27	0.60
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.83	0.60
4:J:15:ASN:HD22	4:J:18:ASP:H	1.49	0.60
1:A:232:VAL:HA	1:B:218:ARG:HG3	1.84	0.60
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.37	0.60
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.34	0.60
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.83	0.60
3:D:589:TYR:O	3:D:591:ILE:N	2.34	0.60
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.83	0.60
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.67	0.60
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.84	0.60
3:I:50:LYS:HB3	3:I:50:LYS:NZ	2.16	0.60
1:A:318:LEU:O	1:A:320:ASN:N	2.30	0.60
2:C:897:PRO:HB3	5:X:564:GLY:O	2.02	0.60
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.84	0.60
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.43	0.60
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.31	0.60
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.02	0.60
2:H:1239:VAL:O	2:H:1241:ASP:N	2.35	0.60
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.83	0.59
3:D:213:LYS:O	3:D:217:LEU:HG	2.01	0.59
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.31	0.59
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.31	0.59
2:C:646:SER:HB2	2:C:649:GLN:HG3	1.84	0.59
2:C:1273:MET:HB3	3:D:428:THR:HB	1.83	0.59
4:E:8:ASP:N	4:E:8:ASP:OD1	2.35	0.59
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.84	0.59
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.67	0.59
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.85	0.59
3:I:768:ASN:O	3:I:771:GLN:NE2	2.35	0.59
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.67	0.59
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.85	0.59
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.68	0.59
3:D:827:GLU:O	3:D:831:VAL:HG12	2.02	0.59
5:X:584:ARG:O	5:X:587:ILE:HG22	2.02	0.59
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.68	0.59
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.82	0.59
3:D:768:ASN:O	3:D:771:GLN:NE2	2.35	0.59
4:E:5:THR:CA	4:E:6:VAL:HB	2.31	0.59
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.67	0.59
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.85	0.59
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.67	0.59
3:I:1191:PRO:O	3:I:1193:TRP:N	2.34	0.59
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.37	0.59
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.38	0.59
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.35	0.59
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.85	0.59
3:D:405:GLU:O	3:D:407:VAL:N	2.35	0.59
2:H:20:GLN:O	2:H:22:LEU:N	2.36	0.59
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.85	0.59
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.84	0.59
4:J:15:ASN:ND2	4:J:18:ASP:H	2.01	0.59
4:E:14:GLY:O	4:E:15:ASN:ND2	2.36	0.59
2:H:408:SER:O	2:H:431:LYS:NZ	2.29	0.59
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.83	0.59
2:C:873:ILE:HD11	2:C:931:VAL:HG22	1.84	0.59
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.85	0.59
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.84	0.59
3:D:1191:PRO:O	3:D:1193:TRP:N	2.33	0.59
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.84	0.59
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.67	0.59
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:711:GLY:O	3:I:712:GLN:HG2	2.03	0.59
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.85	0.59
2:C:166:SER:O	2:C:168:GLY:N	2.33	0.59
3:D:85:CYS:HB3	3:D:88:CYS:O	2.03	0.59
4:E:2:ALA:HB1	4:E:6:VAL:HG23	1.84	0.59
1:G:49:SER:HA	1:G:151:GLY:HA2	1.85	0.59
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.59
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.84	0.59
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.66	0.59
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.84	0.59
2:C:202:ARG:HD3	5:X:35:ILE:HB	1.85	0.58
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.68	0.58
2:H:844:LYS:HB2	2:H:844:LYS:HZ3	1.68	0.58
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.68	0.58
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.85	0.58
3:I:77:ARG:HG3	3:I:78:LEU:H	1.67	0.58
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.36	0.58
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.67	0.58
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.85	0.58
4:E:5:THR:HB	4:E:7:GLN:H	1.68	0.58
1:F:134:THR:HG21	2:H:727:VAL:O	2.03	0.58
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.38	0.58
2:H:901:LEU:HD13	5:Y:563:PHE:HE2	1.68	0.58
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.17	0.58
2:H:55:SER:CB	2:H:56:VAL:HG13	2.30	0.58
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.67	0.58
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.26	0.58
3:I:128:LEU:HD12	3:I:192:MET:CE	2.33	0.58
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.85	0.58
2:C:901:LEU:HD13	5:X:559:LEU:HD22	1.86	0.58
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.84	0.58
3:D:125:GLY:O	3:D:129:ASP:N	2.37	0.58
2:H:901:LEU:O	2:H:905:ILE:HG13	2.03	0.58
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.68	0.58
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.84	0.58
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.35	0.58
3:D:18:ASP:HA	3:D:1369:ARG:HH22	1.69	0.58
5:X:240:ARG:O	5:X:242:HIS:N	2.36	0.58
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.68	0.58
3:I:107:LEU:H	3:I:107:LEU:HD12	1.67	0.58
3:I:822:MET:SD	3:I:838:ARG:NH1	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:302:ILE:HA	2:C:309:LEU:HA	1.85	0.58
2:C:808:ASN:H	3:D:633:ALA:HB2	1.68	0.58
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.36	0.58
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.85	0.58
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.83	0.58
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.84	0.58
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.86	0.58
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.86	0.58
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.34	0.58
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.68	0.58
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.39	0.58
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.19	0.58
2:H:55:SER:HB3	2:H:56:VAL:CB	2.34	0.58
2:H:504:GLU:O	2:H:508:SER:HB3	2.03	0.58
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.19	0.58
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.39	0.58
2:C:91:THR:HG22	2:C:139:ASN:H	1.69	0.58
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.86	0.58
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.19	0.58
3:D:107:LEU:H	3:D:107:LEU:HD12	1.69	0.58
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.84	0.58
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.86	0.58
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.84	0.58
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.03	0.58
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.37	0.57
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.69	0.57
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.86	0.57
2:C:55:SER:CB	2:C:56:VAL:HG13	2.33	0.57
3:D:1362:GLY:O	3:D:1364:ALA:N	2.35	0.57
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.38	0.57
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.19	0.57
4:J:5:THR:HA	4:J:6:VAL:CG1	2.33	0.57
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.86	0.57
2:H:660:VAL:O	2:H:661:VAL:HG22	2.04	0.57
3:I:202:ARG:O	3:I:206:ASN:ND2	2.37	0.57
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.86	0.57
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.03	0.57
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.20	0.57
2:C:756:TYR:H	2:C:766:ASN:HB3	1.69	0.57
3:D:145:VAL:HG22	3:D:180:MET:SD	2.44	0.57
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.05	0.57
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.04	0.57
3:I:405:GLU:O	3:I:407:VAL:N	2.37	0.57
2:C:800:MET:HA	2:C:800:MET:CE	2.34	0.57
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.04	0.57
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.69	0.57
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.85	0.57
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.86	0.57
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.87	0.57
1:F:9:LEU:O	1:G:227:GLN:NE2	2.37	0.57
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.87	0.57
1:B:179:PRO:O	1:B:207:THR:OG1	2.19	0.57
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.68	0.57
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.85	0.57
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.20	0.57
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.86	0.57
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.85	0.57
3:I:824:PRO:O	3:I:826:ILE:HG13	2.05	0.57
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.19	0.57
2:C:576:SER:HB3	2:C:579:ALA:HB2	1.87	0.57
2:C:1252:SER:OG	2:C:1255:THR:O	2.21	0.57
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.68	0.57
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.86	0.57
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.87	0.57
1:B:86:LYS:NZ	3:D:526:VAL:O	2.37	0.57
2:C:1200:LYS:O	2:C:1202:GLY:N	2.35	0.57
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.38	0.57
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.87	0.57
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.05	0.57
5:Y:585:GLU:O	5:Y:589:GLN:N	2.36	0.57
2:C:1255:THR:O	2:C:1257:GLN:N	2.37	0.57
3:D:202:ARG:O	3:D:206:ASN:ND2	2.38	0.57
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.35	0.57
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.86	0.57
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.70	0.56
1:B:227:GLN:O	1:B:229:GLU:N	2.31	0.56
2:C:901:LEU:O	2:C:905:ILE:HG13	2.04	0.56
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.20	0.56
3:D:246:PRO:HB2	3:D:249:LEU:HD13	1.86	0.56
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.18	0.56
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.33	0.56
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.40	0.56
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.87	0.56
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.87	0.56
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.70	0.56
1:B:49:SER:OG	3:D:538:ARG:NH2	2.39	0.56
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.40	0.56
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.86	0.56
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.87	0.56
3:D:316:ILE:HG23	3:D:317:THR:N	2.17	0.56
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.87	0.56
2:H:496:LYS:N	2:H:497:PRO:HD2	2.19	0.56
2:H:843:THR:HG22	2:H:844:LYS:H	1.70	0.56
3:I:85:CYS:HB3	3:I:88:CYS:O	2.05	0.56
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.88	0.56
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.88	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.05	0.56
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.87	0.56
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.39	0.56
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.06	0.56
3:D:487:THR:HG21	4:E:4:VAL:CG1	2.36	0.56
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.88	0.56
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.87	0.56
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.70	0.56
2:C:542:ARG:O	2:C:544:GLY:N	2.35	0.56
2:C:843:THR:HG22	2:C:844:LYS:H	1.71	0.56
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.41	0.56
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.87	0.56
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.88	0.56
3:I:1345:ARG:HG2	3:I:1370:MET:HE1	1.87	0.56
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.06	0.56
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.86	0.56
5:X:561:MET:HA	5:X:567:MET:SD	2.45	0.56
2:H:548:ARG:NH2	2:H:567:PRO:O	2.38	0.56
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.88	0.56
3:I:309:ASN:HD22	3:I:326:SER:HB3	1.71	0.56
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.86	0.56
3:I:1338:ALA:O	3:I:1340:LYS:N	2.39	0.56
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.36	0.56
3:D:245:LEU:O	3:D:250:ARG:NH1	2.39	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1200:LYS:O	2:H:1202:GLY:N	2.37	0.56
1:B:42:ALA:O	1:B:46:ILE:HG12	2.04	0.56
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.06	0.56
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.38	0.56
1:G:19:VAL:O	1:G:20:SER:OG	2.19	0.56
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.88	0.56
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.35	0.56
3:I:809:VAL:HG13	3:I:912:GLY:H	1.71	0.56
3:I:1362:GLY:O	3:I:1364:ALA:N	2.38	0.56
1:A:118:ASP:OD1	1:A:119:GLY:N	2.39	0.56
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.33	0.56
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.87	0.56
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.06	0.56
3:D:139:LEU:HD13	3:D:140:TYR:N	2.21	0.56
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.87	0.56
2:H:694:ARG:O	2:H:798:GLN:NE2	2.39	0.56
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.87	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.88	0.56
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.71	0.56
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.88	0.56
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.88	0.55
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.40	0.55
4:E:13:ILE:HD11	4:E:19:LEU:HD23	1.88	0.55
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.55	0.55
3:I:41:PRO:HB3	3:I:270:ARG:HG3	1.88	0.55
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.88	0.55
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.70	0.55
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.21	0.55
1:B:65:LEU:HD23	1:B:65:LEU:H	1.70	0.55
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.33	0.55
3:D:1338:ALA:O	3:D:1340:LYS:N	2.39	0.55
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.87	0.55
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.87	0.55
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.41	0.55
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.89	0.55
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.36	0.55
3:D:905:ARG:HG2	3:D:907:HIS:H	1.71	0.55
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.72	0.55
1:G:42:ALA:O	1:G:46:ILE:HG12	2.06	0.55
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.38	0.55
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:496:LYS:N	2:C:497:PRO:HD2	2.21	0.55
5:X:363:ARG:O	5:X:367:ILE:HG12	2.06	0.55
1:F:11:PRO:CG	1:G:228:LEU:H	2.19	0.55
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.22	0.55
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.55
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.71	0.55
2:H:1141:LEU:H	2:H:1141:LEU:CD1	2.19	0.55
3:I:72:CYS:SG	3:I:73:GLY:N	2.78	0.55
3:I:412:LEU:O	3:I:416:ILE:HD12	2.07	0.55
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.70	0.55
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.05	0.55
2:H:9:LYS:HD3	2:H:9:LYS:N	2.22	0.55
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.27	0.55
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.36	0.55
2:C:660:VAL:O	2:C:661:VAL:HG22	2.06	0.55
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.22	0.55
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.41	0.55
7:D:1503:G4P:O1C	7:D:1503:G4P:O2'	2.21	0.55
2:H:699:LEU:HD12	2:H:1121:ALA:HB1	1.87	0.55
3:I:125:GLY:O	3:I:129:ASP:N	2.39	0.55
2:C:740:GLU:HB2	2:C:741:MET:SD	2.47	0.55
2:C:1274:GLU:OE1	2:C:1274:GLU:N	2.39	0.55
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	0.55
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.36	0.55
3:D:450:HIS:NE2	3:D:625:MET:SD	2.80	0.55
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.89	0.55
1:B:64:VAL:HG13	1:B:69:SER:OG	2.06	0.55
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.72	0.55
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.71	0.55
3:D:389:GLY:O	3:D:391:ALA:N	2.40	0.55
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.89	0.55
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.89	0.55
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.88	0.55
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.70	0.55
2:C:634:VAL:H	2:C:645:PHE:HE2	1.53	0.55
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.69	0.55
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.42	0.55
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.41	0.55
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.88	0.55
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.89	0.55
2:C:55:SER:HB3	2:C:56:VAL:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:752:ASN:O	2:C:753:LEU:HG	2.07	0.55
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.32	0.55
3:D:1343:GLU:HA	3:D:1344:LEU:CB	2.34	0.55
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.40	0.55
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.89	0.55
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.22	0.54
2:C:517:GLN:HE21	2:C:760:ASN:H	1.55	0.54
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.89	0.54
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.22	0.54
2:H:494:ASN:OD1	2:H:495:ALA:N	2.39	0.54
3:I:173:GLY:HA2	3:I:176:PHE:HE2	1.72	0.54
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.89	0.54
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.42	0.54
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.89	0.54
3:D:644:MET:O	3:D:764:ARG:NH1	2.40	0.54
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.22	0.54
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.07	0.54
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.72	0.54
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.88	0.54
3:I:709:ARG:O	3:I:711:GLY:N	2.41	0.54
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.90	0.54
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.89	0.54
2:C:898:GLU:OE1	2:C:898:GLU:N	2.37	0.54
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.72	0.54
2:C:1141:LEU:CD1	2:C:1141:LEU:H	2.20	0.54
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.89	0.54
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.40	0.54
4:E:41:GLU:O	4:E:52:ARG:NH2	2.28	0.54
1:G:41:ASN:HD21	2:H:1217:THR:HG22	1.72	0.54
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.23	0.54
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.89	0.54
3:I:491:LEU:HB2	3:I:904:ALA:HA	1.90	0.54
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.89	0.54
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.07	0.54
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.90	0.54
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.89	0.54
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.54
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.71	0.54
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.89	0.54
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.41	0.54
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:GLU:H	2:C:107:ARG:HA	1.72	0.54
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.90	0.54
2:H:664:GLY:O	2:H:686:GLN:NE2	2.41	0.54
3:I:500:ILE:HD13	3:I:500:ILE:H	1.72	0.54
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.90	0.54
2:H:510:GLN:O	2:H:513:GLN:NE2	2.40	0.54
2:H:888:THR:O	2:H:914:LYS:N	2.33	0.54
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.23	0.54
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.73	0.54
2:C:149:LEU:HD12	2:C:452:ARG:O	2.08	0.54
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.90	0.54
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.90	0.54
5:X:515:GLU:N	5:X:516:ASP:HA	2.22	0.54
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.90	0.54
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.89	0.54
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.89	0.54
5:Y:119:ILE:HG21	5:Y:379:MET:HG2	1.90	0.54
3:D:72:CYS:SG	3:D:73:GLY:N	2.81	0.54
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.07	0.54
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.71	0.54
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.89	0.54
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.20	0.54
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.90	0.54
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.23	0.54
3:D:1297:LYS:HA	3:D:1297:LYS:NZ	2.23	0.54
2:H:753:LEU:HD12	2:H:753:LEU:O	2.08	0.54
3:I:88:CYS:O	3:I:90:VAL:N	2.41	0.54
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.90	0.54
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.27	0.53
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.33	0.53
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.90	0.53
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.88	0.53
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.90	0.53
1:G:179:PRO:O	1:G:207:THR:OG1	2.23	0.53
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.08	0.53
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.08	0.53
1:G:86:LYS:NZ	3:I:526:VAL:O	2.42	0.53
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.44	0.53
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.43	0.53
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.90	0.53
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:573:THR:HG22	3:D:576:ARG:CG	2.38	0.53
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.44	0.53
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.72	0.53
2:H:1268:GLN:O	3:I:346:ARG:HA	2.09	0.53
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.41	0.53
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.90	0.53
3:I:905:ARG:HG2	3:I:907:HIS:H	1.74	0.53
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.90	0.53
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.44	0.53
3:D:120:LEU:CB	3:D:121:PRO:CD	2.85	0.53
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.90	0.53
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.38	0.53
2:C:9:LYS:N	2:C:9:LYS:HD3	2.23	0.53
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.39	0.53
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.41	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.38	0.53
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.74	0.53
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.53
2:C:494:ASN:OD1	2:C:495:ALA:N	2.40	0.53
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.89	0.53
4:E:82:ALA:O	4:E:86:ILE:HG13	2.07	0.53
1:G:29:GLU:HA	1:G:200:LYS:CB	2.39	0.53
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.42	0.53
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.09	0.53
2:C:311:CYS:SG	2:C:315:MET:HB2	2.49	0.53
2:C:768:MET:O	2:C:785:ASP:N	2.38	0.53
3:D:42:GLU:HG3	5:X:451:ARG:HH21	1.74	0.53
1:G:118:ASP:OD1	1:G:119:GLY:N	2.42	0.53
2:H:1119:MET:O	2:H:1123:GLY:N	2.40	0.53
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.44	0.53
1:A:263:THR:HG23	1:A:266:SER:H	1.74	0.53
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.24	0.53
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.72	0.53
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.43	0.53
3:D:398:LYS:HD2	5:X:532:LEU:HD11	1.90	0.53
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.91	0.53
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.38	0.53
4:E:45:LYS:O	4:E:49:ILE:HG12	2.08	0.53
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.42	0.53
2:H:747:GLY:O	2:H:748:ILE:HG13	2.08	0.53
3:I:589:TYR:O	3:I:591:ILE:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:VAL:HG13	2:C:22:LEU:H	1.73	0.53
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.90	0.53
3:D:1262:ARG:HH22	3:D:1312:ALA:HB1	1.73	0.53
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.89	0.53
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.53
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.44	0.53
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.38	0.53
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.44	0.53
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.44	0.53
2:C:41:GLN:CD	2:C:42:ASP:H	2.12	0.53
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.90	0.53
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.09	0.53
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.39	0.53
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.44	0.53
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.44	0.53
2:H:741:MET:SD	2:H:741:MET:N	2.81	0.53
1:B:61:ILE:HB	1:B:64:VAL:HB	1.91	0.52
2:C:747:GLY:O	2:C:748:ILE:HG13	2.08	0.52
2:C:753:LEU:O	2:C:753:LEU:HD12	2.09	0.52
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.44	0.52
3:D:546:ALA:HB3	3:D:547:ARG:O	2.09	0.52
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.24	0.52
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.73	0.52
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.38	0.52
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.91	0.52
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.91	0.52
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.09	0.52
2:C:42:ASP:O	2:C:44:GLU:HG2	2.10	0.52
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.73	0.52
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.90	0.52
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.73	0.52
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.73	0.52
5:Y:264:LYS:HD2	5:Y:264:LYS:H	1.75	0.52
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.73	0.52
2:C:975:ILE:O	2:C:975:ILE:HD13	2.09	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.42	0.52
5:X:402:LEU:HD13	5:X:405:ILE:HD11	1.91	0.52
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.45	0.52
3:I:264:ASP:HB3	3:I:324:LEU:HB3	1.90	0.52
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.91	0.52
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.52
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.44	0.52
2:H:91:THR:HG22	2:H:139:ASN:N	2.24	0.52
4:J:4:VAL:O	4:J:5:THR:OG1	2.25	0.52
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.45	0.52
2:C:130:MET:SD	2:C:134:GLY:HA2	2.50	0.52
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.91	0.52
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.44	0.52
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.25	0.52
1:F:42:ALA:O	1:F:46:ILE:HG12	2.10	0.52
3:I:704:GLU:HB2	3:I:718:SER:OG	2.10	0.52
3:I:1297:LYS:HA	3:I:1297:LYS:NZ	2.25	0.52
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.49	0.52
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.45	0.52
3:D:128:LEU:HD12	3:D:192:MET:CE	2.40	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.42	0.52
5:X:17:LYS:N	5:X:18:GLU:HA	2.24	0.52
5:X:442:SER:OG	5:X:446:GLN:NE2	2.38	0.52
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.90	0.52
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.91	0.52
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.90	0.52
5:Y:379:MET:HA	5:Y:379:MET:CE	2.40	0.52
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.90	0.52
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.92	0.52
2:C:142:GLU:HG2	2:C:515:MET:SD	2.50	0.52
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.91	0.52
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.44	0.52
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.92	0.52
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	0.52
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.92	0.52
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.92	0.52
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.38	0.52
3:D:51:PRO:HB3	3:D:57:PHE:O	2.10	0.52
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.92	0.52
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.45	0.52
3:I:733:SER:O	3:I:737:ILE:HG12	2.09	0.52
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.91	0.52
2:C:134:GLY:O	2:C:527:LYS:NZ	2.43	0.52
2:C:892:GLU:O	2:C:893:THR:OG1	2.27	0.52
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.92	0.52
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.44	0.52
2:C:94:ALA:N	2:C:126:GLU:OE2	2.27	0.52
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.45	0.52
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.91	0.52
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.44	0.52
3:D:810:THR:OG1	3:D:811:GLU:N	2.43	0.52
3:D:1344:LEU:H	3:D:1345:ARG:HG3	1.75	0.52
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.92	0.52
2:H:728:ASP:OD2	2:H:729:ALA:N	2.43	0.52
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.91	0.52
1:A:90:VAL:HG13	1:A:121:VAL:HG13	1.92	0.51
1:A:100:LEU:HD11	1:A:121:VAL:HG11	1.92	0.51
3:D:88:CYS:O	3:D:90:VAL:N	2.44	0.51
3:D:141:PHE:O	3:D:297:ARG:HD3	2.10	0.51
3:D:473:THR:HB	3:D:476:ALA:HB2	1.91	0.51
3:D:909:ILE:HD12	3:D:909:ILE:O	2.10	0.51
5:X:355:ILE:O	5:X:355:ILE:HD13	2.10	0.51
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.40	0.51
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.32	0.51
2:H:752:ASN:O	2:H:753:LEU:HG	2.10	0.51
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.25	0.51
3:I:292:VAL:HG22	3:I:296:LYS:HE3	1.92	0.51
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.92	0.51
2:C:317:LEU:HD13	2:C:322:LEU:HD21	1.92	0.51
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.39	0.51
2:H:985:GLU:HG2	2:H:989:LEU:HD13	1.92	0.51
2:H:1273:MET:HB3	3:I:428:THR:HB	1.92	0.51
3:I:707:ILE:HG22	3:I:708:ASN:H	1.75	0.51
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.43	0.51
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.23	0.51
3:D:152:THR:O	3:D:154:LEU:N	2.40	0.51
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.92	0.51
2:H:18:ARG:HD3	2:H:619:ALA:O	2.10	0.51
3:I:389:GLY:O	3:I:391:ALA:N	2.43	0.51
3:I:590:SER:O	3:I:594:GLN:N	2.43	0.51
3:I:611:ILE:HG13	3:I:612:LEU:HD23	1.91	0.51
1:A:256:PRO:HA	1:A:277:TYR:HA	1.90	0.51
2:C:91:THR:HG22	2:C:138:ILE:HA	1.93	0.51
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.75	0.51
5:X:264:LYS:H	5:X:264:LYS:HD2	1.74	0.51
5:X:519:LEU:O	5:X:519:LEU:HD13	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.26	0.51
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.92	0.51
2:H:189:ASP:OD1	2:H:193:ASN:N	2.34	0.51
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.29	0.51
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.26	0.51
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.40	0.51
3:I:546:ALA:HB3	3:I:547:ARG:O	2.10	0.51
3:I:919:ALA:O	3:I:923:ILE:HG12	2.11	0.51
2:C:314:ASN:HD21	2:C:348:SER:HA	1.74	0.51
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.91	0.51
3:D:914:ALA:O	3:D:918:ILE:HG22	2.10	0.51
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.91	0.51
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.74	0.51
2:H:459:MET:SD	2:H:511:LEU:HD22	2.51	0.51
2:H:699:LEU:H	2:H:799:ASN:HD21	1.57	0.51
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.10	0.51
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	1.91	0.51
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.92	0.51
2:C:728:ASP:OD2	2:C:729:ALA:N	2.43	0.51
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.92	0.51
2:H:138:ILE:HB	2:H:143:ARG:HD2	1.93	0.51
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.75	0.51
2:H:963:GLU:O	2:H:967:LEU:HD13	2.11	0.51
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.92	0.51
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.26	0.51
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.92	0.51
3:D:63:GLY:O	3:D:98:ARG:NH2	2.42	0.51
3:D:179:LYS:H	3:D:179:LYS:HD3	1.76	0.51
3:D:474:LEU:HD13	3:D:478:LEU:HD13	1.93	0.51
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.91	0.51
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.92	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.51
2:C:681:MET:O	2:C:685:MET:HG2	2.10	0.51
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.30	0.51
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.44	0.51
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.45	0.51
2:H:844:LYS:HB2	2:H:844:LYS:NZ	2.25	0.51
3:I:473:THR:HB	3:I:476:ALA:HB2	1.93	0.51
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.11	0.51
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.11	0.51
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:ND2	2:C:1217:THR:HG22	2.25	0.51
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.11	0.51
2:C:894:GLN:O	2:C:895:LEU:HB2	2.09	0.51
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.91	0.51
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.92	0.51
3:D:316:ILE:HG13	3:D:317:THR:N	2.26	0.51
5:X:384:LEU:O	5:X:384:LEU:HD13	2.10	0.51
1:F:118:ASP:OD1	1:F:119:GLY:N	2.44	0.51
3:I:325:LYS:HD3	5:Y:508:GLU:OE1	2.11	0.51
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.32	0.51
2:C:946:LEU:O	2:C:949:GLU:HG3	2.10	0.51
2:C:1141:LEU:H	2:C:1141:LEU:HD13	1.76	0.51
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.09	0.51
3:D:1360:GLY:HA2	4:E:17:PHE:CZ	2.46	0.51
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.93	0.51
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.92	0.51
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.92	0.51
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.31	0.51
2:C:12:ARG:O	2:C:13:LYS:HG2	2.11	0.50
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.47	0.50
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.46	0.50
5:X:600:HIS:H	5:X:601:PRO:HD2	1.75	0.50
2:H:989:LEU:HG	2:H:990:ASP:H	1.76	0.50
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.11	0.50
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.93	0.50
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.11	0.50
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.42	0.50
1:A:250:ASP:HB3	1:A:253:LEU:HD13	1.93	0.50
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.46	0.50
2:C:1288:GLN:HE21	2:C:1288:GLN:CA	2.24	0.50
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.11	0.50
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.46	0.50
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.93	0.50
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.12	0.50
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.93	0.50
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.93	0.50
1:A:104:LYS:HD3	1:A:105:SER:N	2.26	0.50
2:C:818:VAL:HG22	2:C:819:SER:H	1.75	0.50
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.47	0.50
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.92	0.50
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:PRO:HG2	1:G:228:LEU:H	1.76	0.50
1:G:176:CYS:O	1:G:178:SER:N	2.42	0.50
2:H:590:PRO:O	2:H:659:GLN:NE2	2.45	0.50
2:H:1252:SER:HA	5:Y:524:GLU:HA	1.93	0.50
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.93	0.50
3:I:546:ALA:N	3:I:547:ARG:CA	2.71	0.50
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.94	0.50
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.11	0.50
4:J:13:ILE:HD11	4:J:19:LEU:HD23	1.94	0.50
1:A:134:THR:HG21	2:C:727:VAL:O	2.12	0.50
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.94	0.50
1:B:118:ASP:OD1	1:B:119:GLY:N	2.44	0.50
2:C:639:LYS:HE2	2:C:639:LYS:HA	1.93	0.50
2:C:989:LEU:HG	2:C:990:ASP:H	1.76	0.50
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.94	0.50
3:D:546:ALA:N	3:D:547:ARG:CA	2.70	0.50
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	0.50
2:H:442:VAL:HG12	2:H:443:ASP:H	1.77	0.50
1:B:9:LEU:H	1:B:9:LEU:HD23	1.77	0.50
2:C:1086:PRO:HG2	2:C:1094:VAL:HG21	1.94	0.50
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.44	0.50
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.77	0.50
3:I:504:GLN:HA	3:I:730:ALA:HA	1.92	0.50
3:I:1343:GLU:HA	3:I:1344:LEU:CB	2.38	0.50
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.94	0.50
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.27	0.50
1:A:231:PHE:HZ	1:B:39:LEU:HD13	1.77	0.50
1:B:19:VAL:O	1:B:20:SER:HB3	2.12	0.50
3:D:393:THR:HG23	3:D:396:ALA:H	1.77	0.50
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.12	0.50
3:D:858:VAL:HB	3:D:859:PRO:CD	2.35	0.50
2:H:106:GLU:H	2:H:107:ARG:HA	1.77	0.50
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.46	0.50
3:I:50:LYS:HB3	3:I:50:LYS:HZ3	1.77	0.50
3:I:128:LEU:HD13	3:I:189:LEU:HD23	1.94	0.50
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.77	0.50
1:B:176:CYS:O	1:B:178:SER:N	2.40	0.50
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.93	0.50
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.38	0.50
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.27	0.50
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:GLU:HG3	1:F:169:GLY:O	2.11	0.50
2:H:38:PHE:CE2	2:H:49:LEU:HD12	2.38	0.50
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.50
3:I:573:THR:HG22	3:I:576:ARG:CG	2.42	0.50
3:I:1266:ILE:HG13	3:I:1274:PHE:O	2.12	0.50
3:D:62:PHE:O	3:D:101:ARG:HG3	2.12	0.50
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.92	0.50
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.32	0.50
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.42	0.50
1:G:16:ILE:HG12	1:G:26:VAL:HG22	1.93	0.50
2:H:892:GLU:O	2:H:893:THR:OG1	2.25	0.50
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.36	0.50
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.50
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.26	0.50
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.94	0.50
2:C:163:LYS:HD3	2:C:163:LYS:N	2.16	0.50
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.41	0.50
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.12	0.50
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.11	0.50
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.12	0.50
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.94	0.50
3:I:843:VAL:HG11	3:I:897:HIS:HB3	1.94	0.50
3:I:918:ILE:HD13	3:I:919:ALA:N	2.27	0.50
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.94	0.49
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.94	0.49
2:C:741:MET:SD	2:C:741:MET:N	2.85	0.49
2:C:820:GLU:HB2	2:C:1081:PRO:HA	1.94	0.49
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.93	0.49
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.93	0.49
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.94	0.49
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.94	0.49
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.46	0.49
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.42	0.49
5:Y:279:ARG:NH2	5:Y:350:GLU:OE1	2.43	0.49
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.77	0.49
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.42	0.49
3:D:33:TRP:O	3:D:102:MET:HB2	2.11	0.49
3:D:452:LEU:HG	3:D:625:MET:SD	2.52	0.49
3:D:932:MET:SD	3:D:932:MET:N	2.75	0.49
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.93	0.49
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.12	0.49
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.94	0.49
2:H:12:ARG:O	2:H:13:LYS:HG2	2.12	0.49
2:H:131:THR:HG22	2:H:135:THR:HG22	1.93	0.49
2:H:637:ARG:HE	3:I:770:LEU:HD23	1.77	0.49
2:H:944:ARG:O	2:H:944:ARG:HD3	2.11	0.49
3:I:166:LEU:HD12	3:I:167:ASP:N	2.26	0.49
3:I:504:GLN:HG3	3:I:505:ASP:H	1.78	0.49
3:I:660:GLU:O	3:I:664:ILE:HG12	2.12	0.49
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.12	0.49
5:Y:278:ASP:OD1	5:Y:281:ARG:NH2	2.45	0.49
1:B:22:THR:HG22	1:B:208:ASN:O	2.12	0.49
2:C:27:LEU:O	2:C:528:ARG:NH1	2.44	0.49
2:C:697:LYS:HZ3	2:C:791:LEU:HD11	1.77	0.49
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.94	0.49
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.42	0.49
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.38	0.49
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.12	0.49
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.95	0.49
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.93	0.49
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.42	0.49
3:I:1171:GLY:N	3:I:1172:LYS:O	2.45	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.28	0.49
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.27	0.49
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.12	0.49
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.93	0.49
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.78	0.49
4:E:5:THR:CA	4:E:6:VAL:CB	2.86	0.49
2:H:119:GLU:HG2	2:H:120:GLN:N	2.27	0.49
2:H:384:LEU:O	2:H:388:LEU:HG	2.11	0.49
3:I:552:ILE:HD13	3:I:570:LYS:HB2	1.94	0.49
3:I:648:GLU:OE2	3:I:648:GLU:N	2.45	0.49
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.45	0.49
1:A:303:ILE:O	1:A:307:LEU:HD13	2.11	0.49
2:C:96:LEU:HD22	2:C:127:ILE:HD12	1.94	0.49
2:C:402:ARG:NH2	2:C:419:ILE:O	2.46	0.49
2:C:442:VAL:HG12	2:C:443:ASP:H	1.77	0.49
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	1.95	0.49
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	1.93	0.49
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.95	0.49
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:678:ARG:HD3	2:H:681:MET:HG3	1.94	0.49
3:I:152:THR:O	3:I:154:LEU:N	2.42	0.49
4:J:60:ASN:H	4:J:63:ILE:HB	1.77	0.49
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.19	0.49
3:D:888:CYS:SG	3:D:890:THR:HB	2.53	0.49
5:X:400:GLN:O	5:X:404:LEU:HD13	2.12	0.49
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.40	0.49
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.93	0.49
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.93	0.49
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.93	0.49
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.49
3:D:646:ILE:HD12	3:D:646:ILE:O	2.12	0.49
5:X:143:TYR:O	5:X:147:GLN:HG2	2.13	0.49
2:H:24:VAL:HG11	2:H:704:MET:HE1	1.94	0.49
2:H:639:LYS:HA	2:H:639:LYS:HE2	1.93	0.49
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.27	0.49
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.28	0.49
4:J:65:ASP:O	4:J:69:ARG:HG3	2.13	0.49
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.45	0.49
2:C:179:TYR:HE2	2:C:462:ASN:HD21	1.61	0.49
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.94	0.49
3:D:797:THR:O	3:D:801:VAL:HG23	2.13	0.49
1:G:9:LEU:HD23	1:G:9:LEU:H	1.78	0.49
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.94	0.49
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.94	0.49
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.12	0.49
2:H:1332:SER:O	3:I:243:PRO:HG2	2.12	0.49
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.95	0.49
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.95	0.49
5:Y:561:MET:HA	5:Y:567:MET:SD	2.53	0.49
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.48	0.49
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.47	0.49
2:C:127:ILE:HD13	2:C:127:ILE:N	2.27	0.49
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.48	0.49
2:C:384:LEU:O	2:C:388:LEU:HG	2.11	0.49
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.45	0.49
3:D:608:CYS:O	3:D:612:LEU:HB2	2.13	0.49
3:D:648:GLU:N	3:D:648:GLU:OE2	2.45	0.49
3:D:856:ILE:HG13	3:D:857:LEU:O	2.12	0.49
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.93	0.49
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.45	0.49
4:J:5:THR:HB	4:J:7:GLN:H	1.78	0.49
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.93	0.49
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.93	0.49
3:D:394:ILE:HG21	5:X:536:THR:HA	1.94	0.49
3:D:589:TYR:O	3:D:591:ILE:HG13	2.13	0.49
3:D:591:ILE:HD12	3:D:592:VAL:N	2.28	0.49
5:X:301:ASN:O	5:X:305:LEU:HD13	2.13	0.49
3:I:316:ILE:HD13	3:I:316:ILE:N	2.28	0.49
3:I:482:ALA:C	3:I:483:LEU:HD12	2.34	0.49
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.12	0.49
4:J:5:THR:HB	4:J:7:GLN:HB2	1.94	0.49
5:Y:400:GLN:O	5:Y:404:LEU:HD13	2.12	0.49
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.78	0.48
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.95	0.48
3:D:515:ARG:HH22	3:D:717:VAL:C	2.16	0.48
5:X:600:HIS:H	5:X:601:PRO:CD	2.26	0.48
3:I:810:THR:OG1	3:I:811:GLU:N	2.44	0.48
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.94	0.48
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.95	0.48
2:C:1119:MET:O	2:C:1123:GLY:N	2.43	0.48
5:X:119:ILE:O	5:X:123:ILE:HG13	2.13	0.48
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.47	0.48
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.95	0.48
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.43	0.48
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.43	0.48
3:D:166:LEU:HD12	3:D:167:ASP:N	2.28	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.12	0.48
3:D:316:ILE:HD11	3:D:320:ASN:O	2.13	0.48
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.43	0.48
5:X:310:GLU:O	5:X:344:LEU:HD23	2.14	0.48
2:H:36:GLN:O	2:H:39:ILE:HG22	2.13	0.48
2:H:489:PRO:HB2	2:H:492:MET:CB	2.39	0.48
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.94	0.48
3:I:197:GLU:O	3:I:201:LEU:HD23	2.12	0.48
3:I:363:LEU:O	3:I:363:LEU:HD23	2.13	0.48
3:I:393:THR:HG23	3:I:396:ALA:H	1.78	0.48
3:I:807:LEU:HD12	3:I:807:LEU:O	2.12	0.48
2:C:72:SER:O	2:C:98:VAL:HG23	2.13	0.48
2:C:91:THR:HG22	2:C:139:ASN:N	2.29	0.48
2:C:106:GLU:HG2	2:C:109:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:756:TYR:H	2:H:766:ASN:HB3	1.78	0.48
3:I:161:THR:HG22	3:I:162:GLU:H	1.78	0.48
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.95	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.14	0.48
1:A:207:THR:OG1	1:A:208:ASN:N	2.47	0.48
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.95	0.48
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.40	0.48
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.44	0.48
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.48	0.48
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.13	0.48
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.27	0.48
5:X:28:ASN:HD22	5:X:29:ASP:N	2.11	0.48
5:X:493:LYS:O	5:X:497:VAL:HG23	2.13	0.48
2:H:38:PHE:O	2:H:39:ILE:HB	2.12	0.48
2:H:149:LEU:HD12	2:H:452:ARG:O	2.13	0.48
2:H:808:ASN:H	3:I:633:ALA:HB2	1.78	0.48
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.46	0.48
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.12	0.48
1:A:241:GLU:OE2	1:A:243:LYS:HE3	2.14	0.48
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.28	0.48
3:D:807:LEU:HD12	3:D:807:LEU:O	2.13	0.48
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.41	0.48
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.49	0.48
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.14	0.48
3:I:56:LEU:HB3	3:I:250:ARG:NH2	2.28	0.48
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.44	0.48
3:I:245:LEU:O	3:I:250:ARG:NH1	2.45	0.48
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.44	0.48
3:I:579:LEU:O	3:I:579:LEU:HD13	2.14	0.48
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.44	0.48
3:I:646:ILE:HD12	3:I:646:ILE:O	2.13	0.48
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.14	0.48
5:Y:437:GLN:HA	5:Y:440:THR:HG22	1.94	0.48
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.96	0.48
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.49	0.48
2:C:891:GLY:O	2:C:893:THR:HG23	2.14	0.48
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.49	0.48
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.96	0.48
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.13	0.48
2:H:660:VAL:HG22	2:H:661:VAL:N	2.25	0.48
2:H:707:ALA:O	2:H:710:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.96	0.48
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.95	0.48
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.95	0.48
2:C:1286:THR:N	3:D:479:GLU:OE2	2.45	0.48
3:D:843:VAL:HG12	3:D:883:ARG:HD3	1.96	0.48
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.48	0.48
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.48	0.48
1:G:33:ARG:HE	1:G:197:ASP:HB2	1.78	0.48
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.78	0.48
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.47	0.48
3:I:513:MET:O	3:I:575:GLY:HA3	2.14	0.48
1:B:18:GLN:C	1:B:20:SER:H	2.17	0.48
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.96	0.48
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.13	0.48
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	1.96	0.48
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.96	0.48
2:H:932:GLN:HE22	2:H:952:GLN:HE22	1.62	0.48
4:J:45:LYS:O	4:J:49:ILE:HG12	2.13	0.48
1:A:192:VAL:O	1:A:194:GLN:N	2.46	0.48
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.94	0.48
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.96	0.48
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.29	0.48
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.95	0.48
5:X:27:VAL:HA	5:X:30:HIS:HD2	1.78	0.48
2:H:73:TYR:HD2	2:H:74:ARG:H	1.58	0.48
2:H:163:LYS:H	2:H:163:LYS:CD	2.22	0.48
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.44	0.48
2:H:1339:LEU:HD12	2:H:1339:LEU:N	2.28	0.48
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.14	0.48
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.96	0.47
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.96	0.47
3:D:840:LEU:HD12	3:D:840:LEU:O	2.14	0.47
5:X:24:TYR:O	5:X:26:GLU:N	2.45	0.47
2:H:152:SER:OG	2:H:404:LYS:NZ	2.24	0.47
2:H:766:ASN:H	2:H:787:PRO:HG3	1.79	0.47
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.96	0.47
3:I:41:PRO:HG3	3:I:273:ILE:HG22	1.96	0.47
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.47	0.47
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.95	0.47
2:C:843:THR:HB	2:C:845:LEU:HD22	1.96	0.47
3:D:613:GLY:O	3:D:617:THR:OG1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.14	0.47
3:D:919:ALA:O	3:D:923:ILE:HG12	2.14	0.47
5:X:130:VAL:O	5:X:134:VAL:HG23	2.14	0.47
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.94	0.47
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.49	0.47
2:H:908:GLU:HG2	2:H:909:LYS:N	2.22	0.47
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.14	0.47
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.96	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.35	0.47
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.96	0.47
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.50	0.47
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.30	0.47
3:D:161:THR:HG22	3:D:162:GLU:H	1.78	0.47
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.43	0.47
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.50	0.47
2:H:1117:LEU:HD21	2:H:1182:ILE:HG21	1.96	0.47
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.30	0.47
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.45	0.47
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.97	0.47
2:C:1058:ARG:HD3	2:C:1240:ASP:OD1	2.14	0.47
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.95	0.47
3:D:316:ILE:O	3:D:317:THR:OG1	2.28	0.47
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.44	0.47
2:H:17:LYS:NZ	2:H:1194:GLU:OE1	2.42	0.47
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.15	0.47
2:H:702:THR:HA	2:H:1184:THR:O	2.14	0.47
2:H:706:ARG:HA	2:H:793:GLU:HA	1.96	0.47
2:H:898:GLU:OE1	2:H:898:GLU:N	2.38	0.47
2:H:1120:ALA:HB1	2:H:1198:LEU:HB3	1.96	0.47
3:I:450:HIS:NE2	3:I:625:MET:SD	2.87	0.47
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.27	0.47
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.14	0.47
2:C:839:VAL:HG13	2:C:1049:ILE:HG22	1.96	0.47
2:C:1106:ARG:O	2:C:1108:ASN:N	2.43	0.47
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.44	0.47
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.96	0.47
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.80	0.47
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.96	0.47
3:I:316:ILE:HD13	3:I:316:ILE:H	1.79	0.47
3:I:608:CYS:O	3:I:612:LEU:HB2	2.14	0.47
3:I:840:LEU:HD12	3:I:840:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.49	0.47
3:D:789:LYS:HD2	3:D:932:MET:SD	2.54	0.47
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.43	0.47
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.30	0.47
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.95	0.47
2:H:634:VAL:H	2:H:645:PHE:HE2	1.62	0.47
2:H:841:ARG:NH1	3:I:256:ASP:HB3	2.28	0.47
3:I:811:GLU:OE2	3:I:890:THR:OG1	2.28	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.65	0.47
2:C:59:ILE:HD11	2:C:63:SER:OG	2.15	0.47
2:C:119:GLU:HG2	2:C:120:GLN:N	2.29	0.47
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.80	0.47
2:C:510:GLN:O	2:C:511:LEU:HB2	2.15	0.47
2:C:963:GLU:O	2:C:966:ILE:HG22	2.15	0.47
3:D:133:ARG:HB2	3:D:133:ARG:NH2	2.30	0.47
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.45	0.47
3:D:482:ALA:C	3:D:483:LEU:HD12	2.34	0.47
3:D:504:GLN:HG3	3:D:505:ASP:H	1.80	0.47
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.96	0.47
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.30	0.47
3:D:1292:LEU:HD21	3:I:1284:ARG:NH2	2.29	0.47
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.14	0.47
5:X:595:LEU:O	5:X:599:ARG:NH1	2.46	0.47
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.95	0.47
1:G:31:LEU:HB2	1:G:199:ASP:O	2.15	0.47
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.49	0.47
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.96	0.47
3:I:290:ILE:O	3:I:293:ARG:HG3	2.15	0.47
3:I:591:ILE:HD12	3:I:592:VAL:N	2.28	0.47
3:I:1196:LEU:HG	3:I:1210:ILE:HD11	1.95	0.47
3:I:1287:ILE:HA	3:I:1290:ARG:HG2	1.97	0.47
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.15	0.47
1:A:42:ALA:O	1:A:46:ILE:HG12	2.14	0.47
2:C:205:PRO:O	2:C:208:ILE:HG22	2.15	0.47
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.44	0.47
2:C:533:LEU:HD23	2:C:533:LEU:H	1.80	0.47
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.79	0.47
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.28	0.47
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.80	0.47
3:D:552:ILE:HD13	3:D:570:LYS:HB2	1.97	0.47
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.14	0.47
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.96	0.47
2:H:106:GLU:HG2	2:H:109:ALA:H	1.78	0.47
2:H:130:MET:SD	2:H:134:GLY:HA2	2.54	0.47
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.97	0.47
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.78	0.47
2:C:127:ILE:HG22	2:C:502:VAL:HG11	1.97	0.47
2:C:893:THR:O	2:C:895:LEU:N	2.40	0.47
3:D:832:LYS:HA	3:D:832:LYS:HZ1	1.79	0.47
5:X:346:GLN:O	5:X:350:GLU:HG3	2.15	0.47
5:X:452:ILE:HG21	5:X:457:ILE:HG12	1.97	0.47
5:X:545:HIS:NE2	5:X:566:ASP:OD2	2.48	0.47
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.49	0.47
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.45	0.47
3:I:120:LEU:CB	3:I:121:PRO:CD	2.90	0.47
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.38	0.47
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.79	0.47
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.96	0.47
3:D:660:GLU:O	3:D:664:ILE:HG12	2.15	0.47
5:X:115:GLY:O	5:X:119:ILE:HG12	2.15	0.47
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.80	0.47
1:F:45:ARG:NE	1:G:38:THR:OG1	2.49	0.47
2:H:356:THR:HG21	2:H:362:ALA:HA	1.96	0.47
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.97	0.47
3:I:8:LEU:HD23	3:I:8:LEU:N	2.30	0.47
3:I:227:PHE:O	3:I:230:SER:OG	2.25	0.47
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.35	0.47
2:C:434:ASP:HB3	2:C:439:LYS:HB2	1.97	0.46
2:C:756:TYR:H	2:C:766:ASN:CB	2.28	0.46
2:C:829:THR:HG22	2:C:1059:ARG:HG2	1.98	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.15	0.46
3:D:56:LEU:HB3	3:D:250:ARG:HH21	1.80	0.46
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.30	0.46
2:H:317:LEU:HD13	2:H:322:LEU:HD21	1.97	0.46
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.81	0.46
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.41	0.46
2:H:895:LEU:HD21	2:H:903:ARG:CZ	2.45	0.46
2:H:975:ILE:HD13	2:H:975:ILE:O	2.14	0.46
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.45	0.46
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.15	0.46
2:C:53:PHE:HD1	2:C:57:PHE:CD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:ASP:O	2:C:437:ASN:ND2	2.48	0.46
2:C:487:LEU:CD1	2:C:488:MET:H	2.28	0.46
2:C:590:PRO:O	2:C:659:GLN:NE2	2.47	0.46
3:D:8:LEU:HD23	3:D:8:LEU:N	2.30	0.46
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.46	0.46
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.45	0.46
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.98	0.46
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.96	0.46
5:X:511:ILE:HG23	5:X:512:GLY:N	2.28	0.46
2:H:11:ILE:HG21	2:H:697:LYS:HZ2	1.80	0.46
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.48	0.46
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.45	0.46
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.97	0.46
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.27	0.46
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.98	0.46
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.16	0.46
3:D:227:PHE:O	3:D:230:SER:OG	2.26	0.46
3:D:240:THR:HG23	3:D:241:VAL:HG23	1.97	0.46
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.97	0.46
3:D:415:VAL:HG23	3:D:416:ILE:HG23	1.97	0.46
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.15	0.46
1:F:79:LEU:HD12	2:H:756:TYR:OH	2.16	0.46
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.96	0.46
3:I:12:THR:O	3:I:13:LYS:HD2	2.15	0.46
3:I:797:THR:O	3:I:801:VAL:HG23	2.15	0.46
1:A:243:LYS:HB2	1:A:243:LYS:HZ2	1.79	0.46
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.15	0.46
2:C:697:LYS:HG3	2:C:698:PRO:HD2	1.98	0.46
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.14	0.46
3:D:27:PRO:O	3:D:31:ARG:HD3	2.15	0.46
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.80	0.46
3:D:733:SER:O	3:D:737:ILE:HG12	2.15	0.46
5:X:271:ASN:O	5:X:275:VAL:HG23	2.14	0.46
5:X:556:ALA:O	5:X:560:ARG:HB2	2.16	0.46
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.96	0.46
3:I:822:MET:HG2	3:I:839:VAL:HG22	1.96	0.46
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.75	0.46
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.15	0.46
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.28	0.46
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.98	0.46
2:C:622:ASN:OD1	2:C:623:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.46	0.46
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.49	0.46
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	1.97	0.46
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.30	0.46
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.37	0.46
5:X:379:MET:CE	5:X:379:MET:HA	2.46	0.46
1:F:80:GLU:HA	2:H:694:ARG:HH22	1.80	0.46
1:G:76:GLU:OE2	1:G:131:CYS:HA	2.16	0.46
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.97	0.46
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.80	0.46
4:J:3:ARG:NH2	4:J:44:ASP:OD2	2.49	0.46
5:Y:105:MET:SD	5:Y:388:ILE:HD12	2.55	0.46
5:Y:303:ILE:O	5:Y:307:THR:OG1	2.30	0.46
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.48	0.46
2:C:216:THR:O	2:C:220:ILE:HG13	2.15	0.46
3:D:378:LYS:HD2	3:D:382:TYR:OH	2.14	0.46
3:D:514:THR:HG21	3:D:595:ALA:O	2.14	0.46
3:D:550:VAL:HG23	3:D:552:ILE:HD11	1.96	0.46
2:H:517:GLN:HE21	2:H:760:ASN:H	1.64	0.46
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.51	0.46
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.36	0.46
2:H:998:LEU:O	2:H:998:LEU:HD13	2.15	0.46
2:H:1042:LEU:HD13	2:H:1042:LEU:N	2.27	0.46
2:H:1142:ARG:HE	2:H:1169:VAL:HB	1.80	0.46
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.30	0.46
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.45	0.46
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.96	0.46
4:J:26:ARG:HD3	4:J:64:LEU:HD21	1.98	0.46
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.46
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.98	0.46
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.98	0.46
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.97	0.46
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.16	0.46
1:G:227:GLN:C	1:G:228:LEU:HD23	2.36	0.46
2:H:902:LEU:HD11	5:Y:608:ARG:HA	1.97	0.46
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.16	0.46
3:I:154:LEU:HD21	3:I:160:LEU:HD21	1.98	0.46
3:I:856:ILE:HG13	3:I:857:LEU:O	2.14	0.46
3:I:1221:LEU:HD23	3:I:1229:VAL:HG11	1.97	0.46
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.26	0.46
2:C:131:THR:HG22	2:C:135:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:682:GLY:HA2	2:C:685:MET:HG2	1.97	0.46
2:C:1211:ARG:HB2	2:C:1220:GLN:HE21	1.80	0.46
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	1.98	0.46
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.46	0.46
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.97	0.46
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.15	0.46
5:X:373:ARG:HG3	5:X:377:LYS:HE3	1.97	0.46
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.96	0.46
3:I:33:TRP:O	3:I:102:MET:HB2	2.16	0.46
3:I:245:LEU:CD1	3:I:246:PRO:HD2	2.45	0.46
1:B:31:LEU:HB2	1:B:199:ASP:O	2.16	0.46
1:B:178:SER:HA	1:B:179:PRO:HD3	1.85	0.46
2:C:372:PRO:CB	5:X:34:ASP:HB3	2.45	0.46
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.37	0.46
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.97	0.46
1:G:110:VAL:HG11	1:G:140:ILE:HD11	1.98	0.46
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.35	0.46
2:C:966:ILE:HG23	2:C:967:LEU:HD12	1.98	0.46
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.97	0.46
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.98	0.46
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.46	0.46
3:D:416:ILE:HD12	3:D:416:ILE:O	2.16	0.46
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.16	0.46
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.15	0.46
1:G:191:ARG:NH2	3:I:441:LEU:O	2.49	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.51	0.46
2:H:1296:ASP:OD1	3:I:345:LYS:HD2	2.15	0.46
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.97	0.46
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.98	0.45
1:B:16:ILE:HG12	1:B:26:VAL:HG22	1.97	0.45
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.80	0.45
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.98	0.45
2:C:876:GLU:N	2:C:876:GLU:OE2	2.49	0.45
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.46	0.45
3:D:572:THR:HG22	3:D:594:GLN:OE1	2.16	0.45
3:D:720:ASN:ND2	3:D:720:ASN:O	2.49	0.45
3:D:809:VAL:HG13	3:D:912:GLY:H	1.80	0.45
4:E:4:VAL:O	4:E:5:THR:OG1	2.20	0.45
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.16	0.45
5:X:437:GLN:HA	5:X:440:THR:HG22	1.97	0.45
1:F:10:LYS:HD2	1:G:226:GLU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ILE:HD13	2:H:127:ILE:N	2.28	0.45
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.30	0.45
3:I:508:LEU:O	3:I:508:LEU:HD23	2.16	0.45
3:I:909:ILE:HD12	3:I:909:ILE:O	2.16	0.45
1:A:5:VAL:O	1:A:6:THR:OG1	2.32	0.45
1:A:222:THR:O	1:A:226:GLU:HG3	2.17	0.45
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.79	0.45
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	1.99	0.45
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.49	0.45
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.98	0.45
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.31	0.45
2:H:21:VAL:HG13	2:H:22:LEU:N	2.30	0.45
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.46	0.45
2:H:893:THR:O	2:H:895:LEU:N	2.45	0.45
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.97	0.45
3:I:113:HIS:CE1	3:I:115:TRP:HB2	2.51	0.45
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.81	0.45
3:I:430:HIS:HA	3:I:921:GLN:HB3	1.97	0.45
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.16	0.45
3:I:1148:ARG:NH2	3:I:1148:ARG:HB2	2.32	0.45
5:Y:379:MET:HA	5:Y:379:MET:HE2	1.97	0.45
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.16	0.45
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.48	0.45
1:A:234:LEU:N	1:A:234:LEU:HD12	2.32	0.45
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.98	0.45
1:B:83:LEU:HD23	3:D:551:ARG:HG3	1.96	0.45
2:C:152:SER:HA	2:C:153:PRO:HD3	1.87	0.45
2:C:462:ASN:O	2:C:466:VAL:HG23	2.17	0.45
2:C:777:VAL:HG21	2:C:783:LEU:HD21	1.98	0.45
2:C:963:GLU:O	2:C:967:LEU:HD13	2.16	0.45
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.47	0.45
3:D:504:GLN:HA	3:D:730:ALA:HA	1.98	0.45
3:D:579:LEU:O	3:D:579:LEU:HD13	2.16	0.45
5:X:250:LEU:O	5:X:254:GLU:HG2	2.16	0.45
2:H:768:MET:O	2:H:785:ASP:N	2.47	0.45
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.98	0.45
3:I:524:GLY:HA2	3:I:548:VAL:HG23	1.99	0.45
3:I:640:GLY:N	3:I:643:ASP:OD2	2.45	0.45
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.16	0.45
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.16	0.45
2:C:43:PRO:HD3	2:C:47:TYR:HD2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.51	0.45
2:C:580:GLN:HG2	2:C:581:THR:N	2.32	0.45
2:C:660:VAL:HG22	2:C:661:VAL:N	2.27	0.45
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.98	0.45
3:D:655:SER:HA	3:D:658:GLU:HG2	1.96	0.45
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.36	0.45
4:E:44:ASP:HB2	4:E:52:ARG:HH21	1.82	0.45
1:F:79:LEU:O	1:F:83:LEU:HD13	2.17	0.45
2:H:73:TYR:N	2:H:73:TYR:CD2	2.85	0.45
2:H:680:LEU:HD13	3:I:783:LEU:HD12	1.98	0.45
2:C:57:PHE:HE1	2:C:472:GLU:HA	1.80	0.45
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.44	0.45
3:D:526:VAL:HG12	3:D:549:LYS:O	2.16	0.45
3:D:915:ILE:O	3:D:918:ILE:HG23	2.17	0.45
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.99	0.45
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.31	0.45
2:H:876:GLU:N	2:H:876:GLU:OE2	2.49	0.45
2:H:972:PHE:HA	2:H:975:ILE:HG22	1.98	0.45
3:I:51:PRO:HB3	3:I:57:PHE:O	2.16	0.45
3:I:235:GLU:OE1	3:I:235:GLU:N	2.50	0.45
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.31	0.45
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.16	0.45
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.15	0.45
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.17	0.45
1:A:33:ARG:HG2	1:A:199:ASP:OD2	2.16	0.45
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.32	0.45
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.32	0.45
2:C:465:ARG:O	2:C:469:VAL:HG23	2.16	0.45
2:C:998:LEU:HD13	2:C:998:LEU:O	2.17	0.45
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.81	0.45
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.65	0.45
3:D:260:PHE:O	5:X:504:PRO:HG2	2.16	0.45
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.30	0.45
3:D:1287:ILE:HA	3:D:1290:ARG:HG2	1.98	0.45
1:F:151:GLY:O	1:F:177:TYR:HB2	2.17	0.45
2:H:1116:HIS:CE1	2:H:1226:THR:HG23	2.50	0.45
3:I:545:HIS:HA	3:I:546:ALA:HA	1.77	0.45
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.56	0.45
2:C:812:PHE:H	2:C:815:SER:HB2	1.81	0.45
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.97	0.45
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:139:GLU:HG3	5:X:351:THR:HA	1.98	0.45
1:F:158:ARG:HE	1:F:172:LEU:HD13	1.81	0.45
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.97	0.45
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.98	0.45
2:H:818:VAL:HG22	2:H:819:SER:N	2.32	0.45
2:H:908:GLU:H	2:H:908:GLU:CD	2.20	0.45
2:H:1006:GLU:H	2:H:1006:GLU:CD	2.20	0.45
3:I:205:LEU:HB3	3:I:217:LEU:HB3	1.99	0.45
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.15	0.45
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.17	0.45
2:C:868:SER:OG	2:C:942:ASP:OD1	2.28	0.45
3:D:531:LYS:HB3	3:D:531:LYS:NZ	2.32	0.45
3:D:619:ILE:HD13	7:D:1503:G4P:O3D	2.17	0.45
3:D:766:GLY:C	3:D:767:LEU:HD22	2.37	0.45
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.80	0.45
1:F:166:ARG:HA	1:F:167:PRO:HD2	1.87	0.45
1:G:47:LEU:HD13	1:G:205:MET:HE2	1.99	0.45
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.38	0.45
2:H:135:THR:OG1	2:H:143:ARG:O	2.29	0.45
2:H:622:ASN:OD1	2:H:623:LEU:N	2.50	0.45
2:H:1294:LYS:HE3	3:I:349:TYR:HB2	1.99	0.45
3:I:326:SER:O	3:I:330:MET:HG3	2.16	0.45
3:I:610:ARG:HG2	3:I:864:LEU:HD22	1.98	0.45
1:B:64:VAL:HG12	1:B:171:LEU:HD11	1.98	0.45
1:B:183:ILE:HD11	1:B:205:MET:HE2	1.99	0.45
2:C:556:GLY:O	2:C:579:ALA:HB2	2.16	0.45
2:C:818:VAL:HG22	2:C:819:SER:N	2.32	0.45
2:C:845:LEU:HD13	2:C:845:LEU:N	2.28	0.45
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.19	0.45
3:D:473:THR:HB	3:D:476:ALA:CB	2.47	0.45
3:D:494:ALA:HA	3:D:1252:HIS:HE1	1.82	0.45
3:D:640:GLY:N	3:D:643:ASP:OD2	2.50	0.45
5:X:101:TYR:CE2	5:X:388:ILE:HD11	2.45	0.45
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.44	0.45
5:X:123:ILE:O	5:X:127:ILE:HG12	2.17	0.45
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.98	0.45
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.98	0.45
1:G:185:TYR:HA	1:G:202:VAL:O	2.17	0.45
2:H:966:ILE:HG23	2:H:967:LEU:HD12	1.97	0.45
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.50	0.45
3:I:325:LYS:HZ1	3:I:330:MET:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:C	1:A:318:LEU:HD13	2.37	0.45
2:C:964:LEU:HD12	2:C:1025:PHE:CG	2.52	0.45
3:D:657:ALA:HB2	3:D:689:ALA:HB2	1.99	0.45
3:D:824:PRO:O	3:D:826:ILE:HG13	2.16	0.45
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.99	0.45
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.98	0.45
2:H:1192:GLU:O	2:H:1196:LYS:HD3	2.17	0.45
3:I:1266:ILE:HA	3:I:1302:TYR:HA	1.99	0.45
1:A:284:ARG:NH1	1:A:288:GLU:HG3	2.32	0.44
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.46	0.44
4:E:5:THR:HB	4:E:7:GLN:N	2.29	0.44
2:H:143:ARG:NH1	2:H:512:SER:O	2.50	0.44
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.99	0.44
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.53	0.44
3:I:269:TYR:HA	3:I:272:VAL:HG12	1.99	0.44
3:I:531:LYS:HB3	3:I:531:LYS:NZ	2.32	0.44
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.16	0.44
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.98	0.44
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.18	0.44
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.99	0.44
1:G:195:ARG:HH21	1:G:198:LEU:HD21	1.81	0.44
2:H:946:LEU:O	2:H:949:GLU:HG3	2.16	0.44
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.98	0.44
2:H:1156:ARG:HH11	2:H:1157:GLN:H	1.64	0.44
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.81	0.44
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.98	0.44
3:I:860:ARG:HD3	3:I:866:GLU:OE2	2.17	0.44
3:I:909:ILE:H	3:I:909:ILE:HG13	1.56	0.44
3:I:911:LYS:HD2	3:I:911:LYS:O	2.17	0.44
1:B:151:GLY:O	1:B:177:TYR:HB2	2.18	0.44
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.33	0.44
2:C:161:LYS:NZ	2:C:161:LYS:HB3	2.32	0.44
2:C:702:THR:HA	2:C:1184:THR:O	2.17	0.44
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.97	0.44
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.47	0.44
3:D:217:LEU:O	3:D:221:ILE:HG12	2.16	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.51	0.44
5:X:277:MET:HE1	5:X:359:LYS:HE2	1.99	0.44
1:F:207:THR:HG23	1:F:209:GLY:H	1.82	0.44
2:H:994:ARG:HD3	2:H:994:ARG:N	2.31	0.44
3:I:214:ARG:O	3:I:218:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:681:LYS:O	3:I:685:ILE:HG13	2.18	0.44
3:I:720:ASN:ND2	3:I:720:ASN:O	2.50	0.44
3:I:1358:PRO:HB3	3:I:1366:HIS:CG	2.52	0.44
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.18	0.44
5:Y:451:ARG:O	5:Y:452:ILE:HG13	2.18	0.44
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.52	0.44
2:C:169:LYS:HD3	2:C:169:LYS:HA	1.80	0.44
2:C:813:GLU:HG2	3:D:504:GLN:NE2	2.31	0.44
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.33	0.44
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.38	0.44
3:D:154:LEU:HD21	3:D:160:LEU:HD21	1.99	0.44
3:D:252:LEU:HD23	3:D:252:LEU:N	2.32	0.44
3:D:356:THR:O	3:D:448:GLN:HA	2.17	0.44
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.31	0.44
1:F:182:ARG:NH1	2:H:1092:THR:HG22	2.33	0.44
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.51	0.44
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.99	0.44
3:I:221:ILE:HG13	3:I:222:LYS:N	2.33	0.44
3:I:240:THR:HG23	3:I:241:VAL:HG23	1.98	0.44
3:I:899:TYR:CD2	3:I:909:ILE:HG12	2.53	0.44
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.16	0.44
5:Y:448:ARG:NH1	5:Y:452:ILE:HD12	2.32	0.44
5:Y:544:THR:O	5:Y:548:LEU:HG	2.17	0.44
2:C:56:VAL:HB	2:C:57:PHE:H	1.51	0.44
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.51	0.44
3:D:525:MET:O	3:D:535:ARG:NH2	2.50	0.44
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.47	0.44
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.50	0.44
1:G:65:LEU:HD23	1:G:65:LEU:N	2.27	0.44
2:H:27:LEU:O	2:H:528:ARG:NH1	2.44	0.44
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.35	0.44
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.20	0.44
3:I:217:LEU:O	3:I:221:ILE:HG12	2.17	0.44
3:I:543:SER:O	3:I:574:VAL:HB	2.18	0.44
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.18	0.44
1:B:19:VAL:O	1:B:20:SER:CB	2.65	0.44
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.99	0.44
2:C:812:PHE:N	2:C:815:SER:HB2	2.31	0.44
2:C:985:GLU:HG3	2:C:988:LYS:HB2	2.00	0.44
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.17	0.44
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:514:THR:HG23	3:D:576:ARG:HE	1.83	0.44
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.47	0.44
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.83	0.44
5:X:133:SER:OG	5:X:365:MET:HB2	2.17	0.44
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.83	0.44
2:H:1042:LEU:HB2	2:H:1043:ALA:H	1.68	0.44
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.98	0.44
3:I:131:PRO:CG	3:I:135:ILE:HD13	2.45	0.44
3:I:843:VAL:HG21	3:I:897:HIS:HA	1.99	0.44
3:I:885:VAL:O	3:I:1258:ARG:HD3	2.17	0.44
5:Y:130:VAL:O	5:Y:134:VAL:HG23	2.17	0.44
2:C:397:LEU:O	2:C:398:SER:OG	2.35	0.44
2:C:707:ALA:O	2:C:710:VAL:HG12	2.18	0.44
3:D:107:LEU:HD23	3:D:299:LEU:HD21	1.99	0.44
3:D:539:SER:OG	3:D:540:GLY:N	2.51	0.44
3:D:1297:LYS:HE3	3:I:1267:VAL:HB	1.99	0.44
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.99	0.44
2:H:71:VAL:O	2:H:72:SER:OG	2.29	0.44
2:H:500:ALA:O	2:H:504:GLU:HB2	2.18	0.44
3:I:704:GLU:HB3	3:I:705:THR:H	1.72	0.44
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.18	0.44
5:Y:586:ARG:HH22	5:Y:590:ILE:HD11	1.82	0.44
5:Y:604:SER:HA	5:Y:607:LEU:HB2	2.00	0.44
1:A:110:VAL:HG21	1:A:140:ILE:HD11	2.00	0.44
2:C:80:PHE:O	2:C:84:GLU:HB3	2.18	0.44
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.53	0.44
2:C:475:VAL:HG23	2:C:492:MET:SD	2.58	0.44
2:C:1212:LEU:HD11	2:C:1227:VAL:HG21	2.00	0.44
2:C:1244:HIS:HB3	2:C:1265:PHE:CG	2.53	0.44
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.17	0.44
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	2.00	0.44
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.82	0.44
5:X:126:GLY:O	5:X:130:VAL:HG23	2.18	0.44
1:G:64:VAL:HG13	1:G:69:SER:OG	2.18	0.44
2:H:551:HIS:CE1	2:H:553:THR:HG1	2.36	0.44
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.41	0.44
2:H:866:ASP:HA	2:H:872:TYR:OH	2.18	0.44
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.18	0.44
3:I:149:GLY:HA2	3:I:156:ARG:HG2	2.00	0.44
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.86	0.44
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	2.00	0.44
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.17	0.44
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.48	0.44
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.98	0.44
2:C:475:VAL:O	2:C:479:LEU:HB2	2.18	0.44
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.33	0.44
2:C:1042:LEU:HB2	2:C:1043:ALA:H	1.70	0.44
2:C:1322:SER:OG	3:D:345:LYS:NZ	2.37	0.44
3:D:221:ILE:HG13	3:D:222:LYS:N	2.33	0.44
3:D:596:LEU:N	3:D:596:LEU:HD23	2.33	0.44
4:E:60:ASN:H	4:E:63:ILE:HB	1.83	0.44
1:G:227:GLN:C	1:G:229:GLU:H	2.21	0.44
2:H:505:PHE:O	2:H:512:SER:OG	2.30	0.44
2:H:681:MET:O	2:H:685:MET:HG2	2.17	0.44
2:H:685:MET:CE	2:H:1073:LYS:HE2	2.48	0.44
3:I:138:VAL:O	3:I:143:SER:HB3	2.18	0.44
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.17	0.44
3:I:526:VAL:CG1	3:I:549:LYS:HB2	2.48	0.44
5:Y:264:LYS:HD2	5:Y:264:LYS:N	2.33	0.44
1:A:300:LEU:O	1:A:300:LEU:HD13	2.18	0.43
1:A:313:SER:OG	1:A:314:LEU:N	2.50	0.43
2:C:22:LEU:HD13	2:C:23:ASP:O	2.18	0.43
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.51	0.43
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.47	0.43
3:D:580:TRP:HE1	3:D:589:TYR:HB3	1.82	0.43
3:D:746:LEU:H	3:D:746:LEU:HD22	1.82	0.43
3:D:1369:ARG:HB3	3:D:1369:ARG:HH11	1.83	0.43
5:X:119:ILE:HG21	5:X:379:MET:HG2	1.98	0.43
5:X:264:LYS:HD2	5:X:264:LYS:N	2.33	0.43
2:H:365:GLU:OE2	2:H:368:ARG:NH2	2.51	0.43
2:H:800:MET:HG2	2:H:1096:ILE:HD13	2.00	0.43
2:H:1109:ILE:HG12	3:I:644:MET:SD	2.58	0.43
3:I:288:PRO:O	3:I:292:VAL:HG12	2.18	0.43
3:I:317:THR:H	3:I:324:LEU:HD21	1.83	0.43
3:I:800:LEU:O	3:I:803:VAL:HG12	2.18	0.43
3:I:1297:LYS:HA	3:I:1297:LYS:HZ3	1.83	0.43
4:J:48:VAL:O	4:J:52:ARG:HG3	2.18	0.43
2:C:73:TYR:N	2:C:73:TYR:CD2	2.86	0.43
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.52	0.43
2:C:1332:SER:O	3:D:243:PRO:HG2	2.18	0.43
3:D:99:ARG:HA	3:D:248:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:138:VAL:O	3:D:143:SER:HB3	2.18	0.43
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.81	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.51	0.43
3:D:901:ARG:HB3	3:D:908:ILE:HA	2.00	0.43
3:D:1247:LYS:H	3:D:1247:LYS:CD	2.24	0.43
2:H:153:PRO:HD2	2:H:404:LYS:HZ1	1.82	0.43
2:H:923:GLY:HA2	3:I:371:LYS:HE3	2.00	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.33	0.43
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.99	0.43
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.17	0.43
1:A:310:ARG:HA	1:A:310:ARG:HE	1.83	0.43
2:C:71:VAL:O	2:C:72:SER:OG	2.32	0.43
2:C:442:VAL:HG12	2:C:443:ASP:N	2.33	0.43
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.18	0.43
3:D:450:HIS:HE2	3:D:625:MET:CE	2.30	0.43
3:D:488:ASN:HD21	4:E:6:VAL:CG1	2.32	0.43
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.82	0.43
5:X:35:ILE:HG23	5:X:36:VAL:N	2.33	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.53	0.43
2:H:964:LEU:HD12	2:H:1025:PHE:CG	2.53	0.43
3:I:205:LEU:HB3	3:I:217:LEU:HD13	2.00	0.43
3:I:252:LEU:HD23	3:I:252:LEU:N	2.31	0.43
3:I:363:LEU:O	3:I:486:SER:OG	2.22	0.43
3:I:589:TYR:O	3:I:591:ILE:HG13	2.19	0.43
3:I:1194:ARG:N	3:I:1194:ARG:HD2	2.33	0.43
1:A:248:GLU:OE1	1:A:248:GLU:N	2.50	0.43
1:A:311:GLY:O	5:X:599:ARG:NE	2.52	0.43
1:B:207:THR:OG1	1:B:208:ASN:N	2.51	0.43
3:D:290:ILE:O	3:D:293:ARG:HG3	2.18	0.43
3:D:1322:ALA:HB1	3:D:1326:GLN:HE21	1.82	0.43
4:E:16:ARG:O	4:E:19:LEU:HB3	2.18	0.43
5:X:551:LEU:HD22	5:X:597:LYS:HD2	2.01	0.43
1:G:51:MET:HA	1:G:52:PRO:HD3	1.87	0.43
2:H:49:LEU:HG	2:H:461:GLU:HB2	2.01	0.43
2:H:127:ILE:O	2:H:127:ILE:HG12	2.19	0.43
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.53	0.43
2:H:735:LYS:HA	2:H:748:ILE:HA	2.01	0.43
2:H:840:SER:HB3	2:H:850:ILE:HD11	2.00	0.43
2:H:1058:ARG:HD3	2:H:1240:ASP:OD1	2.19	0.43
2:H:1268:GLN:NE2	3:I:352:ARG:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:233:LYS:CD	3:I:234:PRO:HD2	2.47	0.43
3:I:539:SER:OG	3:I:540:GLY:N	2.50	0.43
3:I:832:LYS:HB2	3:I:832:LYS:HZ2	1.82	0.43
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.54	0.43
5:Y:573:LEU:HD22	5:Y:588:ARG:HB2	1.99	0.43
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.58	0.43
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.85	0.43
2:C:21:VAL:HG13	2:C:22:LEU:N	2.33	0.43
2:C:221:LEU:HD21	2:C:314:ASN:HD22	1.83	0.43
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.53	0.43
3:D:235:GLU:OE1	3:D:235:GLU:N	2.52	0.43
3:D:620:PHE:O	3:D:624:ILE:HG23	2.18	0.43
3:D:1303:SER:HB2	3:I:1297:LYS:HG2	2.01	0.43
1:F:51:MET:HA	1:F:52:PRO:HD3	1.82	0.43
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.53	0.43
2:H:1185:PRO:HB2	2:H:1186:VAL:H	1.64	0.43
3:I:385:LEU:HD21	3:I:411:ILE:HG13	2.00	0.43
3:I:766:GLY:C	3:I:767:LEU:HD22	2.39	0.43
5:Y:240:ARG:O	5:Y:242:HIS:N	2.51	0.43
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.18	0.43
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.19	0.43
1:A:167:PRO:HG2	1:A:170:ARG:HG3	2.00	0.43
1:A:310:ARG:HA	1:A:310:ARG:NE	2.34	0.43
2:C:888:THR:O	2:C:914:LYS:N	2.41	0.43
3:D:116:PHE:HB3	3:D:237:MET:CE	2.48	0.43
3:D:790:THR:HG22	3:D:928:THR:HG23	2.00	0.43
5:X:333:VAL:HG22	5:X:336:GLU:HB2	2.00	0.43
2:H:153:PRO:HD2	2:H:452:ARG:HD3	1.99	0.43
2:H:1027:LYS:HB2	2:H:1027:LYS:NZ	2.34	0.43
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.53	0.43
2:H:1276:TRP:HA	2:H:1276:TRP:HE3	1.84	0.43
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.80	0.43
3:I:423:LEU:HG	3:I:468:VAL:HG12	2.00	0.43
3:I:704:GLU:HB2	3:I:718:SER:HG	1.84	0.43
3:I:1343:GLU:CA	3:I:1344:LEU:HB2	2.43	0.43
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.31	0.43
1:A:79:LEU:O	1:A:83:LEU:HD13	2.18	0.43
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.53	0.43
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	2.00	0.43
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.19	0.43
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1340:GLU:OE2	3:D:1341:ARG:NH1	2.31	0.43
3:D:239:LEU:HD12	3:D:239:LEU:O	2.19	0.43
5:X:439:ILE:O	5:X:443:ILE:HG13	2.18	0.43
1:G:227:GLN:O	1:G:229:GLU:N	2.52	0.43
2:H:843:THR:HB	2:H:845:LEU:HD22	2.01	0.43
2:H:866:ASP:HA	2:H:872:TYR:CZ	2.54	0.43
3:I:539:SER:O	3:I:541:LEU:N	2.52	0.43
3:I:746:LEU:H	3:I:746:LEU:HD22	1.84	0.43
3:I:1154:ALA:HB1	3:I:1211:SER:HB3	2.00	0.43
1:A:11:PRO:HA	1:A:30:PRO:O	2.18	0.43
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.46	0.43
1:B:232:VAL:O	1:B:233:ASP:HB2	2.18	0.43
2:C:348:SER:O	2:C:352:ARG:HG3	2.19	0.43
2:C:843:THR:HB	2:C:845:LEU:CD2	2.49	0.43
3:D:688:ALA:O	3:D:692:ARG:HG2	2.18	0.43
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.48	0.43
5:X:291:CYS:O	5:X:295:CYS:HB2	2.19	0.43
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.19	0.43
3:I:161:THR:HG22	3:I:162:GLU:N	2.34	0.43
3:I:205:LEU:HD13	3:I:217:LEU:CD2	2.48	0.43
3:I:239:LEU:HD12	3:I:239:LEU:O	2.19	0.43
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.49	0.43
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.36	0.43
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.18	0.43
5:Y:562:ARG:HG3	5:Y:591:GLU:OE1	2.19	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.52	0.43
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.49	0.43
2:C:408:SER:O	2:C:431:LYS:NZ	2.33	0.43
2:C:958:LYS:O	2:C:962:GLU:HG2	2.19	0.43
3:D:173:GLY:O	3:D:175:GLU:HG3	2.18	0.43
3:D:658:GLU:HA	3:D:661:VAL:CG1	2.48	0.43
5:X:465:ARG:O	5:X:468:ARG:HG2	2.19	0.43
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.43
2:H:617:ALA:HB2	2:H:650:VAL:HG21	1.99	0.43
2:H:1233:LEU:HD12	2:H:1233:LEU:O	2.19	0.43
3:I:596:LEU:N	3:I:596:LEU:HD23	2.33	0.43
5:Y:596:ARG:HH21	5:Y:599:ARG:CZ	2.32	0.43
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.84	0.43
1:B:65:LEU:HD23	1:B:65:LEU:N	2.33	0.43
1:B:179:PRO:HB2	1:B:211:ILE:HG22	2.00	0.43
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:HB3	2:C:88:ARG:NH1	2.34	0.43
2:C:270:THR:H	2:C:273:HIS:HD2	1.66	0.43
2:C:337:PHE:O	2:C:338:THR:OG1	2.30	0.43
2:C:345:PRO:O	2:C:349:GLU:HG2	2.18	0.43
2:C:694:ARG:O	2:C:798:GLN:NE2	2.50	0.43
2:C:1258:PRO:HB3	3:D:348:ASP:OD2	2.19	0.43
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.48	0.43
3:D:501:VAL:HG21	3:D:602:SER:HB2	2.00	0.43
5:X:608:ARG:NH1	5:X:608:ARG:HB3	2.33	0.43
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.34	0.43
1:G:182:ARG:CG	1:G:206:GLU:HB3	2.48	0.43
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.84	0.43
2:H:747:GLY:C	2:H:748:ILE:HG13	2.39	0.43
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	2.01	0.43
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.51	0.43
3:I:584:PRO:HD3	3:I:620:PHE:CD1	2.54	0.43
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.19	0.43
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.40	0.42
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.19	0.42
2:C:1027:LYS:HB2	2:C:1027:LYS:NZ	2.34	0.42
2:C:1161:LEU:HD21	2:C:1172:LEU:HD11	2.01	0.42
3:D:165:TYR:O	3:D:169:LEU:HB2	2.19	0.42
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.88	0.42
5:X:278:ASP:O	5:X:282:THR:OG1	2.24	0.42
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.86	0.42
2:H:812:PHE:H	2:H:815:SER:HB2	1.84	0.42
2:H:845:LEU:HD13	2:H:845:LEU:N	2.31	0.42
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.79	0.42
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.49	0.42
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.49	0.42
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.01	0.42
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.44	0.42
1:A:318:LEU:HD13	1:A:318:LEU:N	2.34	0.42
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.83	0.42
2:C:1086:PRO:HA	2:C:1213:TYR:O	2.19	0.42
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.55	0.42
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	2.01	0.42
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.35	0.42
5:X:108:VAL:HB	5:X:110:LEU:HG	2.01	0.42
5:X:456:MET:O	5:X:460:ILE:HG13	2.19	0.42
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ARG:HG3	1:F:183:ILE:HG22	2.01	0.42
1:F:190:ALA:HB2	1:F:200:LYS:HB3	2.01	0.42
1:G:83:LEU:HD11	3:I:527:LEU:O	2.19	0.42
1:G:110:VAL:HG21	1:G:140:ILE:HD11	2.00	0.42
2:H:362:ALA:O	2:H:366:ILE:HG13	2.19	0.42
3:I:210:SER:O	3:I:214:ARG:HG3	2.19	0.42
1:A:253:LEU:HB3	1:A:321:TRP:CH2	2.55	0.42
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.49	0.42
2:C:68:LEU:HG	2:C:100:LEU:HD23	2.01	0.42
2:C:590:PRO:HB3	2:C:605:TYR:HE1	1.84	0.42
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.49	0.42
3:D:573:THR:HG23	3:D:576:ARG:H	1.83	0.42
3:D:681:LYS:HB2	3:D:681:LYS:HZ2	1.82	0.42
3:D:1282:TYR:HA	3:D:1285:VAL:CG2	2.50	0.42
5:X:9:LEU:HD22	5:X:60:PRO:HB3	2.00	0.42
5:X:457:ILE:HG23	5:X:461:ASN:ND2	2.34	0.42
1:G:185:TYR:HB2	1:G:201:LEU:HD11	2.00	0.42
2:H:56:VAL:HB	2:H:57:PHE:H	1.48	0.42
2:H:469:VAL:O	2:H:472:GLU:HB3	2.19	0.42
2:H:1219:GLU:OE2	3:I:634:ARG:NH1	2.52	0.42
3:I:179:LYS:HD3	3:I:179:LYS:N	2.34	0.42
3:I:1345:ARG:HG2	3:I:1370:MET:CE	2.48	0.42
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.83	0.42
1:A:323:PRO:HA	1:A:324:ALA:HA	1.74	0.42
1:B:51:MET:HA	1:B:52:PRO:HD3	1.87	0.42
2:C:73:TYR:O	2:C:74:ARG:HB2	2.19	0.42
2:C:747:GLY:C	2:C:748:ILE:HG13	2.40	0.42
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.20	0.42
3:D:378:LYS:HD2	3:D:382:TYR:CZ	2.54	0.42
3:D:607:THR:O	3:D:611:ILE:HG12	2.19	0.42
3:D:681:LYS:O	3:D:685:ILE:HG13	2.19	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
5:X:451:ARG:O	5:X:452:ILE:HG13	2.20	0.42
5:X:532:LEU:O	5:X:536:THR:HG23	2.20	0.42
5:X:543:ALA:O	5:X:547:VAL:HG23	2.19	0.42
1:G:191:ARG:HD3	1:G:191:ARG:HA	1.88	0.42
2:H:42:ASP:HB2	2:H:47:TYR:CG	2.53	0.42
2:H:161:LYS:NZ	2:H:161:LYS:HB3	2.33	0.42
2:H:297:VAL:HB	2:H:317:LEU:HD21	2.01	0.42
3:I:573:THR:CG2	3:I:576:ARG:HG3	2.49	0.42
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:555:TYR:OH	2:C:654:ASP:OD2	2.36	0.42
2:C:1105:SER:HB2	3:D:731:ARG:HD3	2.01	0.42
3:D:74:LYS:HB3	3:D:74:LYS:NZ	2.35	0.42
3:D:130:MET:HA	3:D:131:PRO:HD3	1.96	0.42
3:D:238:ILE:HG13	3:D:238:ILE:O	2.18	0.42
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.20	0.42
3:D:857:LEU:HB2	3:D:860:ARG:HB2	2.02	0.42
3:D:910:ASN:HB3	4:E:15:ASN:HA	2.02	0.42
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	2.02	0.42
5:X:311:THR:HG21	5:X:348:GLU:CD	2.40	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.84	0.42
3:I:238:ILE:O	3:I:238:ILE:HG13	2.19	0.42
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.42
1:A:158:ARG:HB2	1:A:158:ARG:HH21	1.84	0.42
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.54	0.42
2:C:896:THR:O	2:C:899:GLU:N	2.50	0.42
2:C:1111:GLN:HG3	2:C:1230:MET:HE2	2.01	0.42
3:D:77:ARG:HA	3:D:77:ARG:HD2	1.76	0.42
3:D:384:LYS:HA	3:D:384:LYS:HD2	1.85	0.42
5:X:299:LYS:O	5:X:303:ILE:HG12	2.19	0.42
1:F:163:GLU:HG3	1:F:170:ARG:NH1	2.20	0.42
1:G:110:VAL:HB	1:G:131:CYS:HB2	2.00	0.42
2:H:106:GLU:CB	2:H:107:ARG:HA	2.49	0.42
3:I:12:THR:C	3:I:13:LYS:HD2	2.40	0.42
3:I:700:ASN:O	3:I:704:GLU:HG2	2.19	0.42
3:I:1341:ARG:HD3	3:I:1343:GLU:CD	2.39	0.42
1:A:29:GLU:O	1:A:31:LEU:N	2.52	0.42
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.49	0.42
2:C:814:ASP:OD1	2:C:1106:ARG:NH1	2.50	0.42
3:D:50:LYS:HB3	3:D:50:LYS:HZ2	1.85	0.42
3:D:1372:ARG:NH2	3:I:853:THR:HG21	2.35	0.42
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.54	0.42
2:H:593:LYS:HD2	2:H:604:HIS:NE2	2.35	0.42
2:H:632:ASP:O	2:H:633:LEU:HD23	2.20	0.42
2:H:843:THR:HB	2:H:845:LEU:CD2	2.50	0.42
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.34	0.42
3:I:378:LYS:HD2	3:I:382:TYR:OH	2.19	0.42
3:I:1307:LEU:N	3:I:1307:LEU:HD23	2.35	0.42
1:B:22:THR:HB	1:B:207:THR:O	2.20	0.42
2:C:49:LEU:HG	2:C:461:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:VAL:HG22	2:C:123:TYR:N	2.34	0.42
2:C:551:HIS:CE1	2:C:553:THR:HG1	2.37	0.42
2:C:943:LYS:O	2:C:947:GLU:HG2	2.19	0.42
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.34	0.42
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	2.00	0.42
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.79	0.42
3:D:122:SER:HB2	3:D:132:LEU:HB2	2.00	0.42
3:D:535:ARG:HB3	3:D:541:LEU:HD11	2.02	0.42
1:G:178:SER:HA	1:G:179:PRO:HD3	1.88	0.42
2:H:59:ILE:HG12	2:H:65:ASN:O	2.20	0.42
2:H:72:SER:O	2:H:98:VAL:HG23	2.20	0.42
2:H:91:THR:HG22	2:H:138:ILE:HA	2.02	0.42
2:H:620:ASN:ND2	3:I:768:ASN:HB2	2.35	0.42
2:H:848:GLU:CD	2:H:888:THR:HG22	2.40	0.42
2:H:1238:LEU:HD12	2:H:1239:VAL:N	2.34	0.42
3:I:267:ASP:OD2	3:I:270:ARG:NH2	2.52	0.42
3:I:370:LYS:HG3	3:I:371:LYS:H	1.84	0.42
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.43	0.42
2:C:127:ILE:O	2:C:127:ILE:HG12	2.20	0.42
2:C:237:LEU:HB2	2:C:287:VAL:O	2.19	0.42
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.34	0.42
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.34	0.42
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.34	0.42
3:D:205:LEU:HB3	3:D:217:LEU:HB3	2.01	0.42
3:D:646:ILE:HG22	3:D:741:ALA:O	2.19	0.42
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.20	0.42
5:X:448:ARG:HD3	5:X:450:ILE:HG13	2.01	0.42
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.35	0.42
2:H:685:MET:HE1	2:H:1073:LYS:HE2	2.00	0.42
3:I:222:LYS:HZ1	3:I:1276:GLU:HB2	1.84	0.42
3:I:515:ARG:HH22	3:I:717:VAL:C	2.21	0.42
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.20	0.42
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.85	0.42
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.84	0.42
2:C:429:MET:O	2:C:433:ILE:HG13	2.20	0.42
2:C:686:GLN:O	2:C:688:GLN:N	2.47	0.42
2:C:961:SER:O	2:C:965:GLN:HG3	2.20	0.42
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.20	0.42
3:D:161:THR:HG22	3:D:162:GLU:N	2.35	0.42
3:D:313:GLY:H	5:X:38:SER:HB3	1.83	0.42
3:D:390:LEU:N	3:D:390:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:543:SER:O	3:D:574:VAL:HB	2.20	0.42
3:D:1343:GLU:CA	3:D:1344:LEU:HB2	2.36	0.42
1:F:11:PRO:HA	1:F:30:PRO:O	2.20	0.42
1:F:31:LEU:HB2	1:F:199:ASP:O	2.20	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.42
2:H:122:VAL:HG22	2:H:123:TYR:N	2.35	0.42
2:H:488:MET:HE3	2:H:490:GLN:N	2.35	0.42
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.53	0.42
2:H:1117:LEU:HD11	2:H:1182:ILE:HD13	2.02	0.42
2:H:1146:GLN:CD	2:H:1160:ASP:HB2	2.41	0.42
2:H:1269:ARG:HD3	2:H:1269:ARG:N	2.35	0.42
3:I:31:ARG:HD2	3:I:104:HIS:CD2	2.55	0.42
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.85	0.42
3:I:492:SER:HA	3:I:493:PRO:HD3	1.94	0.42
5:Y:99:ARG:O	5:Y:99:ARG:HD3	2.20	0.42
1:A:45:ARG:NE	1:B:38:THR:OG1	2.53	0.41
1:A:246:LYS:HD3	1:A:246:LYS:N	2.35	0.41
1:A:299:SER:O	1:A:303:ILE:HG12	2.20	0.41
2:C:208:ILE:HD11	2:C:365:GLU:HB3	2.01	0.41
2:C:221:LEU:HD13	2:C:298:ALA:HA	2.01	0.41
2:C:517:GLN:NE2	2:C:760:ASN:OD1	2.53	0.41
2:C:669:PRO:HG2	2:C:1070:HIS:HE1	1.85	0.41
2:C:1272:GLU:HG3	2:C:1276:TRP:CE2	2.55	0.41
3:D:66:LYS:NZ	3:D:66:LYS:HB3	2.35	0.41
3:D:800:LEU:O	3:D:803:VAL:HG12	2.20	0.41
3:D:1290:ARG:HH22	3:I:1301:THR:HG22	1.85	0.41
5:X:147:GLN:O	5:X:151:VAL:HG23	2.20	0.41
1:F:182:ARG:HH11	2:H:1092:THR:HG22	1.83	0.41
1:G:52:PRO:HB2	1:G:53:GLY:H	1.59	0.41
2:H:59:ILE:HB	2:H:480:SER:OG	2.20	0.41
2:H:255:ILE:HD12	2:H:263:VAL:HB	2.02	0.41
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.35	0.41
3:I:109:SER:OG	3:I:296:LYS:HE2	2.20	0.41
3:I:293:ARG:NH1	5:Y:104:GLU:HB2	2.34	0.41
3:I:356:THR:O	3:I:448:GLN:HA	2.20	0.41
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.45	0.41
2:C:115:LYS:O	2:C:116:ASP:HB2	2.20	0.41
2:C:1004:ASP:OD1	2:C:1004:ASP:N	2.53	0.41
2:C:1211:ARG:H	2:C:1211:ARG:HG3	1.68	0.41
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.34	0.41
3:D:26:SER:O	3:D:30:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:646:ILE:H	3:D:646:ILE:HG13	1.65	0.41
3:D:789:LYS:HB3	3:D:932:MET:SD	2.60	0.41
3:D:822:MET:HG2	3:D:839:VAL:HG22	2.02	0.41
3:D:887:SER:HA	3:I:1292:LEU:HD23	2.02	0.41
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.35	0.41
5:X:112:THR:HG22	5:X:113:ARG:N	2.31	0.41
2:H:208:ILE:HD11	2:H:365:GLU:HB3	2.02	0.41
2:H:560:PRO:HA	3:I:780:ARG:NH2	2.35	0.41
3:I:305:ALA:O	3:I:309:ASN:ND2	2.53	0.41
3:I:492:SER:HB2	3:I:499:ILE:HB	2.01	0.41
3:I:605:LEU:O	3:I:605:LEU:HD13	2.20	0.41
3:I:607:THR:O	3:I:611:ILE:HG12	2.20	0.41
5:Y:122:ARG:NH2	5:Y:378:GLU:OE2	2.50	0.41
5:Y:316:PHE:CZ	5:Y:320:ILE:HD11	2.55	0.41
1:A:183:ILE:HD11	1:A:205:MET:HG3	2.02	0.41
2:C:51:ALA:C	2:C:53:PHE:H	2.23	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.55	0.41
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.55	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.41
3:D:275:ARG:HD2	3:D:302:ALA:HB2	2.03	0.41
3:D:382:TYR:CE1	3:D:401:VAL:HG21	2.56	0.41
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.20	0.41
4:E:65:ASP:O	4:E:69:ARG:HG3	2.21	0.41
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.50	0.41
1:G:56:VAL:HG12	1:G:173:VAL:HG11	2.01	0.41
2:H:582:ASN:HB2	2:H:588:GLU:HG3	2.01	0.41
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	2.02	0.41
2:H:704:MET:HA	2:H:704:MET:HE2	2.02	0.41
2:H:773:LEU:CD1	2:H:773:LEU:H	2.32	0.41
2:H:1195:ILE:O	2:H:1199:LEU:HG	2.21	0.41
2:H:1286:THR:N	3:I:479:GLU:OE2	2.50	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.02	0.41
3:I:50:LYS:HA	3:I:51:PRO:HD3	1.95	0.41
3:I:646:ILE:H	3:I:646:ILE:HG13	1.66	0.41
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.31	0.41
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.20	0.41
5:Y:143:TYR:O	5:Y:147:GLN:HG2	2.19	0.41
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.46	0.41
2:C:773:LEU:C	2:C:773:LEU:HD22	2.41	0.41
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.35	0.41
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:377:PHE:O	3:D:381:ILE:HG13	2.20	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.03	0.41
3:D:533:ALA:HB2	3:D:578:ILE:HD13	2.02	0.41
3:D:700:ASN:O	3:D:704:GLU:HG2	2.21	0.41
3:D:905:ARG:NE	3:D:907:HIS:HB2	2.29	0.41
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.35	0.41
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.83	0.41
5:X:276:MET:O	5:X:280:VAL:HG23	2.20	0.41
5:X:453:PRO:HB2	5:X:455:HIS:CE1	2.55	0.41
5:X:598:LEU:O	5:X:599:ARG:HD2	2.19	0.41
2:H:148:GLN:HB2	2:H:511:LEU:HD21	2.02	0.41
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	2.01	0.41
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	2.02	0.41
3:I:325:LYS:HB3	5:Y:508:GLU:HG3	2.02	0.41
3:I:438:GLU:HA	3:I:439:PRO:HD3	1.87	0.41
3:I:591:ILE:HD12	3:I:592:VAL:HG13	2.03	0.41
3:I:809:VAL:CG1	3:I:913:GLU:H	2.34	0.41
3:I:899:TYR:CZ	3:I:915:ILE:HD12	2.55	0.41
3:I:910:ASN:OD1	4:J:15:ASN:HA	2.21	0.41
3:I:1357:ILE:HD12	3:I:1357:ILE:N	2.35	0.41
3:I:1368:ASP:O	3:I:1372:ARG:HB2	2.19	0.41
5:Y:383:ASN:HB2	5:Y:412:LEU:HD21	2.02	0.41
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.20	0.41
2:C:1210:ILE:HG23	2:C:1211:ARG:NH1	2.35	0.41
3:D:113:HIS:O	3:D:117:LEU:HB2	2.19	0.41
3:D:605:LEU:O	3:D:605:LEU:HD13	2.21	0.41
3:D:803:VAL:HG11	3:D:1309:ILE:HG13	2.01	0.41
3:D:1257:VAL:HA	3:D:1260:MET:CB	2.50	0.41
5:X:45:ILE:C	5:X:45:ILE:HD12	2.41	0.41
5:X:283:GLN:NE2	5:X:343:LYS:HD2	2.35	0.41
5:X:290:LEU:O	5:X:294:GLN:HB3	2.20	0.41
5:X:561:MET:SD	5:X:576:VAL:HG22	2.61	0.41
1:F:33:ARG:HA	1:F:33:ARG:HD3	1.89	0.41
1:G:82:LEU:O	1:G:86:LYS:HG3	2.20	0.41
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.40	0.41
2:H:57:PHE:HA	2:H:476:LYS:NZ	2.35	0.41
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.19	0.41
2:H:1313:HIS:HD2	3:I:474:LEU:HD23	1.86	0.41
3:I:233:LYS:HB3	3:I:236:TRP:CE2	2.55	0.41
3:I:473:THR:HB	3:I:476:ALA:CB	2.49	0.41
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:790:THR:HG22	3:I:928:THR:HG23	2.01	0.41
3:I:850:LYS:NZ	3:I:873:GLU:HB3	2.36	0.41
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.45	0.41
1:B:118:ASP:HB3	1:B:121:VAL:HB	2.03	0.41
2:C:500:ALA:O	2:C:504:GLU:HB2	2.20	0.41
2:C:560:PRO:HB2	3:D:776:THR:OG1	2.20	0.41
2:C:905:ILE:HG12	5:X:595:LEU:HD22	2.02	0.41
3:D:843:VAL:HG11	3:D:897:HIS:HB3	2.01	0.41
5:X:410:ILE:O	5:X:414:LYS:HG3	2.21	0.41
1:G:33:ARG:NE	1:G:197:ASP:HB2	2.36	0.41
2:H:333:ILE:N	2:H:333:ILE:HD12	2.36	0.41
2:H:453:ILE:O	2:H:453:ILE:HG23	2.21	0.41
2:H:680:LEU:O	2:H:680:LEU:HD23	2.21	0.41
2:H:759:SER:HB3	2:H:763:THR:H	1.85	0.41
2:H:896:THR:O	2:H:899:GLU:N	2.50	0.41
2:H:943:LYS:O	2:H:947:GLU:HG2	2.19	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.51	0.41
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.56	0.41
3:I:534:GLU:O	3:I:538:ARG:HB2	2.20	0.41
3:I:679:TYR:O	3:I:683:ILE:HG13	2.19	0.41
1:A:107:ILE:HG12	1:A:134:THR:O	2.21	0.41
1:B:7:GLU:O	1:B:8:PHE:CG	2.74	0.41
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.56	0.41
2:C:68:LEU:HD22	2:C:475:VAL:HG21	2.02	0.41
2:C:177:ILE:HD12	2:C:177:ILE:N	2.36	0.41
5:X:240:ARG:HD3	5:X:244:THR:CB	2.44	0.41
2:H:120:GLN:HG3	2:H:121:GLU:N	2.35	0.41
2:H:453:ILE:HG22	2:H:585:GLY:O	2.21	0.41
2:H:902:LEU:HD21	5:Y:608:ARG:CG	2.45	0.41
2:H:1270:PHE:HB3	2:H:1271:GLY:H	1.61	0.41
3:I:362:ARG:HB3	3:I:363:LEU:H	1.65	0.41
3:I:450:HIS:CE1	3:I:452:LEU:HB2	2.55	0.41
3:I:646:ILE:HG22	3:I:741:ALA:O	2.21	0.41
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.50	0.41
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.21	0.41
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.21	0.41
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.02	0.41
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.93	0.41
2:C:529:ARG:HB2	2:C:529:ARG:NH1	2.35	0.41
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.48	0.41
2:C:1293:VAL:HA	2:C:1297:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:288:PRO:O	3:D:292:VAL:HG12	2.20	0.41
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.51	0.41
5:X:113:ARG:O	5:X:117:ILE:HD13	2.21	0.41
2:H:69:GLN:HE22	2:H:101:ARG:NH2	2.13	0.41
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.81	0.41
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.86	0.41
2:H:429:MET:O	2:H:433:ILE:HG13	2.21	0.41
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.21	0.41
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.35	0.41
2:H:1314:GLN:HG2	2:H:1315:MET:H	1.86	0.41
3:I:412:LEU:O	3:I:415:VAL:HG22	2.21	0.41
3:I:479:GLU:O	3:I:483:LEU:HB2	2.21	0.41
3:I:1361:THR:O	4:J:21:LEU:HD21	2.20	0.41
1:B:74:VAL:HG12	1:B:76:GLU:H	1.85	0.41
1:B:152:TYR:OH	3:D:535:ARG:NH1	2.47	0.41
2:C:453:ILE:O	2:C:453:ILE:HG23	2.21	0.41
2:C:521:LEU:HD22	2:C:667:LEU:HD12	2.02	0.41
2:C:699:LEU:H	2:C:799:ASN:ND2	2.16	0.41
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.20	0.41
2:C:980:VAL:O	2:C:984:VAL:HG22	2.21	0.41
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.86	0.41
3:D:12:THR:C	3:D:13:LYS:HD2	2.42	0.41
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.38	0.41
3:D:214:ARG:O	3:D:218:THR:HG22	2.21	0.41
3:D:423:LEU:HB3	3:D:466:MET:CE	2.50	0.41
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.86	0.41
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.21	0.41
1:F:222:THR:O	1:F:226:GLU:HG3	2.21	0.41
1:G:152:TYR:OH	3:I:535:ARG:NH1	2.45	0.41
1:G:207:THR:OG1	1:G:208:ASN:N	2.53	0.41
1:G:222:THR:O	1:G:226:GLU:HG2	2.21	0.41
2:H:176:ILE:HD12	2:H:184:LEU:HD23	2.02	0.41
2:H:177:ILE:HD12	2:H:177:ILE:N	2.36	0.41
2:H:205:PRO:O	2:H:208:ILE:HG22	2.21	0.41
2:H:221:LEU:HD22	2:H:336:LEU:HD11	2.02	0.41
2:H:225:PHE:CE2	2:H:347:ILE:HB	2.56	0.41
2:H:302:ILE:HA	2:H:309:LEU:HA	2.03	0.41
2:H:431:LYS:O	2:H:435:ILE:HG13	2.20	0.41
2:H:961:SER:O	2:H:965:GLN:HG3	2.21	0.41
2:H:999:GLU:HG2	2:H:1000:LEU:H	1.85	0.41
2:H:1043:ALA:C	2:H:1045:GLY:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1107:MET:N	2:H:1107:MET:SD	2.94	0.41
2:H:1169:VAL:HG23	2:H:1172:LEU:HD11	2.02	0.41
3:I:390:LEU:N	3:I:390:LEU:HD12	2.34	0.41
3:I:500:ILE:H	3:I:500:ILE:CD1	2.34	0.41
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.41	0.41
5:Y:456:MET:O	5:Y:460:ILE:HG13	2.19	0.41
5:Y:477:GLU:OE1	5:Y:477:GLU:N	2.53	0.41
1:B:129:VAL:HG11	1:B:132:HIS:HE1	1.86	0.41
2:C:310:ILE:O	2:C:311:CYS:HB3	2.21	0.41
2:C:563:THR:HG21	3:D:780:ARG:CZ	2.50	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CZ3	2.56	0.41
3:D:583:VAL:HG13	3:D:584:PRO:HD2	2.03	0.41
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.43	0.41
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.51	0.41
2:H:22:LEU:HD13	2:H:23:ASP:O	2.21	0.41
2:H:145:ILE:CG2	2:H:456:VAL:HG22	2.51	0.41
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.53	0.41
3:I:620:PHE:O	3:I:624:ILE:HG23	2.21	0.41
1:B:181:GLU:HG2	3:D:531:LYS:HD3	2.02	0.40
2:C:54:ARG:HG2	2:C:55:SER:CB	2.49	0.40
2:C:68:LEU:HD12	2:C:68:LEU:HA	1.91	0.40
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.56	0.40
2:C:1092:THR:HA	2:C:1093:PRO:HD3	1.88	0.40
3:D:52:GLU:OE1	5:X:451:ARG:HD2	2.21	0.40
3:D:746:LEU:HD22	3:D:746:LEU:N	2.36	0.40
5:X:431:ALA:O	5:X:435:ILE:HG13	2.21	0.40
1:F:82:LEU:O	1:F:86:LYS:HG3	2.21	0.40
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.03	0.40
2:H:88:ARG:NH1	2:H:88:ARG:HB3	2.36	0.40
2:H:94:ALA:O	2:H:126:GLU:HG2	2.21	0.40
2:H:202:ARG:NE	2:H:369:MET:HG2	2.36	0.40
2:H:668:ILE:HD12	2:H:671:LEU:HD13	2.02	0.40
2:H:816:ILE:HG13	2:H:1098:LEU:CD2	2.35	0.40
3:I:139:LEU:C	3:I:139:LEU:HD22	2.41	0.40
3:I:194:LEU:O	3:I:198:CYS:HB2	2.21	0.40
3:I:773:PHE:O	3:I:776:THR:HG22	2.21	0.40
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.90	0.40
2:C:174:ALA:HB2	2:C:432:LEU:HD13	2.03	0.40
2:C:619:ALA:HA	2:C:653:MET:HE2	2.02	0.40
2:C:843:THR:HG22	2:C:844:LYS:N	2.36	0.40
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.86	0.40
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.21	0.40
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	2.03	0.40
4:E:77:ALA:O	4:E:80:LEU:HD22	2.20	0.40
5:X:343:LYS:O	5:X:346:GLN:HB3	2.21	0.40
2:H:54:ARG:N	2:H:55:SER:C	2.75	0.40
2:H:977:ALA:O	2:H:980:VAL:HG12	2.21	0.40
2:H:1108:ASN:O	2:H:1108:ASN:ND2	2.54	0.40
3:I:122:SER:OG	3:I:132:LEU:HD13	2.21	0.40
3:I:155:GLU:H	3:I:155:GLU:CD	2.25	0.40
3:I:475:GLU:HG2	3:I:475:GLU:H	1.74	0.40
3:I:810:THR:HG22	3:I:893:GLY:HA3	2.02	0.40
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	2.02	0.40
5:Y:281:ARG:HD3	5:Y:359:LYS:NZ	2.37	0.40
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.40
2:C:1060:ILE:H	2:C:1060:ILE:HG12	1.70	0.40
3:D:292:VAL:HG22	3:D:296:LYS:HE3	2.03	0.40
3:D:832:LYS:HZ2	3:D:832:LYS:HB2	1.86	0.40
5:X:254:GLU:O	5:X:258:GLN:HG3	2.21	0.40
5:X:580:PHE:O	5:X:582:VAL:N	2.55	0.40
2:H:103:VAL:HG22	2:H:104:ILE:H	1.86	0.40
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.56	0.40
2:H:488:MET:HE2	2:H:488:MET:N	2.36	0.40
2:H:1106:ARG:O	2:H:1108:ASN:N	2.43	0.40
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.22	0.40
2:H:1241:ASP:N	2:H:1241:ASP:OD2	2.54	0.40
1:A:22:THR:HB	1:A:207:THR:O	2.21	0.40
1:A:91:ARG:NH2	1:A:209:GLY:O	2.55	0.40
1:B:52:PRO:HB2	1:B:53:GLY:H	1.61	0.40
2:C:697:LYS:HD2	2:C:793:GLU:OE2	2.22	0.40
2:C:898:GLU:HG3	5:X:565:ILE:CD1	2.51	0.40
2:C:1166:ASP:C	2:C:1168:GLU:H	2.23	0.40
3:D:182:ALA:O	3:D:185:ILE:HG22	2.21	0.40
3:D:217:LEU:O	3:D:221:ILE:HG23	2.21	0.40
3:D:586:GLY:O	3:D:587:LEU:HB2	2.22	0.40
3:D:704:GLU:O	3:D:705:THR:OG1	2.30	0.40
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.22	0.40
5:X:459:THR:O	5:X:463:LEU:HD13	2.21	0.40
1:F:167:PRO:HG2	1:F:170:ARG:HG3	2.03	0.40
3:I:801:VAL:O	3:I:805:GLN:HG2	2.21	0.40
3:I:1290:ARG:HD2	3:I:1299:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:O	1:B:19:VAL:HG12	2.22	0.40
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.85	0.40
2:C:542:ARG:HG2	2:C:543:ALA:N	2.36	0.40
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	2.02	0.40
3:D:42:GLU:HG3	5:X:451:ARG:NH2	2.37	0.40
3:D:286:ALA:HB3	5:X:413:MET:SD	2.62	0.40
3:D:310:GLY:O	3:D:314:ARG:HG2	2.20	0.40
3:D:428:THR:HG23	3:D:433:GLY:HA3	2.03	0.40
5:X:295:CYS:SG	5:X:330:LEU:HD23	2.61	0.40
1:F:207:THR:OG1	1:F:208:ASN:N	2.54	0.40
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.51	0.40
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.03	0.40
2:H:517:GLN:NE2	2:H:760:ASN:OD1	2.54	0.40
2:H:773:LEU:O	2:H:773:LEU:HD22	2.22	0.40
2:H:1314:GLN:O	3:I:473:THR:HG23	2.21	0.40
3:I:555:TYR:HD1	3:I:589:TYR:HE2	1.68	0.40
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.48	0.40
3:I:1195:GLN:OE1	3:I:1195:GLN:N	2.50	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	321/329 (98%)	266 (83%)	41 (13%)	14 (4%)	2 25
1	B	217/329 (66%)	186 (86%)	24 (11%)	7 (3%)	4 32
1	F	227/329 (69%)	196 (86%)	26 (12%)	5 (2%)	6 38
1	G	213/329 (65%)	188 (88%)	21 (10%)	4 (2%)	8 41
2	C	1333/1342 (99%)	1069 (80%)	213 (16%)	51 (4%)	3 28
2	H	1333/1342 (99%)	1070 (80%)	213 (16%)	50 (4%)	3 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1154/1407 (82%)	922 (80%)	189 (16%)	43 (4%)	3	29
3	I	1154/1407 (82%)	929 (80%)	183 (16%)	42 (4%)	3	29
4	E	88/91 (97%)	76 (86%)	8 (9%)	4 (4%)	2	25
4	J	74/91 (81%)	64 (86%)	6 (8%)	4 (5%)	2	22
5	X	511/613 (83%)	450 (88%)	45 (9%)	16 (3%)	4	32
5	Y	454/613 (74%)	411 (90%)	32 (7%)	11 (2%)	6	37
All	All	7079/8222 (86%)	5827 (82%)	1001 (14%)	251 (4%)	3	30

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	B	20	SER
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	686	GLN
2	C	748	ILE
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
2	C	1341	ASP
3	D	120	LEU
3	D	311	ARG
3	D	406	ALA
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1344	LEU
4	E	6	VAL
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
2	H	21	VAL

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Mol	Chain	Res	Type
2	H	39	ILE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	669	PRO
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP
3	I	120	LEU
3	I	406	ALA
3	I	710	ASP
3	I	847	ASP
3	I	851	PRO
5	Y	241	SER
1	A	52	PRO
1	B	19	VAL
2	C	79	VAL
2	C	669	PRO
2	C	699	LEU
2	C	753	LEU
2	C	1239	VAL
2	C	1256	GLN
3	D	89	GLY
3	D	155	GLU
3	D	255	LEU
3	D	316	ILE
3	D	390	LEU
3	D	404	GLU
3	D	542	ALA
3	D	595	ALA
3	D	703	THR
3	D	708	ASN
3	D	721	SER
3	D	851	PRO
3	D	887	SER
3	D	901	ARG
3	D	913	GLU
3	D	1274	PHE
3	D	1339	GLY
4	E	35	LYS

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Mol	Chain	Res	Type
5	X	20	GLY
5	X	25	ALA
1	F	160	HIS
1	G	177	TYR
2	H	78	PRO
2	H	170	VAL
2	H	535	PRO
2	H	736	VAL
2	H	753	LEU
2	H	1186	VAL
3	I	53	ARG
3	I	89	GLY
3	I	155	GLU
3	I	390	LEU
3	I	404	GLU
3	I	540	GLY
3	I	542	ALA
3	I	595	ALA
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	913	GLU
3	I	914	ALA
3	I	1268	ASN
3	I	1339	GLY
3	I	1344	LEU
4	J	6	VAL
4	J	35	LYS
5	Y	108	VAL
5	Y	490	PRO
1	A	14	VAL
1	A	193	GLU
1	B	177	TYR
1	B	235	ARG
2	C	53	PHE
2	C	56	VAL
2	C	78	PRO
2	C	143	ARG
2	C	437	ASN
2	C	487	LEU
2	C	740	GLU
2	C	908	GLU

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Mol	Chain	Res	Type
2	C	1107	MET
2	C	1236	ASN
2	C	1240	ASP
2	C	1270	PHE
3	D	53	ARG
3	D	559	ALA
3	D	707	ILE
3	D	902	ASP
5	X	23	THR
5	X	491	GLU
5	X	581	ASP
1	F	188	GLU
1	G	188	GLU
1	G	228	LEU
2	H	13	LYS
2	H	56	VAL
2	H	298	ALA
2	H	437	ASN
2	H	740	GLU
2	H	908	GLU
2	H	1236	ASN
2	H	1239	VAL
2	H	1240	ASP
2	H	1256	GLN
2	H	1270	PHE
3	I	255	LEU
3	I	345	LYS
3	I	559	ALA
3	I	703	THR
3	I	901	ARG
3	I	1195	GLN
5	Y	491	GLU
5	Y	504	PRO
5	Y	564	GLY
1	A	93	GLN
1	A	160	HIS
1	A	166	ARG
1	A	187	VAL
1	A	188	GLU
1	A	194	GLN
1	B	188	GLU
2	C	13	LYS

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Mol	Chain	Res	Type
2	C	44	GLU
2	C	69	GLN
2	C	167	SER
2	C	736	VAL
2	C	812	PHE
2	C	1080	ASN
2	C	1139	ALA
2	C	1237	HIS
3	D	731	ARG
3	D	848	VAL
3	D	914	ALA
3	D	1195	GLN
5	X	50	ASP
5	X	108	VAL
5	X	308	GLY
5	X	504	PRO
5	X	514	ASP
1	F	153	VAL
2	H	43	PRO
2	H	44	GLU
2	H	143	ARG
2	H	167	SER
2	H	699	LEU
2	H	812	PHE
2	H	895	LEU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1107	MET
2	H	1181	PRO
3	I	210	SER
3	I	731	ARG
3	I	848	VAL
3	I	887	SER
3	I	888	CYS
3	I	902	ASP
5	Y	308	GLY
5	Y	514	ASP
5	Y	581	ASP
2	C	298	ALA
2	C	746	ALA
2	C	895	LEU

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Mol	Chain	Res	Type
2	C	1093	PRO
2	C	1238	LEU
3	D	598	LYS
3	D	888	CYS
3	D	1174	ARG
4	E	5	THR
5	X	564	GLY
5	X	600	HIS
1	F	166	ARG
2	H	53	PHE
2	H	104	ILE
2	H	487	LEU
2	H	488	MET
2	H	1139	ALA
2	H	1237	HIS
3	I	62	PHE
3	I	1174	ARG
3	I	1194	ARG
3	I	1274	PHE
4	J	5	THR
5	Y	600	HIS
1	A	163	GLU
1	B	49	SER
2	C	543	ALA
3	D	62	PHE
3	D	210	SER
3	D	590	SER
3	D	1173	ARG
3	D	1184	ASP
3	D	1194	ARG
4	E	59	ILE
2	H	746	ALA
3	I	598	LYS
3	I	712	GLN
4	J	59	ILE
1	A	232	VAL
1	A	322	PRO
2	C	104	ILE
3	D	540	GLY
2	H	1045	GLY
3	I	1184	ASP
3	D	742	GLY

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Mol	Chain	Res	Type
5	X	97	PRO
3	I	742	GLY
5	Y	97	PRO
2	C	373	GLY
2	H	373	GLY
2	C	117	ILE
2	C	1045	GLY
5	X	35	ILE
2	H	489	PRO
1	A	153	VAL
3	I	850	LYS
2	C	1181	PRO

5.3.2 Protein sidechains (i)

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	281/286 (98%)	274 (98%)	7 (2%)	47	69
1	B	189/286 (66%)	185 (98%)	4 (2%)	53	73
1	F	197/286 (69%)	192 (98%)	5 (2%)	47	69
1	G	185/286 (65%)	180 (97%)	5 (3%)	44	67
2	C	1150/1157 (99%)	1087 (94%)	63 (6%)	21	51
2	H	1150/1157 (99%)	1092 (95%)	58 (5%)	24	53
3	D	971/1168 (83%)	919 (95%)	52 (5%)	22	52
3	I	971/1168 (83%)	921 (95%)	50 (5%)	24	53
4	E	74/75 (99%)	71 (96%)	3 (4%)	30	58
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	460/540 (85%)	442 (96%)	18 (4%)	32	59
5	Y	407/540 (75%)	391 (96%)	16 (4%)	32	59
All	All	6100/7024 (87%)	5819 (95%)	281 (5%)	27	55

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	117	HIS
1	A	158	ARG
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	77	ASP
1	B	196	THR
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	73	TYR
2	C	80	PHE
2	C	88	ARG
2	C	114	VAL
2	C	121	GLU
2	C	127	ILE
2	C	133	ASN
2	C	150	HIS
2	C	163	LYS
2	C	479	LEU
2	C	487	LEU
2	C	514	PHE
2	C	554	HIS
2	C	600	THR
2	C	645	PHE
2	C	661	VAL
2	C	690	VAL
2	C	741	MET
2	C	773	LEU
2	C	800	MET
2	C	807	TRP
2	C	817	LEU
2	C	845	LEU

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Mol	Chain	Res	Type
2	C	908	GLU
2	C	941	LYS
2	C	944	ARG
2	C	953	LEU
2	C	955	GLN
2	C	964	LEU
2	C	975	ILE
2	C	994	ARG
2	C	1002	LEU
2	C	1010	GLN
2	C	1011	LEU
2	C	1017	GLN
2	C	1032	LYS
2	C	1042	LEU
2	C	1106	ARG
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1211	ARG
2	C	1233	LEU
2	C	1248	THR
2	C	1259	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1276	TRP
2	C	1288	GLN
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
2	C	1341	ASP
3	D	13	LYS
3	D	20	ILE
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET

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Mol	Chain	Res	Type
3	D	169	LEU
3	D	175	GLU
3	D	179	LYS
3	D	188	LEU
3	D	235	GLU
3	D	239	LEU
3	D	250	ARG
3	D	309	ASN
3	D	430	HIS
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	668	PHE
3	D	678	ARG
3	D	681	LYS
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR
3	D	816	THR
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1227	HIS
3	D	1247	LYS
3	D	1306	LEU
3	D	1341	ARG
4	E	6	VAL

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Mol	Chain	Res	Type
4	E	8	ASP
4	E	15	ASN
5	X	21	TYR
5	X	28	ASN
5	X	99	ARG
5	X	136	GLU
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	400	GLN
5	X	401	PHE
5	X	452	ILE
5	X	457	ILE
5	X	471	LEU
5	X	476	ARG
5	X	495	ARG
5	X	545	HIS
5	X	562	ARG
5	X	607	LEU
1	F	37	HIS
1	F	77	ASP
1	F	158	ARG
1	F	160	HIS
1	F	163	GLU
1	G	13	LEU
1	G	37	HIS
1	G	88	LEU
1	G	218	ARG
1	G	228	LEU
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS

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Mol	Chain	Res	Type
2	H	127	ILE
2	H	150	HIS
2	H	163	LYS
2	H	311	CYS
2	H	464	PHE
2	H	479	LEU
2	H	488	MET
2	H	513	GLN
2	H	514	PHE
2	H	600	THR
2	H	645	PHE
2	H	661	VAL
2	H	690	VAL
2	H	773	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	845	LEU
2	H	941	LYS
2	H	944	ARG
2	H	955	GLN
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	994	ARG
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1032	LYS
2	H	1034	ARG
2	H	1042	LEU
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1211	ARG
2	H	1233	LEU
2	H	1241	ASP
2	H	1264	GLN
2	H	1270	PHE
2	H	1288	GLN

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Mol	Chain	Res	Type
2	H	1291	LEU
2	H	1326	LEU
2	H	1339	LEU
2	H	1341	ASP
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL
3	I	114	ILE
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	169	LEU
3	I	176	PHE
3	I	179	LYS
3	I	188	LEU
3	I	239	LEU
3	I	248	ASP
3	I	250	ARG
3	I	316	ILE
3	I	416	ILE
3	I	430	HIS
3	I	475	GLU
3	I	500	ILE
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	594	GLN
3	I	668	PHE
3	I	678	ARG
3	I	681	LYS
3	I	709	ARG
3	I	771	GLN
3	I	795	TYR
3	I	816	THR
3	I	832	LYS
3	I	864	LEU
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS

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Mol	Chain	Res	Type
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1149	ARG
3	I	1247	LYS
3	I	1273	ASP
3	I	1297	LYS
3	I	1306	LEU
3	I	1341	ARG
3	I	1369	ARG
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	477	GLU
5	Y	511	ILE
5	Y	545	HIS
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	239	GLN
1	B	41	ASN
1	B	84	ASN
2	C	41	GLN
2	C	69	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	462	ASN

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Mol	Chain	Res	Type
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	649	GLN
2	C	673	HIS
2	C	799	ASN
2	C	894	GLN
2	C	955	GLN
2	C	1010	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1134	GLN
2	C	1146	GLN
2	C	1175	ASN
2	C	1220	GLN
2	C	1264	GLN
2	C	1288	GLN
2	C	1313	HIS
3	D	94	GLN
3	D	164	GLN
3	D	300	GLN
3	D	504	GLN
3	D	519	ASN
3	D	875	ASN
3	D	907	HIS
3	D	1197	ASN
3	D	1268	ASN
3	D	1350	ASN
4	E	31	GLN
5	X	30	HIS
5	X	46	GLN
5	X	54	GLN
5	X	301	ASN
5	X	406	GLN
5	X	437	GLN
5	X	461	ASN
5	X	469	GLN
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	462	ASN

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Mol	Chain	Res	Type
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	649	GLN
2	H	684	ASN
2	H	894	GLN
2	H	922	ASN
2	H	952	GLN
2	H	1010	GLN
2	H	1108	ASN
2	H	1111	GLN
2	H	1134	GLN
2	H	1175	ASN
2	H	1220	GLN
2	H	1264	GLN
2	H	1288	GLN
2	H	1313	HIS
3	I	94	GLN
3	I	274	ASN
3	I	300	GLN
3	I	309	ASN
3	I	504	GLN
3	I	519	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	242	HIS
5	Y	301	ASN
5	Y	342	GLN
5	Y	400	GLN
5	Y	437	GLN
5	Y	469	GLN
5	Y	589	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	G4P	D	1503	-	30,38,38	2.21	9 (30%)	42,61,61	1.73	8 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	G4P	D	1503	-	-	7/23/43/43	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1503	G4P	C2'-C1'	-5.25	1.45	1.53
7	D	1503	G4P	C5-C6	-4.78	1.37	1.47
7	D	1503	G4P	C6-N1	-4.50	1.31	1.37
7	D	1503	G4P	C5-C4	-4.39	1.31	1.43
7	D	1503	G4P	C2'-C3'	-3.55	1.45	1.52
7	D	1503	G4P	C2-N2	3.40	1.42	1.34
7	D	1503	G4P	C2-N3	2.76	1.39	1.33
7	D	1503	G4P	C8-N7	2.29	1.38	1.35
7	D	1503	G4P	C3'-C4'	-2.07	1.47	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1503	G4P	O3C-PC-O3'	4.89	112.34	102.48
7	D	1503	G4P	O4'-C1'-C2'	-4.68	100.09	106.93
7	D	1503	G4P	PC-O3C-PD	-4.57	117.16	132.83
7	D	1503	G4P	PA-O3A-PB	-3.42	121.10	132.83
7	D	1503	G4P	C5-C6-N1	2.84	118.97	113.95
7	D	1503	G4P	PC-O3'-C3'	2.65	129.04	119.41
7	D	1503	G4P	C2-N1-C6	-2.56	120.39	125.10
7	D	1503	G4P	C8-N7-C5	2.53	107.81	102.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1503	G4P	C5'-O5'-PA-O1A
7	D	1503	G4P	C5'-O5'-PA-O2A
7	D	1503	G4P	O4'-C4'-C5'-O5'
7	D	1503	G4P	C3'-C4'-C5'-O5'
7	D	1503	G4P	C4'-C3'-O3'-PC
7	D	1503	G4P	C2'-C3'-O3'-PC
7	D	1503	G4P	C5'-O5'-PA-O3A

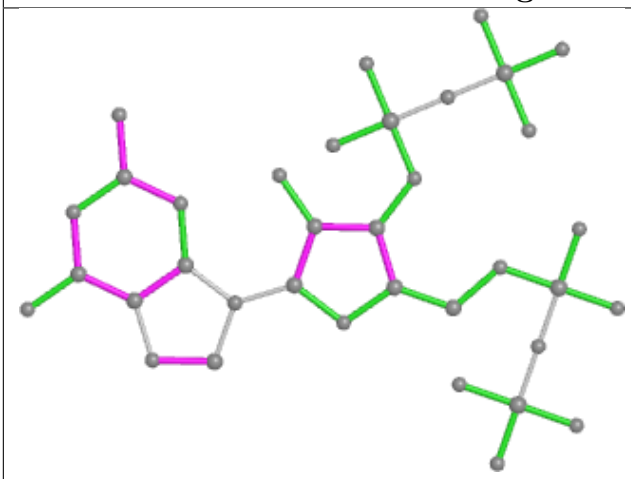
There are no ring outliers.

1 monomer is involved in 2 short contacts:

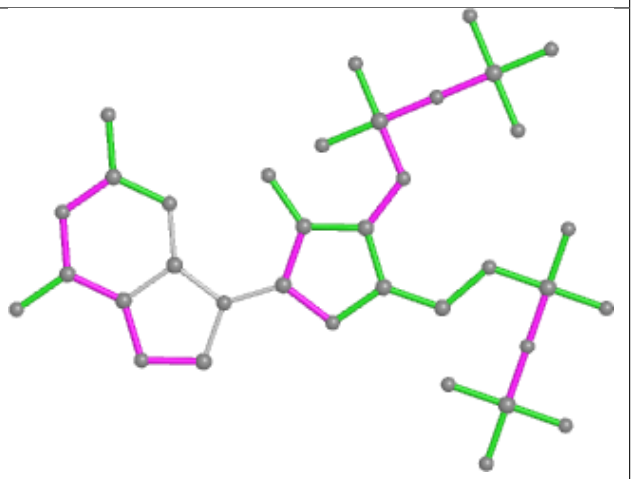
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1503	G4P	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

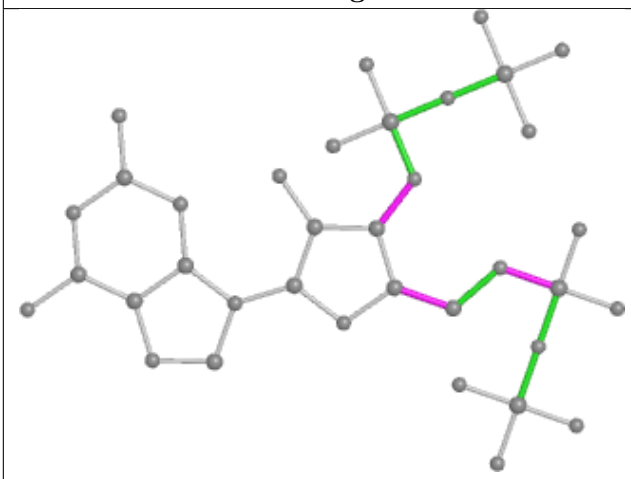
Ligand G4P D 1503



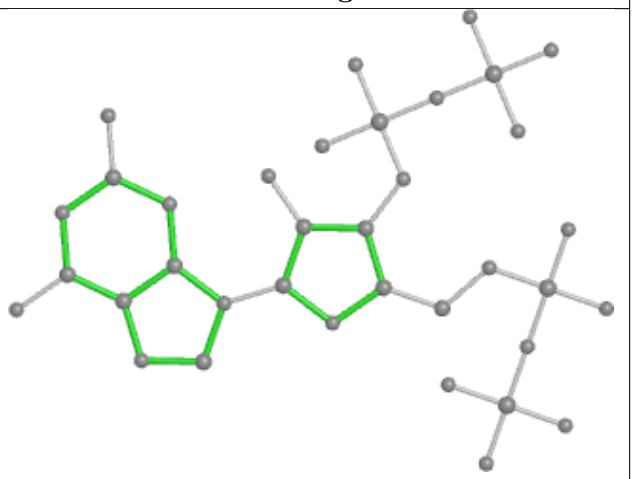
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	323/329 (98%)	-0.01	14 (4%)	35	28	1, 73, 178, 299	0
1	B	221/329 (67%)	0.29	12 (5%)	25	21	5, 98, 204, 259	0
1	F	229/329 (69%)	0.30	15 (6%)	18	13	27, 123, 199, 278	0
1	G	217/329 (65%)	0.34	13 (5%)	21	16	34, 118, 187, 236	0
2	C	1335/1342 (99%)	-0.15	42 (3%)	49	38	0, 48, 170, 262	0
2	H	1335/1342 (99%)	0.09	80 (5%)	21	16	0, 88, 203, 293	0
3	D	1160/1407 (82%)	-0.04	42 (3%)	42	33	0, 42, 158, 289	0
3	I	1160/1407 (82%)	0.09	71 (6%)	21	15	0, 60, 192, 317	0
4	E	90/91 (98%)	-0.27	1 (1%)	80	73	1, 52, 121, 158	0
4	J	76/91 (83%)	0.25	5 (6%)	18	13	10, 89, 165, 211	0
5	X	517/613 (84%)	0.10	42 (8%)	12	9	0, 101, 226, 326	0
5	Y	458/613 (74%)	0.14	29 (6%)	20	14	1, 109, 234, 357	0
All	All	7121/8222 (86%)	0.04	366 (5%)	28	23	0, 73, 197, 357	0

All (366) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	10	ALA	12.6
5	Y	239	GLY	9.4
3	I	212	THR	9.0
3	I	11	GLN	8.3
3	I	1161	GLY	7.6
3	D	1171	GLY	7.0
2	H	1001	GLY	7.0
3	I	1203	ARG	6.8
1	F	162	GLU	6.7
2	C	311	CYS	6.5
5	X	35	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
2	H	1000	LEU	6.2
2	H	999	GLU	6.2
3	I	208	THR	6.2
1	F	161	SER	6.1
2	C	251	ALA	6.0
3	I	9	LYS	6.0
3	I	12	THR	5.8
5	X	36	VAL	5.8
5	Y	315	TRP	5.8
5	Y	319	ALA	5.7
2	H	987	GLU	5.6
5	Y	337	VAL	5.6
3	I	213	LYS	5.6
5	Y	212	ILE	5.4
2	H	986	ALA	5.3
5	X	56	MET	5.3
2	H	996	ARG	5.2
2	H	1002	LEU	5.2
2	H	998	LEU	5.2
5	X	24	TYR	5.2
1	F	148	ARG	5.1
1	B	169	GLY	5.1
5	Y	318	ALA	5.1
5	X	237	ALA	5.0
2	H	334	GLU	5.0
1	G	96	ASP	4.9
5	X	319	ALA	4.9
2	C	231	GLU	4.8
1	F	194	GLN	4.6
2	H	264	GLU	4.6
3	I	1375	ALA	4.6
5	Y	311	THR	4.6
5	X	318	ALA	4.5
5	Y	293	GLU	4.5
2	H	983	GLY	4.5
3	I	218	THR	4.5
2	H	1003	THR	4.5
3	I	1376	GLY	4.4
2	H	990	ASP	4.4
3	I	1162	ILE	4.4
5	X	305	LEU	4.3
3	I	708	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
2	H	912	ASP	4.3
2	H	981	ALA	4.3
2	H	988	LYS	4.3
2	H	61	SER	4.3
2	C	232	ILE	4.3
3	D	1170	LYS	4.1
1	G	172	LEU	4.1
3	I	13	LYS	4.1
1	B	41	ASN	4.1
1	G	75	GLN	4.1
3	I	732	GLY	4.1
3	D	1203	ARG	4.1
5	Y	421	TYR	4.1
2	C	282	VAL	4.1
3	I	830	ASP	4.1
5	X	43	ASP	4.1
5	Y	317	ASN	4.1
3	I	675	ALA	4.0
1	A	165	GLU	3.9
5	X	34	ASP	3.9
2	H	982	GLY	3.9
5	Y	240	ARG	3.9
3	D	1172	LYS	3.9
2	H	60	GLN	3.8
1	A	4	SER	3.8
3	D	1133	ASP	3.8
5	Y	340	ALA	3.8
3	D	211	GLU	3.8
5	X	306	PHE	3.8
2	H	744	GLY	3.7
2	C	116	ASP	3.7
3	D	80	HIS	3.7
3	I	676	GLY	3.7
1	A	162	GLU	3.7
5	Y	336	GLU	3.7
5	Y	316	PHE	3.7
5	Y	320	ILE	3.7
4	J	2	ALA	3.6
3	I	1160	SER	3.6
3	D	89	GLY	3.6
1	A	41	ASN	3.5
3	D	831	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
5	X	310	GLU	3.5
2	H	1020	GLU	3.5
2	C	331	LYS	3.5
2	C	271	ALA	3.5
5	X	19	GLN	3.5
3	D	1151	LYS	3.5
3	D	1199	PHE	3.5
2	C	270	THR	3.5
2	C	252	SER	3.4
2	C	165	HIS	3.4
1	B	168	ILE	3.4
5	X	53	ILE	3.4
2	C	1002	LEU	3.4
2	C	332	ARG	3.4
3	D	333	GLY	3.3
3	D	1273	ASP	3.3
2	C	238	GLN	3.3
3	I	1273	ASP	3.3
2	H	332	ARG	3.3
1	F	193	GLU	3.3
2	H	165	HIS	3.3
2	H	979	LEU	3.3
2	C	996	ARG	3.3
1	B	171	LEU	3.3
3	I	540	GLY	3.3
3	I	521	LYS	3.3
5	X	315	TRP	3.3
2	H	742	TYR	3.3
2	C	310	ILE	3.2
2	H	1070	HIS	3.2
2	C	1000	LEU	3.2
3	I	204	GLU	3.2
5	X	6	GLN	3.2
2	H	913	VAL	3.2
5	X	236	LYS	3.2
5	X	293	GLU	3.2
3	I	216	LYS	3.2
5	X	313	ASP	3.2
2	C	233	ARG	3.2
2	H	262	TYR	3.1
2	H	258	ASN	3.1
3	I	712	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
3	I	1204	VAL	3.1
1	F	96	ASP	3.1
1	A	324	ALA	3.1
2	C	77	GLU	3.1
2	H	263	VAL	3.1
3	D	212	THR	3.1
3	I	1167	LYS	3.1
5	Y	241	SER	3.1
5	X	44	ILE	3.1
5	X	54	GLN	3.1
2	C	164	THR	3.1
1	A	193	GLU	3.1
5	Y	310	GLU	3.1
2	H	1008	GLN	3.0
4	J	59	ILE	3.0
5	X	485	GLU	3.0
3	D	1198	VAL	3.0
3	D	875	ASN	3.0
2	C	236	LYS	3.0
3	I	1172	LYS	3.0
1	B	147	GLN	3.0
1	G	13	LEU	3.0
2	C	230	PHE	3.0
2	C	999	GLU	3.0
2	H	1009	ASN	3.0
2	H	375	PRO	3.0
3	D	344	GLY	3.0
3	I	477	GLN	3.0
3	D	1302	TYR	2.9
1	F	163	GLU	2.9
3	I	1373	ARG	2.9
4	J	56	GLU	2.9
2	H	1007	LYS	2.9
3	I	855	ASP	2.9
2	C	266	GLY	2.9
2	H	727	VAL	2.9
2	H	252	SER	2.9
3	I	541	LEU	2.9
1	F	191	ARG	2.8
2	H	172	TYR	2.8
1	F	192	VAL	2.8
2	C	483	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	251	ALA	2.8
5	X	515	GLU	2.8
2	H	229	ILE	2.8
3	D	210	SER	2.8
5	Y	578	LYS	2.8
2	H	167	SER	2.8
3	I	210	SER	2.8
2	H	1032	LYS	2.8
1	G	173	VAL	2.8
2	H	107	ARG	2.8
2	H	108	GLU	2.8
5	X	317	ASN	2.8
3	D	832	LYS	2.8
3	I	831	VAL	2.8
3	D	477	GLN	2.8
1	F	160	HIS	2.7
1	B	97	GLU	2.7
2	H	1021	LEU	2.7
3	I	748	ALA	2.7
2	H	911	SER	2.7
1	A	272	ALA	2.7
5	X	8	GLN	2.7
2	C	1001	GLY	2.7
2	C	172	TYR	2.7
3	D	830	ASP	2.7
2	H	725	GLN	2.7
1	A	245	GLU	2.6
2	C	908	GLU	2.6
2	H	473	ARG	2.6
4	J	37	PRO	2.6
2	H	895	LEU	2.6
3	I	564	VAL	2.6
2	H	787	PRO	2.6
2	C	305	SER	2.6
3	D	878	ASP	2.6
3	I	562	GLU	2.6
2	H	614	TYR	2.6
1	B	172	LEU	2.6
1	F	147	GLN	2.6
2	H	299	LYS	2.6
3	D	1185	PRO	2.6
5	X	425	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	1169	THR	2.6
1	G	24	ALA	2.6
3	D	471	PRO	2.6
2	H	121	GLU	2.6
3	D	207	GLU	2.6
2	H	984	VAL	2.5
3	I	211	GLU	2.5
5	Y	574	GLU	2.5
5	X	283	GLN	2.5
1	F	95	LYS	2.5
1	G	106	GLY	2.5
2	C	257	ALA	2.5
2	H	1134	GLN	2.5
1	B	157	THR	2.5
5	X	328	GLU	2.5
3	D	879	ALA	2.5
5	X	31	LEU	2.5
3	I	217	LEU	2.5
3	D	932	MET	2.5
1	G	18	GLN	2.5
5	Y	305	LEU	2.5
2	H	168	GLY	2.5
1	G	107	ILE	2.5
5	X	482	GLU	2.5
2	H	254	ASP	2.5
5	X	20	GLY	2.5
3	I	133	ARG	2.5
5	Y	113	ARG	2.5
2	H	1130	ALA	2.5
3	I	1133	ASP	2.5
5	X	240	ARG	2.5
2	H	111	GLU	2.5
2	H	972	PHE	2.5
5	Y	238	LYS	2.4
1	G	23	HIS	2.4
4	J	36	ASP	2.4
3	I	707	ILE	2.4
1	B	70	THR	2.4
5	X	325	PRO	2.4
1	F	149	GLY	2.4
5	Y	117	ILE	2.4
2	H	1153	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	1294	ALA	2.4
3	I	392	THR	2.4
2	H	1152	GLY	2.4
2	C	304	GLU	2.4
2	C	120	GLN	2.4
3	D	1186	TYR	2.4
3	I	207	GLU	2.4
2	H	333	ILE	2.4
2	H	1071	GLY	2.4
1	G	171	LEU	2.4
5	X	57	GLU	2.4
5	X	289	LYS	2.4
3	D	68	TYR	2.4
3	D	208	THR	2.4
5	Y	514	ASP	2.4
2	H	106	GLU	2.3
2	H	413	GLU	2.3
3	I	542	ALA	2.3
5	X	307	THR	2.3
3	I	177	ASP	2.3
5	X	39	ASP	2.3
2	C	987	GLU	2.3
3	I	1215	GLU	2.3
3	I	1297	LYS	2.3
3	D	547	ARG	2.3
2	H	1089	GLU	2.3
1	B	148	ARG	2.3
2	C	261	VAL	2.3
3	I	1202	GLU	2.3
2	C	267	ARG	2.3
1	F	184	ALA	2.3
4	E	91	ARG	2.3
3	I	174	ASP	2.3
3	I	1296	GLY	2.2
1	A	164	ASP	2.2
1	A	191	ARG	2.2
1	G	12	ARG	2.2
5	Y	306	PHE	2.2
3	I	789	LYS	2.2
1	A	19	VAL	2.2
2	H	376	PRO	2.2
1	G	205	MET	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	563	LEU	2.2
1	A	262	LEU	2.2
2	H	1166	ASP	2.2
5	Y	299	LYS	2.2
3	I	747	MET	2.2
5	X	514	ASP	2.2
3	D	1215	GLU	2.2
3	I	344	GLY	2.2
2	C	272	ARG	2.2
2	H	110	PRO	2.2
5	X	52	GLY	2.2
1	B	19	VAL	2.2
3	D	76	LYS	2.2
3	I	1295	ASN	2.1
3	I	1179	PRO	2.1
5	X	16	GLY	2.1
2	H	1029	LEU	2.1
3	D	390	LEU	2.1
2	H	734	ILE	2.1
3	I	76	LYS	2.1
3	I	587	LEU	2.1
5	Y	452	ILE	2.1
3	I	1168	GLU	2.1
3	D	1268	ASN	2.1
1	A	133	LEU	2.1
2	H	265	LYS	2.1
2	H	997	TRP	2.1
3	I	15	GLU	2.1
5	Y	515	GLU	2.1
2	H	733	VAL	2.1
2	H	937	ASP	2.1
3	D	849	LEU	2.1
5	Y	490	PRO	2.1
3	D	829	GLY	2.1
3	I	565	ALA	2.1
2	C	625	GLU	2.1
5	X	239	GLY	2.1
2	H	483	ASP	2.1
3	I	473	THR	2.1
2	C	844	LYS	2.1
3	D	82	GLY	2.1
2	H	169	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	672	LEU	2.1
5	X	336	GLU	2.1
3	I	711	GLY	2.1
1	B	62	ASP	2.1
3	I	674	THR	2.1
1	A	242	VAL	2.1
2	H	442	VAL	2.1
3	I	813	ASP	2.0
2	C	258	ASN	2.0
3	I	683	ILE	2.0
2	C	57	PHE	2.0
3	I	153	ASN	2.0
2	H	492	MET	2.0
3	D	673	VAL	2.0
1	F	19	VAL	2.0
2	C	1134	GLN	2.0
2	C	237	LEU	2.0
2	H	662	SER	2.0
3	D	148	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	G4P	D	1503	36/36	0.83	0.20	31,56,93,118	0
6	ZN	I	1501	1/1	0.97	0.07	60,60,60,60	0
6	ZN	I	1502	1/1	0.98	0.15	49,49,49,49	0
6	ZN	D	1501	1/1	0.98	0.08	54,54,54,54	0

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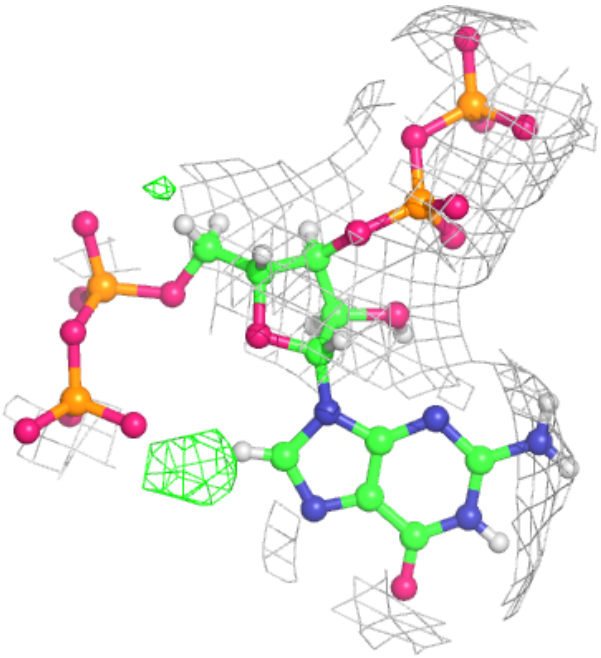
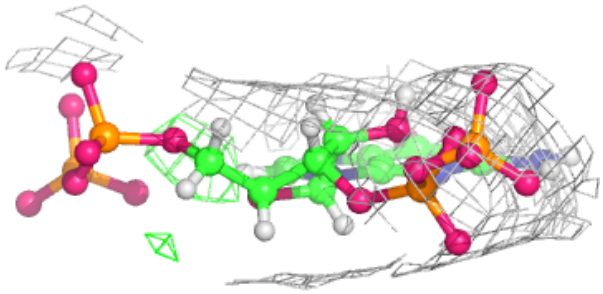
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ZN	D	1502	1/1	0.99	0.18	8,8,8,8	0

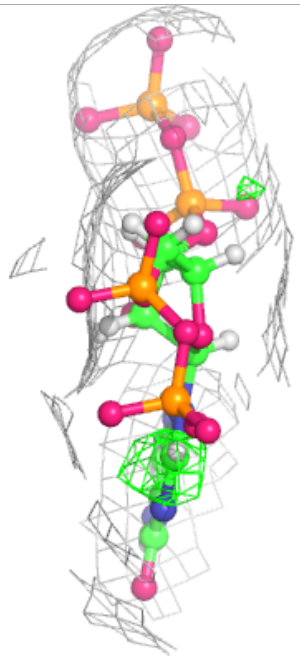
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G4P D 1503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.