Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:06 AM GMT

PDB ID	:	2PFD
Title	:	Anisotropically refined structure of FTCD
Authors	:	Poon, B.K.; Chen, X.; Lu, M.; Quiocho, F.A.; Wang, Q.; Ma, J.
Deposited on	:	2007-04-04
Resolution	:	3.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

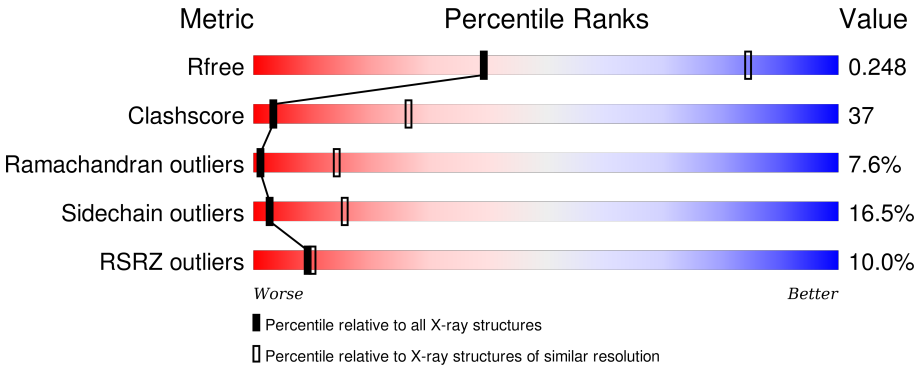
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	541	9% 47% 39% 12% •
1	B	541	8% 45% 40% 13% •
1	C	541	10% 47% 38% 13% •
1	D	541	12% 48% 38% 12% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16524 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Formimidoyltransferase-cyclodeaminase.

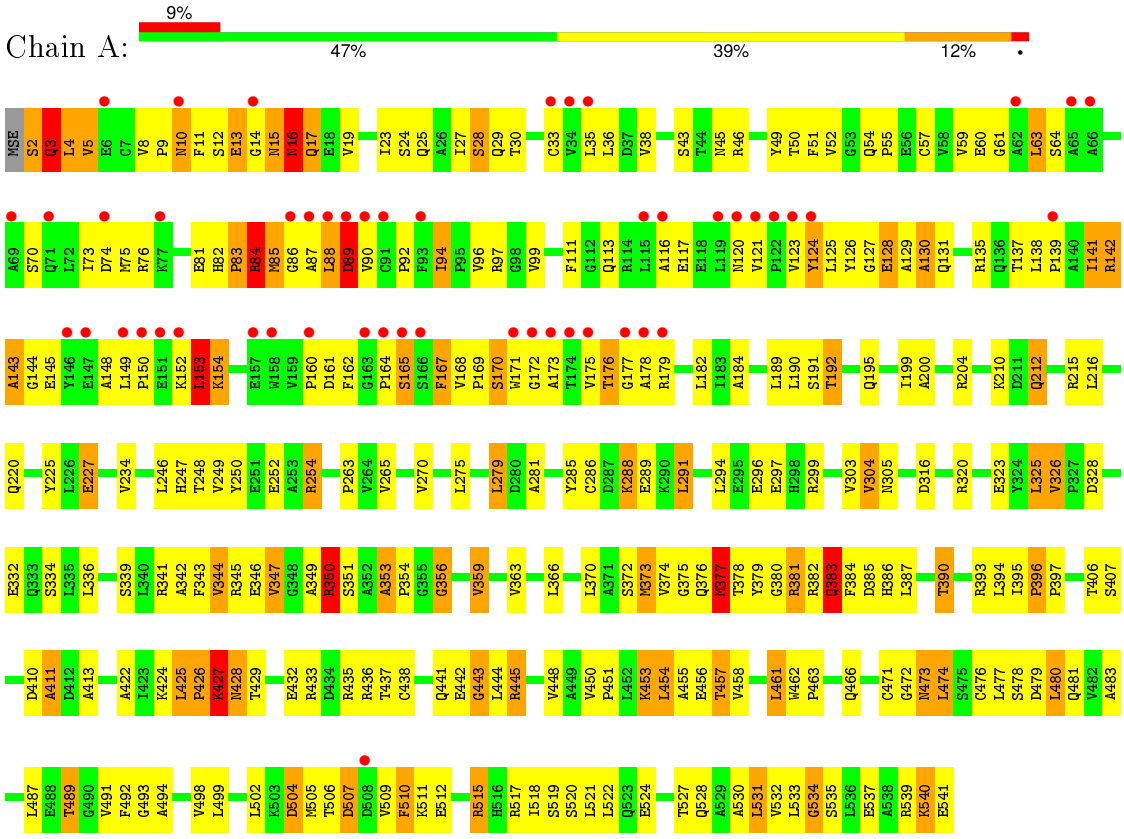
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	Se	0	0	0
			4131	2602	731	779	11	8			
1	B	540	Total	C	N	O	S	Se	0	0	0
			4131	2602	731	779	11	8			
1	C	540	Total	C	N	O	S	Se	0	0	0
			4131	2602	731	779	11	8			
1	D	540	Total	C	N	O	S	Se	0	0	0
			4131	2602	731	779	11	8			

3 Residue-property plots (i)

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

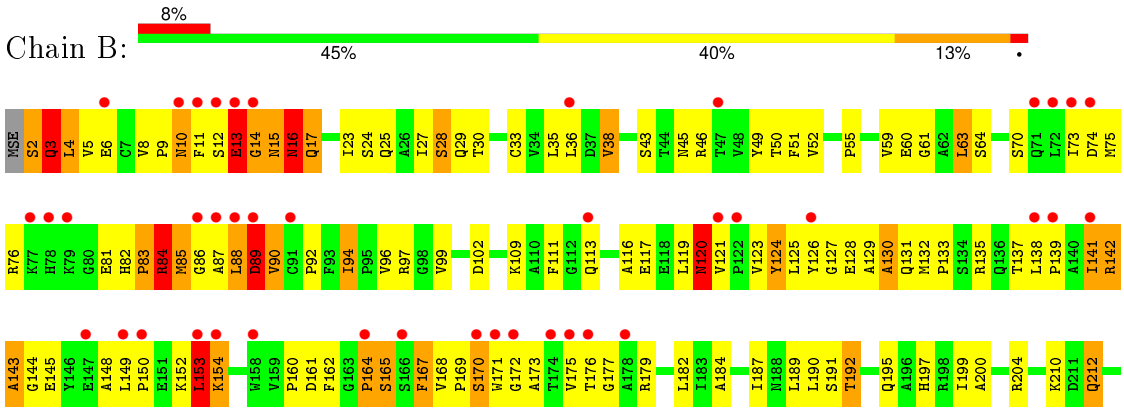
- Molecule 1: Formimidoyltransferase-cyclodeaminase

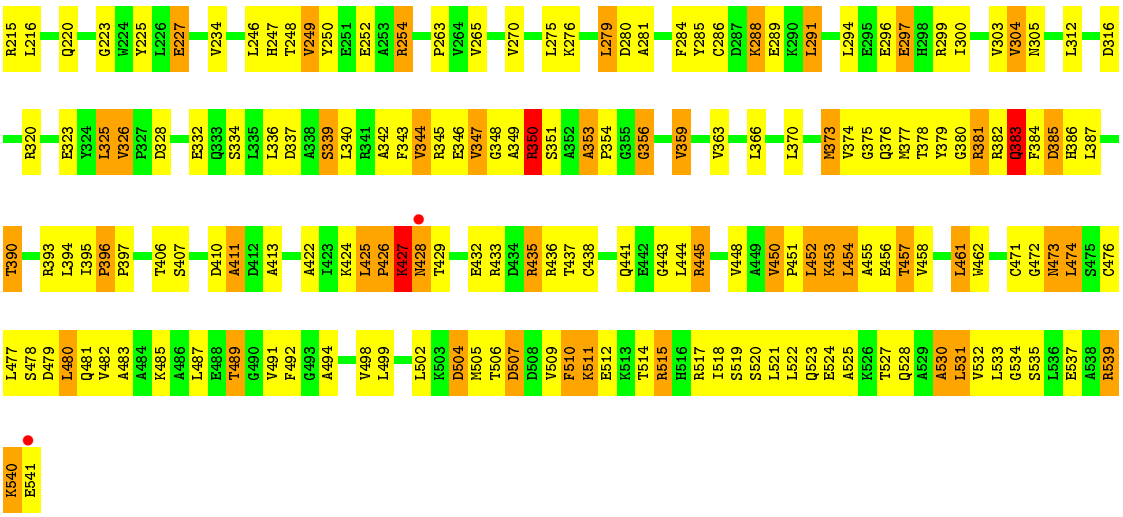
Chain A:



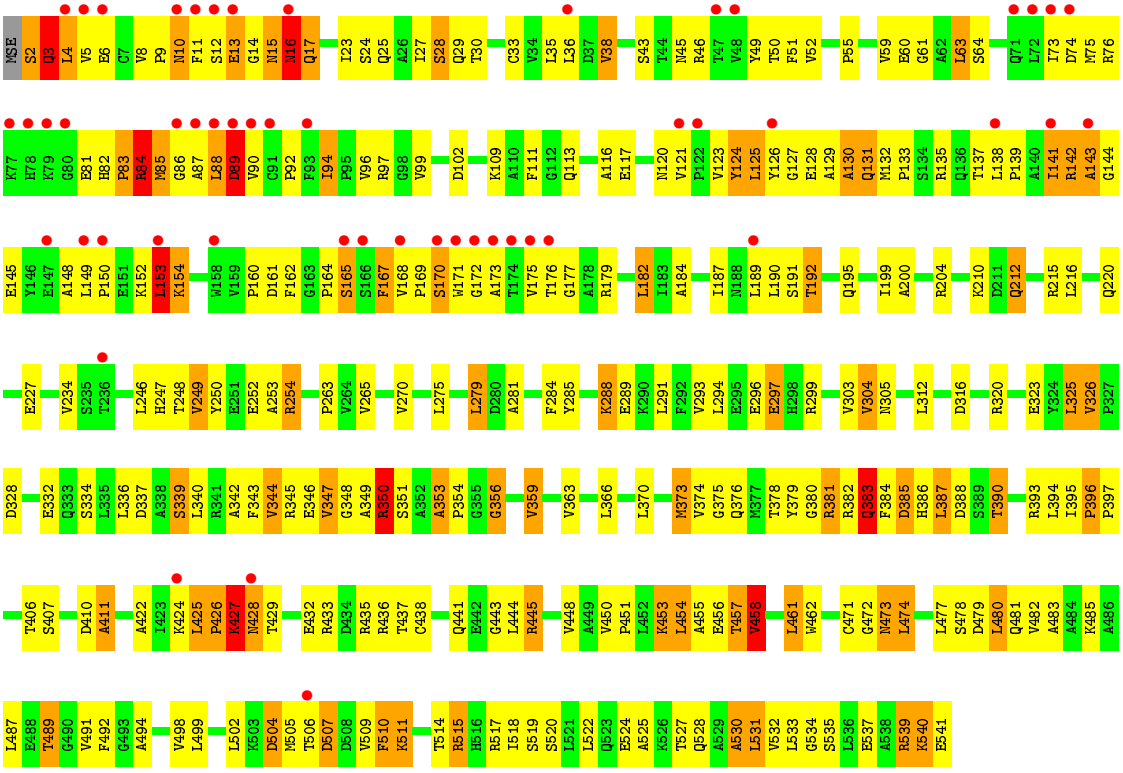
- Molecule 1: Formimidoyltransferase-cyclodeaminase

Chain B:

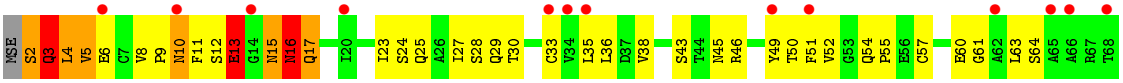


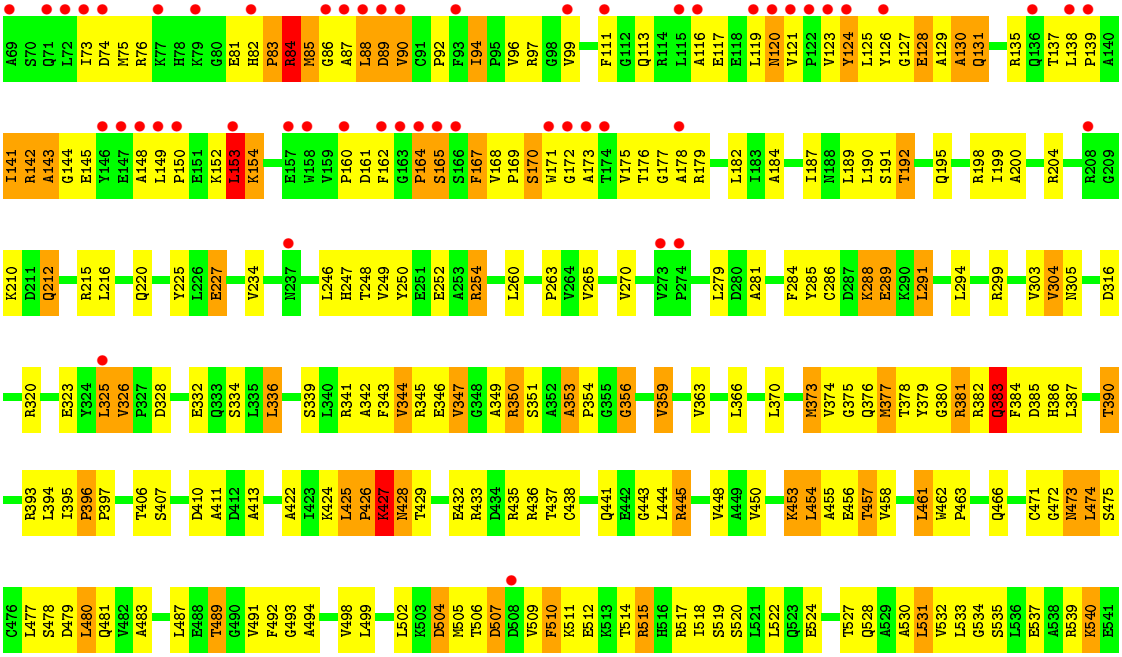


• Molecule 1: Formimidoyltransferase-cyclodeaminase



• Molecule 1: Formimidoyltransferase-cyclodeaminase




A69 S70 Q71 L72 I73 D74 M75 R76 K77 H78 K79 G80 E81 H82 P83 R84 M85 G86 A87 L88 D89 V90 C91 P92 F93 I94 P95 V96 R97 G98 V99 F111 G112 Q113 R114 L115 A116 E117 E118 L119 N120 V121 P122 V123 Y124 L125 Y126 G127 E128 A129 A130 Q131 R135 Q136 T137 L138 P139 A140
I141 R142 A143 G144 E145 Y146 E147 A148 L149 P150 E151 K152 L153 K154 E157 W158 V159 P160 D161 F162 G163 P164 S165 S166 F167 V168 P169 S170 W171 G172 A173 T174 V175 T176 G177 A178 R179 L182 I183 A184 I187 N188 L189 L190 S191 T192 Q195 R198 I199 A200 R204 R208 G209
K210 D211 Q212 R215 L216 Q220 Y225 L226 E227 V234 N237 L246 H247 T248 V249 Y250 E251 E252 A253 R254 L260 P263 V264 V265 V270 V273 P274 L279 D280 A281 F284 Y285 C286 D287 K288 E289 K290 L291 L294 R299 V303 V304 N305 D316
R320 E323 Y324 L325 V326 P327 D328 E332 Q333 S334 L335 L336 S339 L340 R341 A342 F343 V344 R345 E346 V347 G348 A349 R350 S351 A352 A353 P354 G355 G356 V359 V363 L366 L370 M373 V374 G375 Q376 M377 T378 Y379 G380 R381 R382 Q383 P384 D385 H386 L387 T390
R393 L394 I395 P396 P397 T406 S407 D410 A411 D412 A413 A422 I423 K424 L425 P426 K427 N428 T429 E432 R433 D434 R435 R436 T437 C438 Q441 E442 G443 L444 R445 V448 A449 V450 K453 L454 A455 E456 T457 V458 L461 W462 P463 Q466 C471 G472 N473 L474 S475
C476 L477 S478 D479 L480 Q481 V482 A483 L487 E488 T489 G490 V491 F492 G493 A494 V498 L499 L502 K503 D504 M505 T506 D507 D508 V509 F510 K511 E512 K513 T514 R515 H516 R517 I518 S519 S520 L521 L522 Q523 E524 T527 Q528 A529 A530 L531 V532 L533 G534 S535 L536 E537 A538 R539 K540 E541

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	134.85Å 134.85Å 156.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.42 47.75 – 3.42	Depositor EDS
% Data completeness (in resolution range)	94.0 (10.00-3.42) 96.0 (47.75-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.249 0.238 , 0.248	Depositor DCC
R_{free} test set	1717 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 19.2	EDS
Estimated twinning fraction	0.367 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	1 of 36372 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	16524	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	1/4195 (0.0%)	0.76	5/5674 (0.1%)
1	B	0.59	2/4195 (0.0%)	0.82	8/5674 (0.1%)
1	C	0.52	1/4195 (0.0%)	0.75	5/5674 (0.1%)
1	D	0.60	3/4195 (0.1%)	0.75	5/5674 (0.1%)
All	All	0.57	7/16780 (0.0%)	0.77	23/22696 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	13	GLU	CD-OE1	14.62	1.41	1.25
1	D	153	LEU	CG-CD2	-8.97	1.18	1.51
1	B	153	LEU	CG-CD2	-7.96	1.22	1.51
1	A	153	LEU	CG-CD2	-7.45	1.24	1.51
1	C	153	LEU	CG-CD2	-7.37	1.24	1.51
1	B	13	GLU	C-O	-5.96	1.12	1.23
1	D	13	GLU	CD-OE2	5.05	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	435	ARG	NE-CZ-NH2	-14.22	113.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	435	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	D	153	LEU	CB-CG-CD1	11.02	129.73	111.00
1	B	153	LEU	CB-CG-CD1	10.56	128.95	111.00
1	A	153	LEU	CB-CG-CD1	9.31	126.83	111.00
1	A	153	LEU	CB-CG-CD2	-9.16	95.43	111.00
1	C	153	LEU	CB-CG-CD1	8.85	126.04	111.00
1	B	153	LEU	CB-CG-CD2	-8.11	97.21	111.00
1	C	153	LEU	CB-CG-CD2	-7.59	98.10	111.00
1	D	153	LEU	CB-CG-CD2	-7.08	98.96	111.00
1	B	13	GLU	CA-C-N	6.94	130.07	116.20
1	B	435	ARG	CD-NE-CZ	6.68	132.96	123.60
1	A	377	MSE	CB-CG-SE	6.67	132.70	112.70
1	D	153	LEU	CA-CB-CG	6.66	130.61	115.30
1	D	153	LEU	CD1-CG-CD2	-6.54	90.86	110.50
1	A	377	MSE	CG-SE-CE	6.44	113.06	98.90
1	B	153	LEU	CD1-CG-CD2	-6.04	92.37	110.50
1	C	458	VAL	CG1-CB-CG2	-5.94	101.39	110.90
1	A	435	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	C	435	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	435	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	452	LEU	CA-CB-CG	5.09	127.01	115.30
1	C	125	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LYS	Peptide
1	B	427	LYS	Peptide
1	C	427	LYS	Peptide
1	D	427	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4131	0	4175	325	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4131	0	4175	333	0
1	C	4131	0	4175	322	0
1	D	4131	0	4175	315	0
All	All	16524	0	16700	1227	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 37.

All (1227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:SER:O	1:D:373:MSE:HE2	1.37	1.22
1:A:373:MSE:HE2	1:B:351:SER:O	1.44	1.18
1:C:427:LYS:HE3	1:C:436:ARG:NH1	1.63	1.14
1:B:426:PRO:O	1:B:427:LYS:HB2	1.48	1.13
1:B:2:SER:N	1:B:328:ASP:HB2	1.63	1.13
1:B:427:LYS:HE3	1:B:436:ARG:NH1	1.66	1.11
1:A:27:ILE:HD11	1:A:51:PHE:CD1	1.86	1.11
1:C:2:SER:N	1:C:328:ASP:HB2	1.64	1.11
1:A:427:LYS:HE3	1:A:436:ARG:HH12	1.16	1.11
1:C:347:VAL:O	1:D:373:MSE:HE3	1.52	1.10
1:C:489:THR:HG21	1:D:489:THR:HG21	1.11	1.10
1:A:2:SER:N	1:A:328:ASP:HB2	1.67	1.10
1:C:149:LEU:CD2	1:C:153:LEU:HD23	1.81	1.09
1:B:27:ILE:HD11	1:B:51:PHE:CD1	1.87	1.09
1:A:373:MSE:HE3	1:B:347:VAL:O	1.52	1.09
1:A:427:LYS:HE3	1:A:436:ARG:NH1	1.66	1.09
1:D:2:SER:N	1:D:328:ASP:HB2	1.67	1.09
1:C:427:LYS:HE3	1:C:436:ARG:HH12	1.10	1.08
1:B:359:VAL:O	1:B:363:VAL:HG23	1.54	1.08
1:D:427:LYS:HE3	1:D:436:ARG:NH1	1.67	1.07
1:C:359:VAL:O	1:C:363:VAL:HG23	1.54	1.07
1:C:425:LEU:HD22	1:C:426:PRO:HD2	1.35	1.07
1:C:149:LEU:HD22	1:C:153:LEU:HD23	1.16	1.07
1:C:27:ILE:HD11	1:C:51:PHE:CD1	1.89	1.07
1:D:27:ILE:HD11	1:D:51:PHE:CD1	1.90	1.06
1:C:426:PRO:O	1:C:427:LYS:HB2	1.50	1.06
1:D:426:PRO:O	1:D:427:LYS:HB2	1.52	1.06
1:D:531:LEU:H	1:D:531:LEU:HD23	1.20	1.06
1:A:426:PRO:O	1:A:427:LYS:HB2	1.52	1.06
1:D:427:LYS:HE3	1:D:436:ARG:HH12	1.16	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:LEU:HD22	1:D:426:PRO:HD2	1.37	1.05
1:A:359:VAL:O	1:A:363:VAL:HG23	1.56	1.05
1:D:359:VAL:O	1:D:363:VAL:HG23	1.55	1.05
1:D:5:VAL:HG23	1:D:99:VAL:HG11	1.34	1.05
1:A:5:VAL:HG23	1:A:99:VAL:HG11	1.34	1.05
1:A:489:THR:CG2	1:B:489:THR:HG21	1.88	1.04
1:B:425:LEU:HD22	1:B:426:PRO:HD2	1.33	1.04
1:D:149:LEU:O	1:D:153:LEU:HD12	1.57	1.04
1:A:425:LEU:HD22	1:A:426:PRO:HD2	1.37	1.02
1:B:5:VAL:HG23	1:B:99:VAL:HG11	1.38	1.02
1:A:351:SER:O	1:B:373:MSE:HE2	1.58	1.02
1:C:5:VAL:HG23	1:C:99:VAL:HG11	1.38	1.01
1:A:531:LEU:H	1:A:531:LEU:HD23	1.21	1.01
1:A:27:ILE:HD11	1:A:51:PHE:CE1	1.96	1.01
1:B:27:ILE:HD11	1:B:51:PHE:CE1	1.95	1.00
1:D:153:LEU:HD23	1:D:165:SER:O	1.61	1.00
1:B:427:LYS:HE3	1:B:436:ARG:HH12	1.14	0.99
1:C:502:LEU:HA	1:C:505:MSE:HG3	1.42	0.99
1:B:531:LEU:H	1:B:531:LEU:HD23	1.27	0.98
1:C:27:ILE:HD11	1:C:51:PHE:CE1	1.97	0.98
1:A:489:THR:HG21	1:B:489:THR:HG21	1.00	0.98
1:C:458:VAL:HG11	1:C:491:VAL:HG22	1.42	0.98
1:C:531:LEU:H	1:C:531:LEU:HD23	1.27	0.97
1:A:489:THR:HG21	1:B:489:THR:CG2	1.95	0.96
1:D:502:LEU:HA	1:D:505:MSE:HG3	1.48	0.95
1:C:373:MSE:HE2	1:D:351:SER:O	1.67	0.94
1:B:13:GLU:HG2	1:B:13:GLU:O	1.68	0.94
1:C:489:THR:HG21	1:D:489:THR:CG2	1.97	0.94
1:D:27:ILE:HD11	1:D:51:PHE:CE1	2.01	0.94
1:C:445:ARG:HG3	1:C:445:ARG:HH11	1.32	0.93
1:A:373:MSE:HE1	1:B:354:PRO:O	1.68	0.93
1:A:502:LEU:HA	1:A:505:MSE:HG3	1.51	0.93
1:A:422:ALA:O	1:A:425:LEU:HB2	1.69	0.93
1:D:153:LEU:CD2	1:D:165:SER:O	2.17	0.93
1:B:502:LEU:HA	1:B:505:MSE:HG3	1.48	0.93
1:A:149:LEU:CD2	1:A:153:LEU:HD23	1.99	0.92
1:D:422:ALA:O	1:D:425:LEU:HB2	1.69	0.92
1:B:422:ALA:O	1:B:425:LEU:HB2	1.69	0.92
1:C:15:ASN:O	1:C:16:ASN:HB3	1.70	0.91
1:A:363:VAL:HG13	1:B:363:VAL:HG13	1.50	0.91
1:D:227:GLU:HA	1:D:227:GLU:OE1	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ASN:O	1:D:16:ASN:HB3	1.71	0.91
1:D:445:ARG:HG3	1:D:445:ARG:HH11	1.35	0.91
1:B:483:ALA:O	1:B:487:LEU:HD12	1.71	0.90
1:A:370:LEU:HD11	1:B:359:VAL:HG11	1.52	0.90
1:B:445:ARG:HH11	1:B:445:ARG:HG3	1.36	0.90
1:B:15:ASN:O	1:B:16:ASN:HB3	1.70	0.90
1:C:422:ALA:O	1:C:425:LEU:HB2	1.69	0.89
1:A:15:ASN:O	1:A:16:ASN:HB3	1.70	0.89
1:D:149:LEU:O	1:D:153:LEU:CD1	2.21	0.89
1:A:390:THR:HG22	1:A:393:ARG:HH21	1.37	0.88
1:A:149:LEU:HB3	1:A:153:LEU:HD21	1.56	0.88
1:A:356:GLY:H	1:B:370:LEU:HD21	1.38	0.88
1:C:113:GLN:O	1:C:117:GLU:HG2	1.74	0.87
1:C:149:LEU:HD22	1:C:153:LEU:CD2	2.05	0.87
1:C:359:VAL:HG11	1:D:370:LEU:HD11	1.55	0.87
1:C:483:ALA:O	1:C:487:LEU:HD12	1.75	0.86
1:B:113:GLN:O	1:B:117:GLU:HG2	1.75	0.85
1:C:445:ARG:HH11	1:C:445:ARG:CG	1.89	0.85
1:A:445:ARG:HH11	1:A:445:ARG:HG3	1.38	0.85
1:C:390:THR:HG22	1:C:393:ARG:HH21	1.42	0.85
1:D:445:ARG:CG	1:D:445:ARG:HH11	1.89	0.84
1:A:370:LEU:HD21	1:B:356:GLY:H	1.40	0.84
1:A:113:GLN:O	1:A:117:GLU:HG2	1.78	0.83
1:D:483:ALA:O	1:D:487:LEU:HD12	1.78	0.83
1:C:354:PRO:O	1:D:373:MSE:HE1	1.78	0.83
1:A:227:GLU:HA	1:A:227:GLU:OE1	1.76	0.83
1:A:149:LEU:HB3	1:A:153:LEU:CD2	2.08	0.83
1:C:349:ALA:C	1:C:351:SER:H	1.79	0.83
1:A:349:ALA:C	1:A:351:SER:H	1.81	0.82
1:C:345:ARG:HH21	1:D:406:THR:HB	1.43	0.82
1:D:390:THR:HG22	1:D:393:ARG:HH21	1.41	0.82
1:A:373:MSE:CE	1:B:351:SER:OG	2.27	0.82
1:C:351:SER:OG	1:D:373:MSE:CE	2.26	0.82
1:A:90:VAL:HA	1:A:175:VAL:HG23	1.60	0.82
1:C:227:GLU:OE1	1:C:227:GLU:HA	1.79	0.82
1:D:15:ASN:HB2	1:D:45:ASN:OD1	1.80	0.81
1:B:445:ARG:HH11	1:B:445:ARG:CG	1.93	0.81
1:A:445:ARG:HH11	1:A:445:ARG:CG	1.92	0.81
1:C:2:SER:N	1:C:328:ASP:CB	2.43	0.81
1:B:15:ASN:HB2	1:B:45:ASN:OD1	1.80	0.81
1:A:15:ASN:HB2	1:A:45:ASN:OD1	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HG	1:B:165:SER:O	1.80	0.81
1:B:227:GLU:HA	1:B:227:GLU:OE1	1.80	0.81
1:B:390:THR:HG22	1:B:393:ARG:HH21	1.46	0.81
1:B:2:SER:N	1:B:328:ASP:CB	2.43	0.81
1:C:90:VAL:HA	1:C:175:VAL:HG23	1.62	0.81
1:D:113:GLN:O	1:D:117:GLU:HG2	1.80	0.81
1:B:458:VAL:HG11	1:B:491:VAL:HG22	1.61	0.81
1:A:483:ALA:O	1:A:487:LEU:HD12	1.81	0.80
1:A:97:ARG:NH2	1:A:328:ASP:HB3	1.96	0.80
1:D:427:LYS:HB3	1:D:428:ASN:HD22	1.46	0.80
1:D:90:VAL:HA	1:D:175:VAL:HG23	1.62	0.80
1:C:15:ASN:HB2	1:C:45:ASN:OD1	1.81	0.80
1:A:427:LYS:HB3	1:A:428:ASN:HD22	1.47	0.80
1:A:149:LEU:HD22	1:A:153:LEU:CD2	2.11	0.79
1:B:149:LEU:HD23	1:B:153:LEU:HB3	1.64	0.79
1:B:149:LEU:CD2	1:B:153:LEU:HB3	2.11	0.79
1:B:153:LEU:C	1:B:153:LEU:HD23	2.03	0.79
1:D:97:ARG:NH2	1:D:328:ASP:HB3	1.98	0.79
1:D:515:ARG:O	1:D:518:ILE:HG22	1.83	0.78
1:B:90:VAL:HA	1:B:175:VAL:HG23	1.63	0.78
1:B:471:CYS:SG	1:B:472:GLY:N	2.55	0.78
1:B:349:ALA:C	1:B:351:SER:H	1.84	0.78
1:A:363:VAL:CG1	1:B:363:VAL:HG13	2.14	0.77
1:D:149:LEU:HD23	1:D:153:LEU:HB3	1.66	0.77
1:B:190:LEU:HB2	1:B:263:PRO:HG2	1.67	0.77
1:A:2:SER:N	1:A:328:ASP:CB	2.46	0.77
1:D:149:LEU:HD22	1:D:153:LEU:HG	1.66	0.77
1:D:2:SER:N	1:D:328:ASP:CB	2.47	0.77
1:A:515:ARG:O	1:A:518:ILE:HG22	1.84	0.77
1:C:373:MSE:HE3	1:D:347:VAL:O	1.84	0.77
1:C:351:SER:OG	1:D:373:MSE:HE2	1.85	0.76
1:C:370:LEU:HD21	1:D:356:GLY:H	1.50	0.76
1:C:363:VAL:HG13	1:D:363:VAL:HG13	1.66	0.76
1:B:13:GLU:O	1:B:15:ASN:N	2.18	0.76
1:B:97:ARG:NH2	1:B:328:ASP:HB3	2.00	0.76
1:D:494:ALA:O	1:D:498:VAL:HG23	1.84	0.76
1:C:97:ARG:NH2	1:C:328:ASP:HB3	2.00	0.76
1:D:349:ALA:C	1:D:351:SER:H	1.88	0.75
1:C:458:VAL:HG11	1:C:491:VAL:CG2	2.17	0.75
1:D:25:GLN:HB3	1:D:29:GLN:NE2	2.01	0.75
1:A:342:ALA:O	1:A:346:GLU:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:GLN:HB3	1:C:29:GLN:NE2	2.01	0.74
1:C:471:CYS:SG	1:C:472:GLY:N	2.60	0.74
1:C:356:GLY:H	1:D:370:LEU:HD21	1.53	0.74
1:A:494:ALA:O	1:A:498:VAL:HG23	1.86	0.74
1:D:473:ASN:O	1:D:474:LEU:HB2	1.87	0.74
1:B:25:GLN:HB3	1:B:29:GLN:NE2	2.03	0.73
1:B:396:PRO:HB2	1:B:397:PRO:CD	2.18	0.73
1:C:116:ALA:HB2	1:C:123:VAL:HG12	1.69	0.73
1:C:454:LEU:O	1:C:454:LEU:HD12	1.87	0.73
1:D:116:ALA:HB2	1:D:123:VAL:HG12	1.71	0.73
1:C:494:ALA:O	1:C:498:VAL:HG23	1.88	0.73
1:A:116:ALA:HB2	1:A:123:VAL:HG12	1.70	0.73
1:A:25:GLN:HB3	1:A:29:GLN:NE2	2.04	0.72
1:D:216:LEU:HD21	1:D:252:GLU:HG2	1.71	0.72
1:D:342:ALA:O	1:D:346:GLU:HB2	1.88	0.72
1:B:116:ALA:HB2	1:B:123:VAL:HG12	1.69	0.72
1:D:382:ARG:O	1:D:383:GLN:HB3	1.88	0.72
1:A:458:VAL:HG11	1:A:491:VAL:HG22	1.71	0.72
1:A:373:MSE:HE3	1:B:351:SER:OG	1.89	0.71
1:A:347:VAL:O	1:B:373:MSE:HE3	1.90	0.71
1:C:427:LYS:HB3	1:C:428:ASN:HD22	1.54	0.71
1:C:190:LEU:HB2	1:C:263:PRO:HG2	1.72	0.71
1:B:494:ALA:O	1:B:498:VAL:HG23	1.89	0.71
1:D:149:LEU:CD2	1:D:153:LEU:HB3	2.20	0.71
1:C:342:ALA:O	1:C:346:GLU:HB2	1.90	0.71
1:B:342:ALA:O	1:B:346:GLU:HB2	1.91	0.71
1:C:515:ARG:O	1:C:518:ILE:HG22	1.91	0.71
1:C:396:PRO:HB2	1:C:397:PRO:CD	2.20	0.71
1:B:135:ARG:HG2	1:B:141:ILE:HD11	1.73	0.71
1:A:135:ARG:HG2	1:A:141:ILE:HD11	1.73	0.71
1:B:149:LEU:HB3	1:B:153:LEU:HD13	1.73	0.71
1:A:406:THR:HB	1:B:345:ARG:HH21	1.55	0.71
1:C:382:ARG:O	1:C:383:GLN:HB3	1.90	0.71
1:D:11:PHE:CE1	1:D:88:LEU:HD12	2.26	0.71
1:C:135:ARG:HG2	1:C:141:ILE:HD11	1.72	0.70
1:B:427:LYS:HB3	1:B:428:ASN:HD22	1.55	0.70
1:C:13:GLU:HG2	1:C:15:ASN:N	2.06	0.70
1:A:386:HIS:CD2	1:A:387:LEU:HD12	2.26	0.70
1:A:13:GLU:HG2	1:A:15:ASN:N	2.06	0.70
1:C:473:ASN:O	1:C:474:LEU:HB2	1.91	0.70
1:D:190:LEU:HB2	1:D:263:PRO:HG2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ALA:HB2	1:C:123:VAL:CG1	2.22	0.70
1:A:149:LEU:CD2	1:A:153:LEU:CD2	2.68	0.70
1:A:149:LEU:HD23	1:A:153:LEU:HD23	1.72	0.70
1:D:458:VAL:HG11	1:D:491:VAL:HG22	1.73	0.70
1:B:454:LEU:O	1:B:454:LEU:HD12	1.91	0.69
1:A:216:LEU:HD21	1:A:252:GLU:HG2	1.72	0.69
1:A:190:LEU:HB2	1:A:263:PRO:HG2	1.74	0.69
1:D:76:ARG:NH2	1:D:169:PRO:HB3	2.08	0.69
1:B:515:ARG:O	1:B:518:ILE:HG22	1.92	0.69
1:D:13:GLU:H	1:D:46:ARG:HA	1.57	0.69
1:D:458:VAL:HG23	1:D:487:LEU:HD23	1.74	0.69
1:A:471:CYS:SG	1:A:472:GLY:N	2.65	0.69
1:D:424:LYS:HG3	1:D:424:LYS:O	1.93	0.69
1:C:148:ALA:N	1:C:150:PRO:HD2	2.08	0.69
1:B:176:THR:CG2	1:B:177:GLY:N	2.56	0.69
1:C:76:ARG:NH2	1:C:169:PRO:HB3	2.08	0.68
1:B:76:ARG:NH2	1:B:169:PRO:HB3	2.08	0.68
1:A:473:ASN:O	1:A:474:LEU:HB2	1.93	0.68
1:B:116:ALA:HB2	1:B:123:VAL:CG1	2.23	0.68
1:D:148:ALA:C	1:D:150:PRO:HD2	2.14	0.68
1:D:13:GLU:HG2	1:D:15:ASN:N	2.08	0.68
1:D:25:GLN:HB3	1:D:29:GLN:HE21	1.59	0.68
1:A:382:ARG:O	1:A:383:GLN:HB3	1.92	0.68
1:C:148:ALA:C	1:C:150:PRO:HD2	2.13	0.68
1:A:424:LYS:HG3	1:A:424:LYS:O	1.94	0.68
1:A:427:LYS:HB3	1:A:428:ASN:ND2	2.09	0.68
1:C:489:THR:CG2	1:D:489:THR:HG21	2.07	0.68
1:A:396:PRO:HB2	1:A:397:PRO:CD	2.24	0.68
1:B:473:ASN:O	1:B:474:LEU:HB2	1.92	0.68
1:C:445:ARG:HG3	1:C:445:ARG:NH1	2.07	0.68
1:D:471:CYS:SG	1:D:472:GLY:N	2.67	0.68
1:A:373:MSE:HE2	1:B:351:SER:OG	1.93	0.67
1:B:374:VAL:HG21	1:B:480:LEU:HD22	1.76	0.67
1:A:116:ALA:HB2	1:A:123:VAL:CG1	2.24	0.67
1:D:11:PHE:CZ	1:D:88:LEU:HD11	2.29	0.67
1:B:148:ALA:C	1:B:150:PRO:HD2	2.14	0.67
1:D:116:ALA:HB2	1:D:123:VAL:CG1	2.24	0.67
1:C:427:LYS:HG3	1:C:436:ARG:HH11	1.60	0.67
1:B:148:ALA:N	1:B:150:PRO:HD2	2.09	0.67
1:D:316:ASP:O	1:D:320:ARG:HG2	1.95	0.67
1:C:374:VAL:HG21	1:C:480:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CE1	1:A:88:LEU:HD12	2.29	0.67
1:D:427:LYS:HB3	1:D:428:ASN:ND2	2.08	0.67
1:A:531:LEU:H	1:A:531:LEU:CD2	2.01	0.67
1:A:148:ALA:C	1:A:150:PRO:HD2	2.15	0.67
1:A:111:PHE:HD2	1:A:176:THR:HG1	1.40	0.67
1:A:176:THR:CG2	1:A:177:GLY:N	2.58	0.67
1:B:299:ARG:O	1:B:303:VAL:HG12	1.95	0.67
1:D:8:VAL:O	1:D:8:VAL:HG12	1.95	0.67
1:A:76:ARG:NH2	1:A:169:PRO:HB3	2.10	0.67
1:C:351:SER:OG	1:D:373:MSE:HE3	1.95	0.67
1:D:299:ARG:O	1:D:303:VAL:HG12	1.95	0.67
1:D:396:PRO:HB2	1:D:397:PRO:CD	2.25	0.67
1:C:386:HIS:CD2	1:C:387:LEU:HD12	2.30	0.67
1:C:25:GLN:HB3	1:C:29:GLN:HE21	1.58	0.66
1:D:148:ALA:N	1:D:150:PRO:HD2	2.10	0.66
1:A:149:LEU:HD22	1:A:153:LEU:HD22	1.75	0.66
1:C:299:ARG:O	1:C:303:VAL:HG12	1.95	0.66
1:A:373:MSE:CE	1:B:354:PRO:O	2.43	0.66
1:C:76:ARG:CZ	1:C:169:PRO:HB2	2.24	0.66
1:B:13:GLU:CG	1:B:13:GLU:O	2.36	0.66
1:A:76:ARG:CZ	1:A:169:PRO:HB2	2.26	0.66
1:D:386:HIS:CD2	1:D:387:LEU:HD12	2.31	0.66
1:B:76:ARG:CZ	1:B:169:PRO:HB2	2.25	0.66
1:B:386:HIS:CD2	1:B:387:LEU:HD12	2.30	0.66
1:B:427:LYS:HG3	1:B:436:ARG:HH11	1.61	0.66
1:D:531:LEU:CD2	1:D:531:LEU:H	1.99	0.66
1:B:531:LEU:H	1:B:531:LEU:CD2	2.05	0.66
1:B:382:ARG:O	1:B:383:GLN:HB3	1.96	0.66
1:A:13:GLU:H	1:A:46:ARG:HA	1.61	0.66
1:A:374:VAL:HG21	1:A:480:LEU:CD2	2.26	0.66
1:A:148:ALA:N	1:A:150:PRO:HD2	2.10	0.65
1:C:13:GLU:H	1:C:46:ARG:HA	1.60	0.65
1:B:25:GLN:HB3	1:B:29:GLN:HE21	1.61	0.65
1:A:374:VAL:HG21	1:A:480:LEU:HD22	1.78	0.65
1:D:76:ARG:CZ	1:D:169:PRO:HB2	2.25	0.65
1:D:46:ARG:CZ	1:D:82:HIS:HD2	2.10	0.65
1:B:458:VAL:CG1	1:B:491:VAL:HG22	2.27	0.65
1:A:299:ARG:O	1:A:303:VAL:HG12	1.97	0.65
1:B:502:LEU:HA	1:B:505:MSE:CG	2.26	0.65
1:C:8:VAL:HG12	1:C:8:VAL:O	1.96	0.65
1:D:374:VAL:HG21	1:D:480:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:CZ	1:C:82:HIS:HD2	2.10	0.65
1:A:247:HIS:CD2	1:A:281:ALA:HA	2.32	0.65
1:A:189:LEU:HD12	1:A:234:VAL:HG23	1.79	0.65
1:A:316:ASP:O	1:A:320:ARG:HG2	1.97	0.65
1:A:25:GLN:HB3	1:A:29:GLN:HE21	1.61	0.64
1:A:344:VAL:HG22	1:A:345:ARG:HG2	1.78	0.64
1:C:11:PHE:CZ	1:C:88:LEU:HD11	2.32	0.64
1:C:502:LEU:HA	1:C:505:MSE:CG	2.24	0.64
1:D:247:HIS:CD2	1:D:281:ALA:HA	2.31	0.64
1:D:189:LEU:HD12	1:D:234:VAL:HG23	1.79	0.64
1:B:374:VAL:HG21	1:B:480:LEU:CD2	2.27	0.64
1:C:247:HIS:CD2	1:C:281:ALA:HA	2.32	0.64
1:D:176:THR:CG2	1:D:177:GLY:N	2.60	0.64
1:D:351:SER:HB2	1:D:354:PRO:HD2	1.80	0.64
1:B:46:ARG:CZ	1:B:82:HIS:HD2	2.10	0.64
1:C:316:ASP:O	1:C:320:ARG:HG2	1.98	0.64
1:C:189:LEU:HD12	1:C:234:VAL:HG23	1.80	0.64
1:D:149:LEU:C	1:D:153:LEU:HD12	2.18	0.64
1:A:46:ARG:CZ	1:A:82:HIS:HD2	2.10	0.64
1:C:374:VAL:HG21	1:C:480:LEU:CD2	2.27	0.64
1:B:426:PRO:O	1:B:427:LYS:CB	2.35	0.64
1:D:11:PHE:CE1	1:D:88:LEU:CD1	2.81	0.64
1:D:441:GLN:OE1	1:D:505:MSE:HA	1.97	0.64
1:A:373:MSE:CE	1:B:351:SER:O	2.36	0.64
1:B:13:GLU:HG2	1:B:15:ASN:N	2.13	0.64
1:A:441:GLN:OE1	1:A:505:MSE:HA	1.98	0.64
1:A:458:VAL:HG23	1:A:487:LEU:HD23	1.80	0.64
1:A:386:HIS:CD2	1:A:387:LEU:CD1	2.81	0.64
1:A:11:PHE:CZ	1:A:88:LEU:HD11	2.33	0.64
1:D:502:LEU:HA	1:D:505:MSE:CG	2.25	0.63
1:B:441:GLN:OE1	1:B:505:MSE:HA	1.99	0.63
1:C:285:TYR:O	1:C:289:GLU:HB2	1.98	0.63
1:B:8:VAL:HG12	1:B:8:VAL:O	1.97	0.63
1:C:427:LYS:HB3	1:C:428:ASN:ND2	2.12	0.63
1:D:454:LEU:O	1:D:454:LEU:HD12	1.98	0.63
1:B:247:HIS:CD2	1:B:281:ALA:HA	2.33	0.63
1:C:424:LYS:O	1:C:424:LYS:HG3	1.97	0.63
1:C:427:LYS:CE	1:C:436:ARG:HH12	2.00	0.63
1:D:425:LEU:HB3	1:D:436:ARG:HG3	1.80	0.63
1:C:363:VAL:HG13	1:D:363:VAL:CG1	2.27	0.63
1:D:285:TYR:O	1:D:289:GLU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:THR:CG2	1:C:177:GLY:N	2.61	0.63
1:D:382:ARG:O	1:D:383:GLN:CB	2.46	0.63
1:B:424:LYS:O	1:B:424:LYS:HG3	1.98	0.63
1:A:111:PHE:HD2	1:A:176:THR:OG1	1.82	0.62
1:D:374:VAL:HG21	1:D:480:LEU:CD2	2.30	0.62
1:A:200:ALA:HB2	1:A:234:VAL:HG13	1.81	0.62
1:A:8:VAL:O	1:A:8:VAL:HG12	1.97	0.62
1:C:111:PHE:HD2	1:C:176:THR:OG1	1.83	0.62
1:C:425:LEU:HB3	1:C:436:ARG:HG3	1.81	0.62
1:B:427:LYS:HB3	1:B:428:ASN:ND2	2.13	0.62
1:A:425:LEU:HB3	1:A:436:ARG:HG3	1.81	0.62
1:C:149:LEU:HB3	1:C:153:LEU:CD2	2.30	0.62
1:C:458:VAL:HG22	1:C:487:LEU:HD23	1.82	0.62
1:D:200:ALA:HB2	1:D:234:VAL:HG13	1.80	0.62
1:B:453:LYS:O	1:B:457:THR:HG22	1.99	0.62
1:B:425:LEU:HB3	1:B:436:ARG:HG3	1.81	0.62
1:B:189:LEU:HD11	1:B:199:ILE:HD12	1.82	0.62
1:A:370:LEU:HD11	1:B:359:VAL:CG1	2.27	0.62
1:B:200:ALA:HB2	1:B:234:VAL:HG13	1.82	0.62
1:B:506:THR:O	1:B:507:ASP:CB	2.46	0.62
1:B:285:TYR:O	1:B:289:GLU:HB2	1.99	0.62
1:C:351:SER:O	1:D:373:MSE:CE	2.30	0.62
1:A:427:LYS:HG3	1:A:436:ARG:HH11	1.65	0.62
1:C:386:HIS:CD2	1:C:387:LEU:CD1	2.83	0.62
1:C:254:ARG:HH11	1:C:254:ARG:HB3	1.65	0.62
1:D:111:PHE:HD2	1:D:176:THR:OG1	1.83	0.61
1:C:200:ALA:HB2	1:C:234:VAL:HG13	1.81	0.61
1:D:111:PHE:HD2	1:D:176:THR:HG1	1.47	0.61
1:B:11:PHE:CE1	1:B:88:LEU:HD12	2.34	0.61
1:C:149:LEU:HB3	1:C:153:LEU:HD21	1.82	0.61
1:A:11:PHE:CE1	1:A:88:LEU:CD1	2.83	0.61
1:C:441:GLN:OE1	1:C:505:MSE:HA	2.00	0.61
1:D:82:HIS:O	1:D:84:ARG:N	2.34	0.61
1:B:458:VAL:HG23	1:B:487:LEU:HD23	1.82	0.61
1:B:386:HIS:CD2	1:B:387:LEU:CD1	2.83	0.61
1:B:189:LEU:HD12	1:B:234:VAL:HG23	1.82	0.61
1:C:9:PRO:HG2	1:C:49:TYR:HB2	1.83	0.61
1:B:111:PHE:HD2	1:B:176:THR:OG1	1.84	0.61
1:B:349:ALA:C	1:B:351:SER:N	2.54	0.61
1:A:2:SER:O	1:A:3:GLN:HB2	2.01	0.61
1:C:506:THR:O	1:C:507:ASP:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:SER:OG	1:D:479:ASP:N	2.33	0.61
1:B:458:VAL:CG2	1:B:487:LEU:HD23	2.31	0.61
1:A:390:THR:HG22	1:A:393:ARG:NH2	2.14	0.61
1:A:458:VAL:CG2	1:A:487:LEU:HD23	2.31	0.61
1:C:462:TRP:HB3	1:C:528:GLN:HG2	1.83	0.61
1:A:35:LEU:HD12	1:A:51:PHE:HB3	1.83	0.61
1:D:254:ARG:HB3	1:D:254:ARG:HH11	1.65	0.61
1:B:11:PHE:CZ	1:B:88:LEU:HD11	2.36	0.60
1:C:215:ARG:CZ	1:C:252:GLU:OE2	2.49	0.60
1:A:454:LEU:O	1:A:454:LEU:HD12	2.01	0.60
1:A:382:ARG:O	1:A:383:GLN:CB	2.49	0.60
1:A:349:ALA:C	1:A:351:SER:N	2.54	0.60
1:C:11:PHE:CE1	1:C:88:LEU:HD12	2.35	0.60
1:D:506:THR:O	1:D:507:ASP:CB	2.48	0.60
1:B:9:PRO:HG2	1:B:49:TYR:HB2	1.83	0.60
1:A:502:LEU:HA	1:A:505:MSE:CG	2.28	0.60
1:C:453:LYS:O	1:C:457:THR:HG22	2.00	0.60
1:A:506:THR:O	1:A:507:ASP:CB	2.49	0.60
1:D:135:ARG:HH11	1:D:135:ARG:HG3	1.66	0.60
1:A:82:HIS:O	1:A:84:ARG:N	2.34	0.60
1:C:351:SER:HB2	1:C:354:PRO:HD2	1.84	0.60
1:A:149:LEU:CB	1:A:153:LEU:CD2	2.78	0.60
1:A:215:ARG:CZ	1:A:252:GLU:OE2	2.49	0.60
1:D:386:HIS:CD2	1:D:387:LEU:CD1	2.84	0.60
1:D:189:LEU:HD11	1:D:199:ILE:HD12	1.84	0.60
1:C:354:PRO:O	1:D:373:MSE:CE	2.50	0.60
1:A:478:SER:OG	1:A:479:ASP:N	2.34	0.60
1:A:326:VAL:O	1:A:326:VAL:CG2	2.49	0.60
1:D:427:LYS:HG3	1:D:436:ARG:HH11	1.67	0.60
1:A:499:LEU:CD2	1:A:515:ARG:HH11	2.14	0.60
1:D:453:LYS:O	1:D:457:THR:HG22	2.02	0.60
1:A:363:VAL:HG13	1:B:363:VAL:CG1	2.27	0.60
1:A:153:LEU:HD12	1:A:165:SER:O	2.02	0.60
1:B:351:SER:HB2	1:B:354:PRO:HD2	1.83	0.59
1:B:82:HIS:O	1:B:84:ARG:N	2.36	0.59
1:C:382:ARG:O	1:C:383:GLN:CB	2.50	0.59
1:A:353:ALA:HB3	1:A:354:PRO:HD2	1.84	0.59
1:C:10:ASN:OD1	1:C:46:ARG:NH1	2.35	0.59
1:D:135:ARG:HG2	1:D:141:ILE:HD11	1.84	0.59
1:C:248:THR:O	1:C:252:GLU:HB2	2.03	0.59
1:D:2:SER:O	1:D:3:GLN:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:HD21	1:A:515:ARG:HH11	1.68	0.59
1:C:141:ILE:O	1:C:143:ALA:N	2.34	0.59
1:B:316:ASP:O	1:B:320:ARG:HG2	2.02	0.59
1:C:349:ALA:O	1:C:351:SER:N	2.35	0.59
1:C:142:ARG:O	1:C:144:GLY:N	2.35	0.59
1:D:35:LEU:HD12	1:D:51:PHE:HB3	1.85	0.59
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.67	0.59
1:A:138:LEU:HD21	1:A:142:ARG:HH12	1.68	0.59
1:A:142:ARG:O	1:A:144:GLY:N	2.36	0.59
1:B:215:ARG:CZ	1:B:252:GLU:OE2	2.50	0.59
1:B:27:ILE:CD1	1:B:51:PHE:CE1	2.81	0.59
1:B:13:GLU:O	1:B:14:GLY:C	2.36	0.59
1:D:143:ALA:O	1:D:152:LYS:NZ	2.35	0.59
1:C:359:VAL:CG1	1:D:370:LEU:HD11	2.31	0.59
1:D:248:THR:O	1:D:252:GLU:HB2	2.02	0.59
1:C:138:LEU:HD21	1:C:142:ARG:HH12	1.68	0.59
1:D:215:ARG:CZ	1:D:252:GLU:OE2	2.51	0.59
1:C:11:PHE:CE1	1:C:88:LEU:CD1	2.86	0.59
1:A:363:VAL:CG1	1:B:363:VAL:CG1	2.80	0.58
1:A:248:THR:O	1:A:252:GLU:HB2	2.03	0.58
1:B:138:LEU:HD21	1:B:142:ARG:HH12	1.68	0.58
1:B:141:ILE:O	1:B:143:ALA:N	2.34	0.58
1:D:326:VAL:CG2	1:D:326:VAL:O	2.50	0.58
1:A:127:GLY:C	1:A:129:ALA:H	2.06	0.58
1:B:142:ARG:O	1:B:144:GLY:N	2.34	0.58
1:C:35:LEU:HD12	1:C:51:PHE:HB3	1.83	0.58
1:B:499:LEU:CD2	1:B:515:ARG:HH11	2.17	0.58
1:D:445:ARG:NH1	1:D:445:ARG:HG3	2.10	0.58
1:C:43:SER:O	1:C:81:GLU:HB2	2.04	0.58
1:A:4:LEU:HD12	1:A:52:VAL:HB	1.85	0.58
1:A:351:SER:HB2	1:A:354:PRO:HD2	1.85	0.58
1:D:83:PRO:HA	1:D:145:GLU:OE1	2.03	0.58
1:B:153:LEU:HD22	1:B:153:LEU:H	1.68	0.58
1:B:248:THR:O	1:B:252:GLU:HB2	2.04	0.58
1:A:12:SER:HB2	1:A:87:ALA:HA	1.85	0.58
1:A:376:GLN:HG2	1:A:395:ILE:HD13	1.85	0.58
1:D:12:SER:HB2	1:D:87:ALA:HA	1.86	0.58
1:A:453:LYS:O	1:A:457:THR:HG22	2.03	0.58
1:D:462:TRP:HB3	1:D:528:GLN:HG2	1.84	0.58
1:A:458:VAL:CG1	1:A:491:VAL:HG22	2.34	0.58
1:D:376:GLN:HG2	1:D:395:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:THR:O	1:D:531:LEU:HD23	2.03	0.58
1:C:82:HIS:O	1:C:84:ARG:N	2.36	0.58
1:A:189:LEU:HD11	1:A:199:ILE:HD12	1.86	0.58
1:B:304:VAL:HG12	1:B:305:ASN:N	2.18	0.58
1:B:216:LEU:HD21	1:B:252:GLU:HG2	1.85	0.58
1:B:254:ARG:HB3	1:B:254:ARG:HH11	1.69	0.58
1:B:2:SER:O	1:B:3:GLN:HB2	2.03	0.58
1:D:138:LEU:HD21	1:D:142:ARG:HH12	1.69	0.58
1:B:382:ARG:O	1:B:383:GLN:CB	2.52	0.58
1:D:9:PRO:HG2	1:D:49:TYR:HB2	1.86	0.58
1:C:15:ASN:O	1:C:16:ASN:CB	2.49	0.57
1:B:462:TRP:HB3	1:B:528:GLN:HG2	1.86	0.57
1:A:427:LYS:CE	1:A:436:ARG:HH12	2.04	0.57
1:B:373:MSE:O	1:B:373:MSE:HG2	1.95	0.57
1:D:499:LEU:HD21	1:D:515:ARG:HH11	1.69	0.57
1:C:189:LEU:HD11	1:C:199:ILE:HD12	1.86	0.57
1:A:254:ARG:HH11	1:A:254:ARG:HB3	1.69	0.57
1:B:35:LEU:HD12	1:B:51:PHE:HB3	1.84	0.57
1:D:4:LEU:HD12	1:D:52:VAL:HB	1.86	0.57
1:B:143:ALA:O	1:B:152:LYS:NZ	2.38	0.57
1:C:2:SER:O	1:C:3:GLN:HB2	2.03	0.57
1:C:458:VAL:CG1	1:C:491:VAL:HG22	2.27	0.57
1:D:142:ARG:O	1:D:144:GLY:N	2.37	0.57
1:D:127:GLY:C	1:D:129:ALA:H	2.08	0.57
1:C:4:LEU:HD23	1:C:97:ARG:NH2	2.19	0.57
1:A:462:TRP:HB3	1:A:528:GLN:HG2	1.85	0.57
1:A:9:PRO:HG2	1:A:49:TYR:HB2	1.86	0.57
1:A:343:PHE:O	1:A:346:GLU:HB3	2.05	0.57
1:A:143:ALA:O	1:A:152:LYS:NZ	2.37	0.57
1:D:458:VAL:CG1	1:D:491:VAL:HG22	2.34	0.57
1:A:285:TYR:O	1:A:289:GLU:HB2	2.04	0.57
1:B:149:LEU:HD22	1:B:153:LEU:HB3	1.86	0.57
1:C:4:LEU:HB3	1:C:96:VAL:HB	1.87	0.57
1:B:10:ASN:OD1	1:B:46:ARG:NH1	2.38	0.57
1:C:135:ARG:HH11	1:C:135:ARG:HG3	1.68	0.57
1:C:143:ALA:O	1:C:152:LYS:NZ	2.38	0.57
1:D:458:VAL:CG2	1:D:487:LEU:HD23	2.34	0.57
1:B:376:GLN:HG2	1:B:395:ILE:HD13	1.87	0.57
1:D:344:VAL:HG22	1:D:345:ARG:HG2	1.85	0.57
1:A:527:THR:O	1:A:531:LEU:HD23	2.05	0.56
1:B:13:GLU:H	1:B:46:ARG:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:CD2	1:B:426:PRO:HD2	2.23	0.56
1:A:534:GLY:O	1:A:535:SER:C	2.43	0.56
1:C:487:LEU:O	1:C:491:VAL:HG23	2.04	0.56
1:A:141:ILE:HG21	1:A:175:VAL:HG11	1.88	0.56
1:A:83:PRO:HA	1:A:145:GLU:OE1	2.04	0.56
1:B:11:PHE:CE1	1:B:88:LEU:CD1	2.88	0.56
1:A:326:VAL:O	1:A:326:VAL:HG22	2.05	0.56
1:A:149:LEU:CB	1:A:153:LEU:HD23	2.36	0.56
1:C:376:GLN:HG2	1:C:395:ILE:HD13	1.88	0.56
1:D:191:SER:HB2	1:D:195:GLN:OE1	2.06	0.56
1:C:348:GLY:HA2	1:D:373:MSE:HB2	1.88	0.56
1:C:12:SER:HB2	1:C:87:ALA:HA	1.88	0.56
1:D:498:VAL:HG12	1:D:502:LEU:CD1	2.35	0.56
1:D:499:LEU:CD2	1:D:515:ARG:HH11	2.19	0.56
1:B:30:THR:HG21	1:B:61:GLY:N	2.21	0.56
1:C:390:THR:HG22	1:C:393:ARG:NH2	2.17	0.56
1:B:153:LEU:N	1:B:153:LEU:CD2	2.68	0.56
1:B:4:LEU:HB3	1:B:96:VAL:HB	1.87	0.56
1:B:344:VAL:HG22	1:B:345:ARG:HG2	1.86	0.56
1:C:517:ARG:O	1:C:520:SER:OG	2.23	0.56
1:B:43:SER:O	1:B:81:GLU:HB2	2.06	0.56
1:B:127:GLY:C	1:B:129:ALA:H	2.09	0.56
1:A:304:VAL:HG12	1:A:305:ASN:N	2.20	0.56
1:A:36:LEU:HD22	1:A:325:LEU:HD22	1.87	0.56
1:B:4:LEU:HD12	1:B:52:VAL:HB	1.88	0.55
1:A:428:ASN:H	1:A:433:ARG:HB2	1.71	0.55
1:B:498:VAL:HG12	1:B:502:LEU:CD1	2.36	0.55
1:C:111:PHE:HD2	1:C:176:THR:HG1	1.52	0.55
1:B:390:THR:HG22	1:B:393:ARG:NH2	2.18	0.55
1:D:36:LEU:HD22	1:D:325:LEU:HD22	1.88	0.55
1:C:326:VAL:CG2	1:C:326:VAL:O	2.53	0.55
1:C:4:LEU:HD12	1:C:52:VAL:HB	1.89	0.55
1:D:15:ASN:O	1:D:16:ASN:CB	2.49	0.55
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.70	0.55
1:A:141:ILE:O	1:A:143:ALA:N	2.38	0.55
1:A:349:ALA:O	1:A:351:SER:N	2.39	0.55
1:B:499:LEU:HD21	1:B:515:ARG:HH11	1.71	0.55
1:A:492:PHE:CD2	1:A:522:LEU:HD11	2.42	0.55
1:D:353:ALA:HB3	1:D:354:PRO:HD2	1.87	0.55
1:D:141:ILE:O	1:D:143:ALA:N	2.38	0.55
1:B:111:PHE:HD2	1:B:176:THR:HG1	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ARG:O	1:A:520:SER:OG	2.24	0.55
1:B:4:LEU:HD23	1:B:97:ARG:NH2	2.21	0.55
1:B:76:ARG:NH2	1:B:169:PRO:CB	2.69	0.55
1:D:4:LEU:HB3	1:D:96:VAL:HB	1.89	0.55
1:A:124:TYR:HD2	1:A:160:PRO:HA	1.71	0.55
1:B:8:VAL:HG22	1:B:50:THR:HG23	1.89	0.55
1:B:216:LEU:HD13	1:B:249:VAL:HG22	1.89	0.55
1:A:498:VAL:HG12	1:A:502:LEU:CD1	2.36	0.55
1:C:138:LEU:N	1:C:139:PRO:HD2	2.22	0.55
1:D:445:ARG:NH1	1:D:445:ARG:CG	2.60	0.55
1:A:84:ARG:O	1:A:145:GLU:HB2	2.06	0.55
1:B:176:THR:HG22	1:B:177:GLY:N	2.22	0.55
1:A:27:ILE:CD1	1:A:51:PHE:CE1	2.81	0.55
1:D:428:ASN:H	1:D:433:ARG:HB2	1.72	0.55
1:B:124:TYR:HD2	1:B:160:PRO:HA	1.72	0.55
1:D:84:ARG:O	1:D:145:GLU:HB2	2.07	0.55
1:B:343:PHE:O	1:B:347:VAL:HG13	2.07	0.54
1:C:425:LEU:CD2	1:C:426:PRO:HD2	2.24	0.54
1:D:390:THR:HG22	1:D:393:ARG:NH2	2.17	0.54
1:C:477:LEU:O	1:C:481:GLN:HG3	2.07	0.54
1:C:76:ARG:NH2	1:C:169:PRO:CB	2.70	0.54
1:A:359:VAL:HG11	1:B:370:LEU:HD11	1.88	0.54
1:C:124:TYR:HD2	1:C:160:PRO:HA	1.72	0.54
1:C:215:ARG:NH2	1:C:252:GLU:OE2	2.39	0.54
1:C:141:ILE:HG21	1:C:175:VAL:HG11	1.88	0.54
1:C:499:LEU:HD21	1:C:515:ARG:HH11	1.72	0.54
1:B:102:ASP:CG	1:C:109:LYS:HZ1	2.09	0.54
1:D:534:GLY:O	1:D:535:SER:C	2.46	0.54
1:C:498:VAL:HG12	1:C:502:LEU:CD1	2.36	0.54
1:B:141:ILE:HG21	1:B:175:VAL:HG11	1.89	0.54
1:A:10:ASN:OD1	1:A:46:ARG:NH1	2.39	0.54
1:D:76:ARG:NH2	1:D:169:PRO:CB	2.70	0.54
1:C:216:LEU:HD21	1:C:252:GLU:HG2	1.89	0.54
1:D:304:VAL:HG12	1:D:305:ASN:N	2.22	0.54
1:B:12:SER:HB2	1:B:87:ALA:HA	1.89	0.54
1:D:4:LEU:HD23	1:D:97:ARG:NH2	2.23	0.54
1:B:143:ALA:HB1	1:B:152:LYS:NZ	2.23	0.54
1:A:148:ALA:H	1:A:150:PRO:HD2	1.73	0.54
1:D:125:LEU:O	1:D:130:ALA:HB2	2.07	0.54
1:D:531:LEU:N	1:D:531:LEU:HD23	2.05	0.54
1:D:10:ASN:OD1	1:D:46:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ARG:HG3	1:B:445:ARG:NH1	2.11	0.54
1:B:149:LEU:N	1:B:150:PRO:HD2	2.23	0.54
1:C:323:GLU:N	1:C:323:GLU:OE1	2.41	0.54
1:C:83:PRO:HA	1:C:145:GLU:OE1	2.08	0.54
1:D:141:ILE:HG21	1:D:175:VAL:HG11	1.89	0.54
1:A:215:ARG:NH2	1:A:252:GLU:OE2	2.40	0.54
1:C:326:VAL:HG22	1:C:326:VAL:O	2.07	0.54
1:C:30:THR:HG21	1:C:61:GLY:N	2.22	0.54
1:D:30:THR:HG21	1:D:61:GLY:N	2.23	0.54
1:D:326:VAL:HG22	1:D:326:VAL:O	2.07	0.54
1:D:143:ALA:HB1	1:D:152:LYS:NZ	2.23	0.54
1:A:191:SER:HB2	1:A:195:GLN:OE1	2.07	0.54
1:B:455:ALA:O	1:B:456:GLU:C	2.46	0.54
1:C:125:LEU:O	1:C:130:ALA:HB2	2.08	0.54
1:D:427:LYS:CE	1:D:436:ARG:HH12	2.05	0.53
1:A:531:LEU:N	1:A:531:LEU:HD23	2.06	0.53
1:B:527:THR:O	1:B:531:LEU:HD23	2.08	0.53
1:C:143:ALA:HB1	1:C:152:LYS:NZ	2.23	0.53
1:D:382:ARG:HG2	1:D:383:GLN:N	2.23	0.53
1:D:8:VAL:HG22	1:D:50:THR:HG23	1.90	0.53
1:B:349:ALA:O	1:B:351:SER:N	2.42	0.53
1:A:4:LEU:HB3	1:A:96:VAL:HB	1.89	0.53
1:C:345:ARG:HH21	1:D:406:THR:CB	2.18	0.53
1:A:125:LEU:O	1:A:130:ALA:HB2	2.08	0.53
1:A:30:THR:HG21	1:A:61:GLY:N	2.23	0.53
1:D:343:PHE:O	1:D:347:VAL:HG13	2.09	0.53
1:B:138:LEU:N	1:B:139:PRO:HD2	2.22	0.53
1:D:215:ARG:NH2	1:D:252:GLU:OE2	2.40	0.53
1:C:148:ALA:H	1:C:150:PRO:HD2	1.72	0.53
1:B:36:LEU:HD22	1:B:325:LEU:HD22	1.91	0.53
1:A:373:MSE:HG2	1:A:373:MSE:O	2.08	0.53
1:A:149:LEU:N	1:A:150:PRO:HD2	2.24	0.53
1:A:13:GLU:HB2	1:A:46:ARG:C	2.28	0.53
1:B:427:LYS:CE	1:B:436:ARG:HH12	2.03	0.53
1:C:124:TYR:CD2	1:C:160:PRO:HA	2.44	0.53
1:A:143:ALA:HB1	1:A:152:LYS:NZ	2.23	0.53
1:D:11:PHE:CZ	1:D:88:LEU:CD1	2.90	0.53
1:D:43:SER:O	1:D:81:GLU:HB2	2.09	0.53
1:B:124:TYR:CD2	1:B:160:PRO:HA	2.44	0.53
1:A:124:TYR:CD2	1:A:160:PRO:HA	2.44	0.53
1:D:477:LEU:O	1:D:481:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:GLY:C	1:C:129:ALA:H	2.11	0.53
1:B:83:PRO:HA	1:B:145:GLU:OE1	2.09	0.52
1:D:323:GLU:OE1	1:D:323:GLU:N	2.41	0.52
1:B:428:ASN:H	1:B:433:ARG:HB2	1.74	0.52
1:D:149:LEU:N	1:D:150:PRO:HD2	2.24	0.52
1:D:487:LEU:O	1:D:491:VAL:HG23	2.09	0.52
1:A:353:ALA:HB3	1:A:354:PRO:CD	2.38	0.52
1:B:527:THR:O	1:B:530:ALA:HB3	2.09	0.52
1:B:125:LEU:O	1:B:130:ALA:HB2	2.09	0.52
1:C:36:LEU:HD22	1:C:325:LEU:HD22	1.90	0.52
1:C:531:LEU:H	1:C:531:LEU:CD2	2.06	0.52
1:A:138:LEU:N	1:A:139:PRO:HD2	2.25	0.52
1:A:445:ARG:CG	1:A:445:ARG:NH1	2.61	0.52
1:B:126:TYR:O	1:B:129:ALA:HB3	2.10	0.52
1:C:17:GLN:HA	1:C:17:GLN:OE1	2.09	0.52
1:C:149:LEU:N	1:C:150:PRO:HD2	2.24	0.52
1:D:527:THR:O	1:D:530:ALA:HB3	2.10	0.52
1:C:8:VAL:HG22	1:C:50:THR:HG23	1.92	0.52
1:A:8:VAL:HG22	1:A:50:THR:HG23	1.92	0.52
1:A:510:PHE:C	1:A:510:PHE:CD2	2.83	0.52
1:B:326:VAL:CG2	1:B:326:VAL:O	2.57	0.52
1:A:445:ARG:NH1	1:A:445:ARG:HG3	2.12	0.52
1:B:153:LEU:H	1:B:153:LEU:CD2	2.22	0.52
1:A:487:LEU:O	1:A:491:VAL:HG23	2.09	0.52
1:B:517:ARG:O	1:B:520:SER:OG	2.28	0.52
1:D:425:LEU:CD2	1:D:426:PRO:HD2	2.26	0.52
1:A:76:ARG:NH2	1:A:169:PRO:CB	2.71	0.52
1:B:382:ARG:HA	1:B:385:ASP:OD1	2.09	0.52
1:C:13:GLU:HG2	1:C:15:ASN:CA	2.40	0.52
1:D:124:TYR:HD2	1:D:160:PRO:HA	1.74	0.52
1:B:478:SER:OG	1:B:479:ASP:N	2.43	0.52
1:B:506:THR:O	1:B:507:ASP:HB2	2.10	0.52
1:C:36:LEU:HD22	1:C:325:LEU:CD2	2.40	0.52
1:D:148:ALA:H	1:D:150:PRO:HD2	1.72	0.52
1:B:176:THR:HG23	1:B:177:GLY:H	1.75	0.52
1:C:499:LEU:CD2	1:C:515:ARG:HH11	2.22	0.52
1:A:11:PHE:CZ	1:A:88:LEU:CD1	2.93	0.52
1:A:176:THR:HG22	1:A:177:GLY:N	2.25	0.52
1:C:216:LEU:HD13	1:C:249:VAL:HG22	1.91	0.52
1:A:43:SER:O	1:A:81:GLU:HB2	2.10	0.52
1:C:13:GLU:HG2	1:C:15:ASN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:GLU:OE1	1:D:227:GLU:CA	2.50	0.51
1:D:13:GLU:OE1	1:D:45:ASN:HA	2.10	0.51
1:D:27:ILE:CD1	1:D:51:PHE:CE1	2.87	0.51
1:D:123:VAL:HG13	1:D:162:PHE:HB2	1.92	0.51
1:A:176:THR:HG23	1:A:177:GLY:H	1.76	0.51
1:C:84:ARG:O	1:C:145:GLU:HB2	2.10	0.51
1:C:13:GLU:HB2	1:C:46:ARG:C	2.31	0.51
1:B:148:ALA:H	1:B:150:PRO:HD2	1.73	0.51
1:A:506:THR:O	1:A:507:ASP:HB2	2.11	0.51
1:A:265:VAL:HG23	1:A:265:VAL:O	2.10	0.51
1:B:353:ALA:HB3	1:B:354:PRO:HD2	1.92	0.51
1:B:84:ARG:O	1:B:145:GLU:HB2	2.10	0.51
1:A:4:LEU:HD23	1:A:97:ARG:NH2	2.26	0.51
1:C:396:PRO:HB2	1:C:397:PRO:HD2	1.92	0.51
1:B:382:ARG:HG2	1:B:383:GLN:N	2.25	0.51
1:D:124:TYR:CD2	1:D:160:PRO:HA	2.46	0.51
1:D:216:LEU:HD13	1:D:249:VAL:HG22	1.92	0.51
1:D:373:MSE:O	1:D:373:MSE:HG2	2.09	0.51
1:B:487:LEU:O	1:B:491:VAL:HG23	2.10	0.51
1:A:84:ARG:O	1:A:145:GLU:CB	2.59	0.51
1:C:382:ARG:HA	1:C:385:ASP:OD1	2.10	0.51
1:C:528:GLN:O	1:C:532:VAL:HG23	2.11	0.51
1:A:455:ALA:O	1:A:456:GLU:C	2.49	0.51
1:A:378:THR:HG22	1:A:378:THR:O	2.11	0.51
1:B:378:THR:O	1:B:378:THR:HG22	2.10	0.51
1:A:123:VAL:HG13	1:A:162:PHE:HB2	1.93	0.51
1:C:76:ARG:CZ	1:C:169:PRO:CB	2.89	0.51
1:A:376:GLN:HB3	1:B:350:ARG:HD2	1.91	0.51
1:C:382:ARG:HG2	1:C:383:GLN:N	2.25	0.51
1:C:350:ARG:HD2	1:D:376:GLN:O	2.11	0.51
1:D:149:LEU:CA	1:D:153:LEU:HD12	2.40	0.51
1:C:444:LEU:HD11	1:C:504:ASP:HB2	1.93	0.51
1:C:304:VAL:HG12	1:C:305:ASN:N	2.27	0.51
1:D:97:ARG:HH21	1:D:328:ASP:HB3	1.74	0.50
1:A:249:VAL:HG12	1:A:250:TYR:N	2.25	0.50
1:A:382:ARG:HG2	1:A:383:GLN:N	2.25	0.50
1:B:191:SER:HB2	1:B:195:GLN:OE1	2.10	0.50
1:C:373:MSE:HG2	1:C:373:MSE:O	2.03	0.50
1:A:373:MSE:HB2	1:B:348:GLY:HA2	1.93	0.50
1:C:428:ASN:H	1:C:433:ARG:HB2	1.76	0.50
1:C:534:GLY:O	1:C:535:SER:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ILE:N	1:B:396:PRO:CD	2.74	0.50
1:D:383:GLN:HG3	1:D:384:PHE:N	2.26	0.50
1:B:76:ARG:CZ	1:B:169:PRO:CB	2.89	0.50
1:C:11:PHE:CZ	1:C:88:LEU:CD1	2.94	0.50
1:D:192:THR:HG22	1:D:195:GLN:OE1	2.10	0.50
1:C:510:PHE:C	1:C:510:PHE:CD2	2.85	0.50
1:C:60:GLU:O	1:C:64:SER:N	2.35	0.50
1:D:353:ALA:HB3	1:D:354:PRO:CD	2.41	0.50
1:B:444:LEU:HD11	1:B:504:ASP:HB2	1.93	0.50
1:D:73:ILE:HG21	1:D:75:MSE:HE3	1.93	0.50
1:A:379:TYR:CG	1:A:380:GLY:N	2.80	0.50
1:C:478:SER:OG	1:C:479:ASP:N	2.43	0.50
1:A:25:GLN:O	1:A:28:SER:N	2.45	0.50
1:C:378:THR:HG22	1:C:378:THR:O	2.11	0.50
1:A:425:LEU:CD2	1:A:426:PRO:HD2	2.27	0.50
1:D:454:LEU:HG	1:D:494:ALA:HB2	1.94	0.50
1:D:138:LEU:N	1:D:139:PRO:HD2	2.27	0.50
1:D:84:ARG:O	1:D:145:GLU:CB	2.59	0.50
1:A:126:TYR:O	1:A:129:ALA:HB3	2.12	0.50
1:C:527:THR:O	1:C:531:LEU:HD23	2.11	0.50
1:A:15:ASN:O	1:A:16:ASN:CB	2.48	0.50
1:D:76:ARG:CZ	1:D:169:PRO:CB	2.90	0.50
1:B:326:VAL:HG22	1:B:326:VAL:O	2.12	0.50
1:C:455:ALA:O	1:C:456:GLU:C	2.48	0.50
1:D:530:ALA:O	1:D:533:LEU:HB2	2.12	0.50
1:C:383:GLN:HG3	1:C:384:PHE:N	2.27	0.50
1:A:73:ILE:HG21	1:A:75:MSE:HE3	1.92	0.50
1:B:192:THR:HG22	1:B:195:GLN:OE1	2.10	0.50
1:B:510:PHE:CD2	1:B:510:PHE:C	2.85	0.50
1:C:153:LEU:HD13	1:C:165:SER:O	2.12	0.50
1:D:506:THR:O	1:D:507:ASP:HB2	2.12	0.50
1:B:36:LEU:HD22	1:B:325:LEU:CD2	2.41	0.50
1:B:17:GLN:HA	1:B:17:GLN:OE1	2.11	0.50
1:C:395:ILE:N	1:C:396:PRO:CD	2.75	0.49
1:B:323:GLU:N	1:B:323:GLU:OE1	2.44	0.49
1:D:510:PHE:CD2	1:D:510:PHE:C	2.85	0.49
1:A:13:GLU:HG2	1:A:15:ASN:CA	2.41	0.49
1:C:506:THR:O	1:C:507:ASP:HB2	2.11	0.49
1:D:25:GLN:O	1:D:28:SER:N	2.45	0.49
1:B:383:GLN:HG3	1:B:384:PHE:N	2.26	0.49
1:D:176:THR:HG22	1:D:177:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:HH21	1:B:328:ASP:HB3	1.77	0.49
1:A:97:ARG:CZ	1:A:328:ASP:HB3	2.42	0.49
1:B:124:TYR:HD1	1:B:175:VAL:HG12	1.76	0.49
1:D:247:HIS:HD2	1:D:281:ALA:HA	1.77	0.49
1:B:60:GLU:O	1:B:64:SER:N	2.34	0.49
1:C:353:ALA:HB3	1:C:354:PRO:HD2	1.93	0.49
1:C:448:VAL:HG13	1:C:498:VAL:HG13	1.94	0.49
1:A:76:ARG:CZ	1:A:169:PRO:CB	2.90	0.49
1:B:215:ARG:NH2	1:B:252:GLU:OE2	2.44	0.49
1:A:537:GLU:O	1:A:540:LYS:HB2	2.13	0.49
1:A:54:GLN:HB2	1:A:57:CYS:SG	2.52	0.49
1:B:379:TYR:CG	1:B:380:GLY:N	2.81	0.49
1:B:380:GLY:O	1:B:381:ARG:C	2.51	0.49
1:A:124:TYR:HD1	1:A:175:VAL:HG12	1.78	0.49
1:C:344:VAL:HG22	1:C:345:ARG:HG2	1.94	0.49
1:D:265:VAL:HG23	1:D:265:VAL:O	2.13	0.49
1:A:84:ARG:HG2	1:A:85:MSE:N	2.28	0.49
1:B:249:VAL:HG12	1:B:250:TYR:N	2.27	0.49
1:B:427:LYS:O	1:B:428:ASN:HB2	2.12	0.49
1:C:247:HIS:HD2	1:C:281:ALA:HA	1.76	0.49
1:C:191:SER:HB2	1:C:195:GLN:OE1	2.13	0.49
1:C:370:LEU:HD11	1:D:359:VAL:HG11	1.95	0.49
1:A:13:GLU:HG2	1:A:15:ASN:H	1.76	0.49
1:B:511:LYS:O	1:B:514:THR:N	2.46	0.49
1:D:349:ALA:C	1:D:351:SER:N	2.59	0.48
1:C:124:TYR:HD1	1:C:175:VAL:HG12	1.77	0.48
1:B:477:LEU:O	1:B:481:GLN:HG3	2.13	0.48
1:D:303:VAL:O	1:D:303:VAL:HG22	2.12	0.48
1:A:323:GLU:OE1	1:A:323:GLU:N	2.42	0.48
1:A:353:ALA:CB	1:A:354:PRO:CD	2.91	0.48
1:A:527:THR:O	1:A:530:ALA:HB3	2.13	0.48
1:D:84:ARG:HG2	1:D:85:MSE:N	2.29	0.48
1:C:530:ALA:O	1:C:533:LEU:HB2	2.12	0.48
1:A:345:ARG:HH21	1:B:406:THR:HB	1.77	0.48
1:C:192:THR:HG22	1:C:195:GLN:OE1	2.12	0.48
1:C:427:LYS:O	1:C:428:ASN:HB2	2.13	0.48
1:B:530:ALA:O	1:B:533:LEU:HB2	2.13	0.48
1:B:149:LEU:O	1:B:153:LEU:HD22	2.13	0.48
1:A:383:GLN:N	1:A:385:ASP:OD1	2.47	0.48
1:A:192:THR:HG22	1:A:195:GLN:OE1	2.13	0.48
1:C:126:TYR:O	1:C:129:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:PHE:O	1:C:347:VAL:HG13	2.13	0.48
1:D:527:THR:O	1:D:531:LEU:CD2	2.60	0.48
1:D:135:ARG:CG	1:D:135:ARG:HH11	2.26	0.48
1:B:383:GLN:N	1:B:385:ASP:OD1	2.46	0.48
1:C:176:THR:HG22	1:C:177:GLY:N	2.29	0.48
1:A:127:GLY:C	1:A:129:ALA:N	2.67	0.48
1:B:13:GLU:HB3	1:B:46:ARG:HA	1.96	0.48
1:A:390:THR:CG2	1:A:393:ARG:HH21	2.19	0.48
1:A:374:VAL:HA	1:A:377:MSE:HB2	1.95	0.48
1:A:510:PHE:C	1:A:510:PHE:HD2	2.16	0.48
1:A:410:ASP:O	1:A:413:ALA:N	2.46	0.48
1:B:353:ALA:HB3	1:B:354:PRO:CD	2.44	0.48
1:B:97:ARG:CZ	1:B:328:ASP:HB3	2.44	0.48
1:A:97:ARG:HH21	1:A:328:ASP:HB3	1.74	0.48
1:C:527:THR:O	1:C:530:ALA:HB3	2.14	0.48
1:C:84:ARG:O	1:C:145:GLU:CB	2.62	0.48
1:D:13:GLU:HG2	1:D:15:ASN:CA	2.44	0.48
1:D:492:PHE:CD2	1:D:522:LEU:HD11	2.49	0.48
1:B:25:GLN:O	1:B:28:SER:N	2.47	0.48
1:D:379:TYR:CG	1:D:380:GLY:N	2.81	0.48
1:D:427:LYS:O	1:D:428:ASN:HB2	2.13	0.48
1:D:90:VAL:HG11	1:D:138:LEU:HD21	1.95	0.48
1:A:444:LEU:CD1	1:A:504:ASP:HB2	2.44	0.48
1:A:383:GLN:HG3	1:A:384:PHE:N	2.29	0.48
1:A:303:VAL:HG22	1:A:303:VAL:O	2.14	0.48
1:B:11:PHE:CZ	1:B:88:LEU:CD1	2.96	0.48
1:C:76:ARG:HH21	1:C:169:PRO:HB3	1.79	0.48
1:A:454:LEU:HG	1:A:494:ALA:HB2	1.96	0.47
1:D:13:GLU:HB2	1:D:46:ARG:C	2.33	0.47
1:A:216:LEU:HD13	1:A:249:VAL:HG22	1.95	0.47
1:C:510:PHE:C	1:C:510:PHE:HD2	2.17	0.47
1:C:27:ILE:CD1	1:C:51:PHE:CE1	2.83	0.47
1:A:530:ALA:O	1:A:533:LEU:HB2	2.14	0.47
1:B:10:ASN:HB2	1:B:90:VAL:O	2.14	0.47
1:D:76:ARG:NE	1:D:169:PRO:HB2	2.29	0.47
1:C:13:GLU:HB2	1:C:46:ARG:CA	2.44	0.47
1:C:288:LYS:HG3	1:C:289:GLU:N	2.29	0.47
1:D:97:ARG:CZ	1:D:328:ASP:HB3	2.44	0.47
1:B:84:ARG:O	1:B:145:GLU:CB	2.63	0.47
1:B:528:GLN:O	1:B:532:VAL:HG23	2.15	0.47
1:A:350:ARG:HD2	1:B:376:GLN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TYR:O	1:D:129:ALA:HB3	2.14	0.47
1:B:343:PHE:O	1:B:346:GLU:HB3	2.14	0.47
1:A:370:LEU:CD1	1:B:359:VAL:HG11	2.36	0.47
1:A:90:VAL:HG11	1:A:138:LEU:HD21	1.96	0.47
1:A:463:PRO:O	1:A:466:GLN:HB3	2.13	0.47
1:C:171:TRP:CD1	1:C:172:GLY:N	2.83	0.47
1:C:97:ARG:HH21	1:C:328:ASP:HB3	1.79	0.47
1:A:153:LEU:CD1	1:A:165:SER:O	2.62	0.47
1:C:90:VAL:HG11	1:C:138:LEU:HD21	1.96	0.47
1:D:124:TYR:HD1	1:D:175:VAL:HG12	1.78	0.47
1:B:445:ARG:NH1	1:B:445:ARG:CG	2.62	0.47
1:D:378:THR:O	1:D:378:THR:HG22	2.14	0.47
1:B:76:ARG:HH21	1:B:169:PRO:HB3	1.79	0.47
1:A:76:ARG:NE	1:A:169:PRO:HB2	2.29	0.47
1:C:406:THR:HB	1:D:345:ARG:HH21	1.79	0.47
1:B:510:PHE:C	1:B:510:PHE:HD2	2.18	0.47
1:D:74:ASP:OD1	1:D:170:SER:HB3	2.15	0.47
1:D:60:GLU:O	1:D:64:SER:N	2.36	0.47
1:A:17:GLN:HA	1:A:17:GLN:OE1	2.14	0.47
1:B:410:ASP:O	1:B:413:ALA:N	2.47	0.47
1:B:90:VAL:HG11	1:B:138:LEU:HD21	1.96	0.47
1:B:176:THR:HG23	1:B:177:GLY:N	2.29	0.47
1:C:347:VAL:HA	1:C:354:PRO:HG2	1.96	0.47
1:B:347:VAL:HA	1:B:354:PRO:HG2	1.96	0.47
1:A:74:ASP:OD1	1:A:170:SER:HB3	2.14	0.47
1:B:396:PRO:HB2	1:B:397:PRO:HD2	1.93	0.47
1:C:76:ARG:NE	1:C:169:PRO:HB2	2.29	0.47
1:A:395:ILE:N	1:A:396:PRO:CD	2.78	0.47
1:D:176:THR:HG23	1:D:177:GLY:H	1.80	0.47
1:C:351:SER:OG	1:C:351:SER:O	2.32	0.46
1:D:426:PRO:O	1:D:427:LYS:CB	2.39	0.46
1:D:76:ARG:HH21	1:D:169:PRO:HB3	1.79	0.46
1:B:476:CYS:O	1:B:477:LEU:C	2.54	0.46
1:C:265:VAL:O	1:C:265:VAL:HG23	2.14	0.46
1:D:94:ILE:HG22	1:D:179:ARG:O	2.15	0.46
1:C:97:ARG:CZ	1:C:328:ASP:HB3	2.44	0.46
1:C:454:LEU:HG	1:C:494:ALA:HB2	1.97	0.46
1:B:374:VAL:HG11	1:B:480:LEU:HD23	1.97	0.46
1:A:13:GLU:HB2	1:A:46:ARG:CA	2.45	0.46
1:A:60:GLU:O	1:A:64:SER:N	2.34	0.46
1:C:10:ASN:HB2	1:C:90:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:LYS:HG3	1:D:289:GLU:N	2.30	0.46
1:D:129:ALA:O	1:D:130:ALA:C	2.53	0.46
1:B:410:ASP:O	1:B:411:ALA:C	2.53	0.46
1:D:353:ALA:CB	1:D:354:PRO:CD	2.93	0.46
1:B:84:ARG:HG2	1:B:85:MSE:N	2.30	0.46
1:C:123:VAL:HG13	1:C:162:PHE:HB2	1.96	0.46
1:B:123:VAL:HG13	1:B:162:PHE:HB2	1.96	0.46
1:B:76:ARG:NE	1:B:169:PRO:HB2	2.30	0.46
1:B:537:GLU:O	1:B:540:LYS:HB2	2.16	0.46
1:C:522:LEU:O	1:C:525:ALA:HB3	2.16	0.46
1:A:527:THR:O	1:A:531:LEU:CD2	2.64	0.46
1:D:349:ALA:O	1:D:351:SER:N	2.49	0.46
1:A:46:ARG:CZ	1:A:82:HIS:CD2	2.96	0.46
1:A:8:VAL:O	1:A:92:PRO:HD2	2.15	0.46
1:D:380:GLY:O	1:D:381:ARG:C	2.53	0.46
1:D:455:ALA:O	1:D:456:GLU:C	2.51	0.46
1:C:353:ALA:HB3	1:C:354:PRO:CD	2.46	0.46
1:B:534:GLY:O	1:B:535:SER:C	2.52	0.46
1:C:383:GLN:N	1:C:385:ASP:OD1	2.45	0.46
1:D:387:LEU:CD2	1:D:471:CYS:SG	3.04	0.46
1:D:127:GLY:C	1:D:129:ALA:N	2.68	0.46
1:C:380:GLY:O	1:C:381:ARG:C	2.53	0.46
1:C:537:GLU:O	1:C:540:LYS:HB2	2.16	0.46
1:B:296:GLU:O	1:B:297:GLU:C	2.51	0.46
1:A:448:VAL:O	1:A:451:PRO:HD2	2.16	0.46
1:C:84:ARG:HG2	1:C:85:MSE:N	2.30	0.46
1:D:131:GLN:HE21	1:D:131:GLN:HB2	1.58	0.46
1:C:4:LEU:HD23	1:C:97:ARG:HH21	1.80	0.46
1:A:427:LYS:O	1:A:428:ASN:HB2	2.15	0.46
1:A:347:VAL:HA	1:A:354:PRO:HG2	1.98	0.46
1:A:111:PHE:CD2	1:A:176:THR:OG1	2.67	0.46
1:A:176:THR:HG23	1:A:177:GLY:N	2.30	0.46
1:C:379:TYR:CG	1:C:380:GLY:N	2.84	0.46
1:D:517:ARG:O	1:D:520:SER:OG	2.33	0.46
1:B:132:MSE:HA	1:B:133:PRO:HD3	1.76	0.46
1:A:343:PHE:O	1:A:347:VAL:HG13	2.15	0.46
1:B:530:ALA:O	1:B:533:LEU:N	2.48	0.46
1:C:281:ALA:O	1:C:284:PHE:HB3	2.16	0.46
1:B:167:PHE:HD1	1:B:168:VAL:N	2.14	0.46
1:A:184:ALA:HB3	1:A:270:VAL:HB	1.98	0.46
1:D:334:SER:OG	1:D:336:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:PRO:O	1:D:466:GLN:HB3	2.16	0.46
1:A:531:LEU:O	1:A:535:SER:N	2.44	0.46
1:B:531:LEU:O	1:B:535:SER:N	2.44	0.46
1:B:13:GLU:HB3	1:B:46:ARG:CA	2.46	0.46
1:C:13:GLU:HB3	1:C:45:ASN:C	2.36	0.46
1:B:190:LEU:HA	1:B:190:LEU:HD23	1.80	0.46
1:D:249:VAL:HG12	1:D:250:TYR:N	2.29	0.46
1:C:129:ALA:O	1:C:130:ALA:C	2.54	0.46
1:D:510:PHE:HD2	1:D:510:PHE:C	2.18	0.46
1:D:17:GLN:OE1	1:D:17:GLN:HA	2.15	0.46
1:C:343:PHE:O	1:C:346:GLU:HB3	2.17	0.45
1:D:448:VAL:HG13	1:D:498:VAL:HG13	1.99	0.45
1:A:10:ASN:HB2	1:A:90:VAL:O	2.16	0.45
1:C:167:PHE:HD1	1:C:168:VAL:N	2.14	0.45
1:B:265:VAL:O	1:B:265:VAL:HG23	2.16	0.45
1:B:171:TRP:CD1	1:B:172:GLY:N	2.82	0.45
1:A:334:SER:OG	1:A:336:LEU:HB2	2.16	0.45
1:D:143:ALA:HB1	1:D:152:LYS:HZ3	1.80	0.45
1:B:444:LEU:CD1	1:B:504:ASP:HB2	2.47	0.45
1:C:303:VAL:HG22	1:C:303:VAL:O	2.16	0.45
1:C:227:GLU:OE1	1:C:227:GLU:CA	2.58	0.45
1:B:247:HIS:HD2	1:B:281:ALA:HA	1.77	0.45
1:D:537:GLU:O	1:D:540:LYS:HB2	2.16	0.45
1:C:448:VAL:O	1:C:451:PRO:HD2	2.16	0.45
1:C:90:VAL:HG23	1:C:92:PRO:HD3	1.99	0.45
1:D:10:ASN:HB2	1:D:90:VAL:O	2.17	0.45
1:D:524:GLU:O	1:D:528:GLN:HB2	2.16	0.45
1:B:127:GLY:C	1:B:129:ALA:N	2.70	0.45
1:C:337:ASP:OD1	1:D:341:ARG:NH1	2.28	0.45
1:D:347:VAL:HA	1:D:354:PRO:HG2	1.99	0.45
1:A:76:ARG:HH21	1:A:169:PRO:HB3	1.81	0.45
1:A:74:ASP:HA	1:A:170:SER:CB	2.46	0.45
1:D:167:PHE:HD1	1:D:168:VAL:N	2.14	0.45
1:A:354:PRO:O	1:B:373:MSE:HE1	2.17	0.45
1:D:410:ASP:O	1:D:413:ALA:N	2.49	0.45
1:B:450:VAL:HG22	1:B:451:PRO:HD3	1.99	0.45
1:D:444:LEU:CD1	1:D:504:ASP:HB2	2.47	0.45
1:A:531:LEU:O	1:A:532:VAL:C	2.55	0.45
1:B:448:VAL:HG13	1:B:498:VAL:HG13	1.98	0.45
1:C:374:VAL:HG11	1:C:480:LEU:HD23	1.99	0.45
1:B:303:VAL:O	1:B:303:VAL:HG22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:HD2	1:D:376:GLN:HB3	1.98	0.45
1:B:12:SER:O	1:B:73:ILE:HD13	2.16	0.45
1:A:184:ALA:CB	1:A:270:VAL:HB	2.47	0.45
1:D:184:ALA:CB	1:D:270:VAL:HB	2.46	0.45
1:D:184:ALA:HB3	1:D:270:VAL:HB	1.99	0.45
1:A:89:ASP:HB3	1:A:90:VAL:H	1.64	0.45
1:D:474:LEU:HD23	1:D:477:LEU:HD13	1.98	0.45
1:D:395:ILE:N	1:D:396:PRO:CD	2.79	0.45
1:A:86:GLY:HA3	1:A:173:ALA:O	2.16	0.45
1:A:444:LEU:HD11	1:A:504:ASP:HB2	1.99	0.45
1:C:25:GLN:O	1:C:28:SER:N	2.49	0.45
1:C:23:ILE:O	1:C:27:ILE:HG22	2.17	0.45
1:D:531:LEU:O	1:D:535:SER:N	2.44	0.45
1:C:458:VAL:CG2	1:C:487:LEU:HD23	2.47	0.45
1:C:531:LEU:O	1:C:535:SER:N	2.42	0.45
1:C:445:ARG:NH1	1:C:445:ARG:CG	2.58	0.45
1:A:127:GLY:O	1:A:129:ALA:N	2.50	0.45
1:B:129:ALA:O	1:B:130:ALA:C	2.55	0.45
1:B:94:ILE:HG22	1:B:179:ARG:O	2.17	0.45
1:C:179:ARG:HH12	1:C:182:LEU:HB3	1.82	0.45
1:D:444:LEU:HD11	1:D:504:ASP:HB2	1.99	0.44
1:B:6:GLU:OE1	1:B:94:ILE:HG13	2.17	0.44
1:B:74:ASP:OD1	1:B:170:SER:HB3	2.17	0.44
1:B:454:LEU:HG	1:B:494:ALA:HB2	1.98	0.44
1:A:167:PHE:HD1	1:A:168:VAL:N	2.15	0.44
1:D:13:GLU:HB3	1:D:45:ASN:C	2.37	0.44
1:D:383:GLN:N	1:D:385:ASP:OD1	2.47	0.44
1:B:111:PHE:CD2	1:B:176:THR:OG1	2.69	0.44
1:D:129:ALA:O	1:D:130:ALA:O	2.35	0.44
1:C:179:ARG:NH1	1:C:182:LEU:HB3	2.32	0.44
1:B:3:GLN:OE1	1:B:3:GLN:HA	2.17	0.44
1:A:474:LEU:HD11	1:A:541:GLU:OE2	2.17	0.44
1:A:382:ARG:HA	1:A:385:ASP:OD1	2.18	0.44
1:C:249:VAL:HG12	1:C:250:TYR:N	2.32	0.44
1:A:73:ILE:CG2	1:A:75:MSE:HE3	2.47	0.44
1:C:176:THR:HG23	1:C:177:GLY:H	1.81	0.44
1:A:462:TRP:CE3	1:A:462:TRP:HA	2.53	0.44
1:C:379:TYR:CE1	1:C:388:ASP:OD2	2.70	0.44
1:C:539:ARG:O	1:C:541:GLU:N	2.51	0.44
1:B:444:LEU:O	1:B:445:ARG:C	2.56	0.44
1:A:12:SER:O	1:A:73:ILE:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLY:HA3	1:B:173:ALA:O	2.17	0.44
1:B:23:ILE:O	1:B:27:ILE:HG22	2.17	0.44
1:C:461:LEU:N	1:C:461:LEU:CD1	2.79	0.44
1:B:458:VAL:HA	1:B:461:LEU:HD22	2.00	0.44
1:D:8:VAL:O	1:D:92:PRO:HD2	2.16	0.44
1:A:477:LEU:O	1:A:481:GLN:HG3	2.18	0.44
1:D:198:ARG:HD3	1:D:260:LEU:HD11	2.00	0.44
1:D:46:ARG:CZ	1:D:82:HIS:CD2	2.95	0.44
1:B:281:ALA:O	1:B:284:PHE:HB3	2.17	0.44
1:A:492:PHE:CE2	1:A:522:LEU:HD11	2.53	0.44
1:C:6:GLU:OE1	1:C:94:ILE:HG13	2.17	0.44
1:B:492:PHE:CD2	1:B:522:LEU:HD11	2.53	0.44
1:D:86:GLY:HA3	1:D:173:ALA:O	2.17	0.44
1:D:171:TRP:CD1	1:D:172:GLY:N	2.84	0.44
1:D:377:MSE:HE3	1:D:377:MSE:HA	2.00	0.44
1:B:149:LEU:O	1:B:153:LEU:CD2	2.66	0.44
1:D:187:ILE:HD11	1:D:249:VAL:HG12	1.99	0.44
1:A:247:HIS:HD2	1:A:281:ALA:HA	1.79	0.44
1:C:73:ILE:HG21	1:C:75:MSE:HE3	1.99	0.44
1:D:74:ASP:HA	1:D:170:SER:CB	2.47	0.44
1:B:25:GLN:O	1:B:29:GLN:N	2.50	0.44
1:D:374:VAL:HG11	1:D:480:LEU:HD23	2.00	0.44
1:A:336:LEU:O	1:B:339:SER:HB2	2.18	0.44
1:C:94:ILE:HG22	1:C:179:ARG:O	2.18	0.44
1:D:128:GLU:HB2	1:D:178:ALA:O	2.17	0.44
1:A:171:TRP:CD1	1:A:172:GLY:N	2.85	0.44
1:B:184:ALA:CB	1:B:270:VAL:HB	2.48	0.44
1:C:86:GLY:HA3	1:C:173:ALA:O	2.18	0.44
1:A:128:GLU:HB2	1:A:178:ALA:O	2.17	0.44
1:C:38:VAL:HG22	1:C:38:VAL:O	2.18	0.44
1:C:74:ASP:OD1	1:C:170:SER:HB3	2.18	0.44
1:B:15:ASN:O	1:B:16:ASN:CB	2.49	0.43
1:B:46:ARG:CZ	1:B:82:HIS:CD2	2.95	0.43
1:D:176:THR:HG23	1:D:177:GLY:N	2.33	0.43
1:B:8:VAL:O	1:B:92:PRO:HD2	2.18	0.43
1:A:341:ARG:NH1	1:B:337:ASP:OD1	2.34	0.43
1:A:493:GLY:HA2	1:B:482:VAL:HG22	2.00	0.43
1:C:349:ALA:C	1:C:351:SER:N	2.51	0.43
1:D:127:GLY:O	1:D:129:ALA:N	2.52	0.43
1:A:288:LYS:HG3	1:A:289:GLU:N	2.33	0.43
1:B:276:LYS:HE2	1:B:280:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD23	1:B:97:ARG:HH21	1.82	0.43
1:D:153:LEU:HD22	1:D:153:LEU:C	2.38	0.43
1:D:351:SER:OG	1:D:351:SER:O	2.35	0.43
1:C:13:GLU:HG2	1:C:15:ASN:HA	2.01	0.43
1:D:3:GLN:HA	1:D:3:GLN:OE1	2.18	0.43
1:B:13:GLU:HG2	1:B:15:ASN:H	1.83	0.43
1:B:461:LEU:CD1	1:B:461:LEU:N	2.81	0.43
1:A:458:VAL:HA	1:A:461:LEU:HD22	2.00	0.43
1:D:76:ARG:HG3	1:D:76:ARG:H	1.48	0.43
1:D:462:TRP:CE3	1:D:462:TRP:HA	2.54	0.43
1:B:73:ILE:HG21	1:B:75:MSE:HE3	1.99	0.43
1:C:59:VAL:O	1:C:63:LEU:HG	2.18	0.43
1:D:23:ILE:O	1:D:27:ILE:HG22	2.18	0.43
1:C:531:LEU:N	1:C:531:LEU:HD23	2.12	0.43
1:C:13:GLU:C	1:C:15:ASN:H	2.21	0.43
1:A:13:GLU:HB3	1:A:45:ASN:C	2.38	0.43
1:C:113:GLN:O	1:C:117:GLU:CG	2.57	0.43
1:B:288:LYS:HG3	1:B:289:GLU:N	2.33	0.43
1:C:458:VAL:HA	1:C:461:LEU:HD22	2.00	0.43
1:C:444:LEU:O	1:C:445:ARG:C	2.56	0.43
1:A:14:GLY:O	1:A:15:ASN:HB3	2.18	0.43
1:B:396:PRO:CB	1:B:397:PRO:CD	2.92	0.43
1:C:184:ALA:CB	1:C:270:VAL:HB	2.48	0.43
1:D:111:PHE:CD2	1:D:176:THR:OG1	2.68	0.43
1:A:432:GLU:HG2	1:A:432:GLU:O	2.19	0.43
1:D:432:GLU:O	1:D:432:GLU:HG2	2.17	0.43
1:C:482:VAL:HG22	1:D:493:GLY:HA2	2.01	0.43
1:A:448:VAL:HG13	1:A:498:VAL:HG13	2.01	0.43
1:D:382:ARG:HA	1:D:385:ASP:OD1	2.19	0.43
1:C:378:THR:OG1	1:C:473:ASN:N	2.47	0.43
1:B:478:SER:HA	1:B:481:GLN:HE21	1.83	0.43
1:B:524:GLU:O	1:B:528:GLN:HB2	2.18	0.43
1:C:127:GLY:C	1:C:129:ALA:N	2.71	0.43
1:C:46:ARG:CZ	1:C:82:HIS:CD2	2.95	0.43
1:C:135:ARG:CG	1:C:135:ARG:HH11	2.31	0.43
1:D:12:SER:O	1:D:73:ILE:HD13	2.19	0.43
1:A:286:CYS:HA	1:A:291:LEU:CD1	2.49	0.43
1:A:154:LYS:HE2	1:A:154:LYS:HB3	1.70	0.43
1:C:3:GLN:HA	1:C:3:GLN:OE1	2.18	0.42
1:C:444:LEU:CD1	1:C:504:ASP:HB2	2.49	0.42
1:C:8:VAL:O	1:C:92:PRO:HD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:LEU:N	1:D:461:LEU:CD1	2.82	0.42
1:C:375:GLY:HA3	1:C:395:ILE:HG12	1.99	0.42
1:A:380:GLY:O	1:A:381:ARG:C	2.58	0.42
1:B:74:ASP:HA	1:B:170:SER:CB	2.49	0.42
1:A:406:THR:CB	1:B:345:ARG:HH21	2.27	0.42
1:A:377:MSE:CE	1:A:377:MSE:HA	2.49	0.42
1:C:12:SER:HB3	1:C:75:MSE:HE1	2.00	0.42
1:D:36:LEU:HD22	1:D:325:LEU:CD2	2.49	0.42
1:C:425:LEU:O	1:C:426:PRO:C	2.58	0.42
1:B:518:ILE:HD12	1:B:518:ILE:HA	1.89	0.42
1:D:13:GLU:CB	1:D:46:ARG:HA	2.50	0.42
1:A:375:GLY:HA3	1:A:395:ILE:HG12	2.00	0.42
1:A:524:GLU:O	1:A:528:GLN:HB2	2.19	0.42
1:B:12:SER:HB3	1:B:75:MSE:HE1	2.00	0.42
1:B:432:GLU:O	1:B:432:GLU:HG2	2.18	0.42
1:D:498:VAL:HG12	1:D:502:LEU:HD13	2.01	0.42
1:D:82:HIS:ND1	1:D:83:PRO:HD2	2.35	0.42
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.81	0.42
1:A:94:ILE:HG22	1:A:179:ARG:O	2.19	0.42
1:A:346:GLU:HG3	1:A:354:PRO:HG3	2.01	0.42
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.89	0.42
1:C:187:ILE:HD11	1:C:249:VAL:HG12	2.01	0.42
1:D:73:ILE:CG2	1:D:75:MSE:HE3	2.50	0.42
1:B:59:VAL:O	1:B:63:LEU:HG	2.19	0.42
1:A:3:GLN:HA	1:A:3:GLN:OE1	2.18	0.42
1:D:149:LEU:HB3	1:D:153:LEU:HD12	2.00	0.42
1:A:149:LEU:CD2	1:A:153:LEU:HB3	2.49	0.42
1:C:82:HIS:ND1	1:C:83:PRO:HD2	2.35	0.42
1:C:524:GLU:O	1:C:528:GLN:HB2	2.19	0.42
1:B:520:SER:O	1:B:523:GLN:HB3	2.19	0.42
1:B:522:LEU:O	1:B:525:ALA:HB3	2.19	0.42
1:C:74:ASP:HA	1:C:170:SER:CB	2.49	0.42
1:A:275:LEU:HG	1:A:279:LEU:HD12	2.01	0.42
1:C:511:LYS:O	1:C:514:THR:N	2.53	0.42
1:C:275:LEU:HG	1:C:279:LEU:HD12	2.01	0.42
1:B:425:LEU:O	1:B:426:PRO:C	2.58	0.42
1:A:90:VAL:HG12	1:A:138:LEU:HD11	2.01	0.42
1:B:113:GLN:HA	1:B:162:PHE:CD2	2.55	0.42
1:A:443:GLY:O	1:A:444:LEU:C	2.58	0.42
1:A:36:LEU:HD22	1:A:325:LEU:CD2	2.50	0.42
1:B:520:SER:HG	1:B:521:LEU:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:MSE:O	1:B:377:MSE:HB2	2.19	0.42
1:D:343:PHE:O	1:D:346:GLU:HB3	2.20	0.42
1:C:14:GLY:O	1:C:15:ASN:HB3	2.20	0.42
1:B:480:LEU:O	1:B:483:ALA:HB3	2.20	0.42
1:A:461:LEU:CD1	1:A:461:LEU:N	2.82	0.42
1:C:190:LEU:CB	1:C:263:PRO:HG2	2.47	0.42
1:C:339:SER:HB2	1:D:336:LEU:O	2.19	0.42
1:B:154:LYS:HE2	1:B:154:LYS:HB3	1.80	0.42
1:D:54:GLN:HB2	1:D:57:CYS:SG	2.60	0.42
1:B:353:ALA:CB	1:B:354:PRO:CD	2.97	0.42
1:C:13:GLU:O	1:C:15:ASN:N	2.51	0.42
1:A:13:GLU:CB	1:A:46:ARG:HA	2.50	0.42
1:A:344:VAL:HG21	1:B:406:THR:OG1	2.20	0.42
1:C:132:MSE:HA	1:C:133:PRO:HD3	1.76	0.42
1:C:334:SER:OG	1:C:336:LEU:HB2	2.19	0.42
1:B:38:VAL:HG22	1:B:38:VAL:O	2.20	0.42
1:A:23:ILE:O	1:A:27:ILE:HG22	2.19	0.42
1:C:25:GLN:O	1:C:29:GLN:N	2.52	0.42
1:C:492:PHE:CD2	1:C:522:LEU:HD11	2.55	0.42
1:B:539:ARG:O	1:B:541:GLU:N	2.53	0.42
1:B:275:LEU:HG	1:B:279:LEU:HD12	2.01	0.42
1:D:4:LEU:HD23	1:D:97:ARG:HH21	1.85	0.41
1:B:13:GLU:HG2	1:B:15:ASN:CA	2.50	0.41
1:D:25:GLN:O	1:D:29:GLN:N	2.51	0.41
1:C:176:THR:HG23	1:C:177:GLY:N	2.34	0.41
1:B:184:ALA:HB3	1:B:270:VAL:HB	2.01	0.41
1:C:353:ALA:CB	1:C:354:PRO:CD	2.98	0.41
1:C:390:THR:CG2	1:C:393:ARG:HH21	2.23	0.41
1:C:154:LYS:HB3	1:C:154:LYS:HE2	1.79	0.41
1:B:119:LEU:O	1:B:120:ASN:CB	2.68	0.41
1:B:82:HIS:ND1	1:B:83:PRO:HD2	2.34	0.41
1:A:444:LEU:O	1:A:445:ARG:C	2.57	0.41
1:A:376:GLN:O	1:B:350:ARG:HD2	2.20	0.41
1:C:254:ARG:HH11	1:C:254:ARG:CB	2.32	0.41
1:A:129:ALA:O	1:A:130:ALA:C	2.57	0.41
1:A:12:SER:HB3	1:A:75:MSE:HE1	2.02	0.41
1:D:153:LEU:HD23	1:D:165:SER:C	2.35	0.41
1:B:135:ARG:CG	1:B:135:ARG:HH11	2.29	0.41
1:B:13:GLU:OE1	1:B:45:ASN:HA	2.20	0.41
1:A:227:GLU:OE1	1:A:227:GLU:CA	2.54	0.41
1:C:474:LEU:HD23	1:C:477:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLY:O	1:B:129:ALA:N	2.53	0.41
1:C:129:ALA:O	1:C:130:ALA:O	2.39	0.41
1:D:154:LYS:HE2	1:D:154:LYS:HB3	1.78	0.41
1:A:518:ILE:HA	1:A:521:LEU:HD12	2.02	0.41
1:C:13:GLU:CB	1:C:46:ARG:HA	2.50	0.41
1:A:82:HIS:ND1	1:A:83:PRO:HD2	2.35	0.41
1:B:375:GLY:HA3	1:B:395:ILE:HG12	2.02	0.41
1:D:149:LEU:CD2	1:D:153:LEU:HG	2.45	0.41
1:B:135:ARG:CG	1:B:141:ILE:HD11	2.48	0.41
1:A:150:PRO:HD3	1:A:167:PHE:CE2	2.56	0.41
1:A:14:GLY:O	1:A:15:ASN:CB	2.69	0.41
1:C:340:LEU:O	1:C:344:VAL:HG12	2.21	0.41
1:D:113:GLN:HA	1:D:162:PHE:CD2	2.55	0.41
1:D:375:GLY:HA3	1:D:395:ILE:HG12	2.01	0.41
1:C:111:PHE:CD2	1:C:176:THR:OG1	2.67	0.41
1:B:187:ILE:HD11	1:B:249:VAL:HG12	2.02	0.41
1:C:12:SER:O	1:C:73:ILE:HD13	2.19	0.41
1:C:432:GLU:O	1:C:432:GLU:HG2	2.20	0.41
1:A:351:SER:OG	1:A:351:SER:O	2.38	0.41
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.32	0.41
1:D:6:GLU:OE1	1:D:94:ILE:HG13	2.20	0.41
1:B:70:SER:HA	1:B:171:TRP:HZ3	1.85	0.41
1:C:410:ASP:O	1:C:411:ALA:C	2.59	0.41
1:B:4:LEU:HB2	1:B:97:ARG:HG2	2.03	0.41
1:D:498:VAL:O	1:D:499:LEU:C	2.58	0.41
1:A:13:GLU:OE1	1:A:45:ASN:HA	2.21	0.41
1:B:149:LEU:N	1:B:150:PRO:CD	2.84	0.41
1:A:25:GLN:O	1:A:29:GLN:N	2.51	0.41
1:A:303:VAL:CG2	1:A:303:VAL:O	2.69	0.41
1:A:476:CYS:O	1:A:477:LEU:C	2.59	0.41
1:B:197:HIS:HB2	1:B:223:GLY:HA3	2.02	0.41
1:D:373:MSE:O	1:D:377:MSE:HB2	2.21	0.41
1:C:426:PRO:O	1:C:427:LYS:CB	2.37	0.41
1:C:149:LEU:HB3	1:C:153:LEU:HD23	2.03	0.41
1:C:363:VAL:CG1	1:D:363:VAL:CG1	2.97	0.41
1:D:531:LEU:O	1:D:532:VAL:C	2.57	0.41
1:C:461:LEU:N	1:C:461:LEU:HD13	2.36	0.41
1:D:502:LEU:HD21	1:D:514:THR:HB	2.03	0.41
1:B:498:VAL:O	1:B:499:LEU:C	2.58	0.41
1:C:89:ASP:HB3	1:C:90:VAL:H	1.63	0.41
1:D:90:VAL:HG12	1:D:138:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:GLU:C	1:D:15:ASN:H	2.24	0.41
1:C:113:GLN:HA	1:C:162:PHE:CD2	2.55	0.41
1:D:458:VAL:HA	1:D:461:LEU:HD22	2.02	0.41
1:B:153:LEU:N	1:B:153:LEU:HD23	2.23	0.41
1:B:164:PRO:HB2	1:B:165:SER:H	1.60	0.41
1:D:378:THR:OG1	1:D:473:ASN:N	2.49	0.41
1:A:406:THR:OG1	1:B:344:VAL:HG21	2.21	0.41
1:C:76:ARG:HG3	1:C:76:ARG:H	1.48	0.41
1:C:187:ILE:HD12	1:C:253:ALA:CB	2.51	0.41
1:C:184:ALA:HB3	1:C:270:VAL:HB	2.02	0.41
1:D:119:LEU:O	1:D:120:ASN:CB	2.69	0.41
1:C:296:GLU:O	1:C:297:GLU:C	2.59	0.41
1:D:164:PRO:HB2	1:D:165:SER:H	1.59	0.41
1:A:498:VAL:O	1:A:499:LEU:C	2.59	0.41
1:A:113:GLN:HA	1:A:162:PHE:CD2	2.56	0.41
1:A:372:SER:O	1:A:376:GLN:HG3	2.21	0.41
1:B:339:SER:O	1:B:340:LEU:C	2.59	0.41
1:C:485:LYS:HD3	1:C:485:LYS:HA	1.96	0.41
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.81	0.41
1:C:131:GLN:HB2	1:C:131:GLN:HE21	1.59	0.41
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.89	0.40
1:A:124:TYR:N	1:A:124:TYR:CD1	2.89	0.40
1:B:286:CYS:HA	1:B:291:LEU:CD1	2.52	0.40
1:D:518:ILE:HA	1:D:518:ILE:HD12	1.89	0.40
1:A:396:PRO:O	1:A:397:PRO:C	2.58	0.40
1:B:474:LEU:HD23	1:B:477:LEU:HD13	2.02	0.40
1:D:303:VAL:CG2	1:D:303:VAL:O	2.70	0.40
1:D:12:SER:HB3	1:D:75:MSE:HE1	2.02	0.40
1:D:125:LEU:HD12	1:D:129:ALA:HB1	2.04	0.40
1:B:485:LYS:HD3	1:B:485:LYS:HA	1.97	0.40
1:D:2:SER:HA	1:D:97:ARG:HE	1.86	0.40
1:B:89:ASP:HB3	1:B:90:VAL:H	1.63	0.40
1:C:135:ARG:HG2	1:C:141:ILE:CD1	2.47	0.40
1:A:395:ILE:HB	1:A:396:PRO:HD3	2.04	0.40
1:D:281:ALA:O	1:D:284:PHE:HB3	2.21	0.40
1:A:410:ASP:O	1:A:411:ALA:C	2.59	0.40
1:A:70:SER:HA	1:A:171:TRP:HZ3	1.86	0.40
1:B:351:SER:O	1:B:351:SER:OG	2.38	0.40
1:C:149:LEU:N	1:C:150:PRO:CD	2.85	0.40
1:D:124:TYR:N	1:D:124:TYR:CD1	2.88	0.40
1:A:377:MSE:HA	1:A:377:MSE:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:SER:OG	1:B:336:LEU:HB2	2.22	0.40
1:B:109:LYS:HZ3	1:C:102:ASP:CG	2.24	0.40
1:D:286:CYS:HA	1:D:291:LEU:CD1	2.52	0.40
1:A:498:VAL:HG12	1:A:502:LEU:HD13	2.03	0.40
1:A:19:VAL:HG11	1:A:73:ILE:HD11	2.03	0.40
1:C:125:LEU:HD12	1:C:129:ALA:HB1	2.04	0.40
1:A:296:GLU:O	1:A:297:GLU:C	2.59	0.40
1:A:59:VAL:O	1:A:63:LEU:HG	2.21	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	538/541 (99%)	401 (74%)	97 (18%)	40 (7%)	1	15
1	B	538/541 (99%)	407 (76%)	88 (16%)	43 (8%)	1	13
1	C	538/541 (99%)	404 (75%)	94 (18%)	40 (7%)	1	15
1	D	538/541 (99%)	404 (75%)	94 (18%)	40 (7%)	1	15
All	All	2152/2164 (99%)	1616 (75%)	373 (17%)	163 (8%)	1	14

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	89	ASP
1	A	142	ARG
1	A	164	PRO
1	A	350	ARG
1	A	353	ALA
1	A	383	GLN

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Mol	Chain	Res	Type
1	A	426	PRO
1	A	427	LYS
1	A	428	ASN
1	A	473	ASN
1	A	507	ASP
1	A	511	LYS
1	A	540	LYS
1	B	13	GLU
1	B	14	GLY
1	B	16	ASN
1	B	89	ASP
1	B	142	ARG
1	B	143	ALA
1	B	164	PRO
1	B	350	ARG
1	B	383	GLN
1	B	426	PRO
1	B	427	LYS
1	B	428	ASN
1	B	473	ASN
1	B	507	ASP
1	B	511	LYS
1	B	540	LYS
1	C	16	ASN
1	C	89	ASP
1	C	130	ALA
1	C	142	ARG
1	C	143	ALA
1	C	164	PRO
1	C	350	ARG
1	C	353	ALA
1	C	383	GLN
1	C	426	PRO
1	C	427	LYS
1	C	428	ASN
1	C	473	ASN
1	C	507	ASP
1	C	511	LYS
1	C	540	LYS
1	D	16	ASN
1	D	89	ASP
1	D	130	ALA

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Mol	Chain	Res	Type
1	D	142	ARG
1	D	143	ALA
1	D	164	PRO
1	D	350	ARG
1	D	353	ALA
1	D	383	GLN
1	D	426	PRO
1	D	427	LYS
1	D	428	ASN
1	D	473	ASN
1	D	507	ASP
1	D	511	LYS
1	D	540	LYS
1	A	13	GLU
1	A	83	PRO
1	A	128	GLU
1	A	130	ALA
1	A	143	ALA
1	A	210	LYS
1	A	356	GLY
1	A	381	ARG
1	A	411	ALA
1	A	474	LEU
1	B	83	PRO
1	B	128	GLU
1	B	130	ALA
1	B	165	SER
1	B	210	LYS
1	B	304	VAL
1	B	353	ALA
1	B	356	GLY
1	B	381	ARG
1	B	411	ALA
1	B	474	LEU
1	C	13	GLU
1	C	83	PRO
1	C	128	GLU
1	C	165	SER
1	C	210	LYS
1	C	356	GLY
1	C	381	ARG
1	C	411	ALA

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Mol	Chain	Res	Type
1	C	474	LEU
1	D	13	GLU
1	D	83	PRO
1	D	128	GLU
1	D	210	LYS
1	D	356	GLY
1	D	381	ARG
1	D	411	ALA
1	D	474	LEU
1	A	3	GLN
1	A	17	GLN
1	A	165	SER
1	A	304	VAL
1	A	339	SER
1	B	3	GLN
1	C	3	GLN
1	C	17	GLN
1	D	3	GLN
1	D	17	GLN
1	D	165	SER
1	D	332	GLU
1	D	336	LEU
1	D	339	SER
1	A	15	ASN
1	A	212	GLN
1	B	17	GLN
1	B	512	GLU
1	C	15	ASN
1	C	304	VAL
1	C	332	GLU
1	C	339	SER
1	D	15	ASN
1	D	212	GLN
1	D	304	VAL
1	D	512	GLU
1	A	84	ARG
1	A	85	MSE
1	A	332	GLU
1	A	396	PRO
1	A	512	GLU
1	B	15	ASN
1	B	55	PRO

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Mol	Chain	Res	Type
1	B	84	ARG
1	B	85	MSE
1	B	212	GLN
1	B	332	GLU
1	B	339	SER
1	B	530	ALA
1	C	84	ARG
1	C	85	MSE
1	C	212	GLN
1	C	530	ALA
1	D	84	ARG
1	D	85	MSE
1	D	509	VAL
1	A	55	PRO
1	A	443	GLY
1	A	509	VAL
1	B	120	ASN
1	B	396	PRO
1	C	55	PRO
1	C	396	PRO
1	C	509	VAL
1	D	55	PRO
1	D	396	PRO
1	D	443	GLY
1	B	249	VAL
1	B	443	GLY
1	C	443	GLY
1	B	509	VAL
1	C	249	VAL
1	A	534	GLY

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	437/429 (102%)	365 (84%)	72 (16%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	437/429 (102%)	363 (83%)	74 (17%)	2 14
1	C	437/429 (102%)	366 (84%)	71 (16%)	3 16
1	D	437/429 (102%)	365 (84%)	72 (16%)	3 15
All	All	1748/1716 (102%)	1459 (84%)	289 (16%)	3 15

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	GLN
1	A	4	LEU
1	A	5	VAL
1	A	10	ASN
1	A	16	ASN
1	A	24	SER
1	A	28	SER
1	A	33	CYS
1	A	38	VAL
1	A	63	LEU
1	A	84	ARG
1	A	88	LEU
1	A	89	ASP
1	A	94	ILE
1	A	120	ASN
1	A	121	VAL
1	A	124	TYR
1	A	131	GLN
1	A	137	THR
1	A	141	ILE
1	A	153	LEU
1	A	154	LYS
1	A	161	ASP
1	A	167	PHE
1	A	170	SER
1	A	176	THR
1	A	182	LEU
1	A	192	THR
1	A	204	ARG
1	A	212	GLN
1	A	220	GLN
1	A	225	TYR

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Mol	Chain	Res	Type
1	A	227	GLU
1	A	246	LEU
1	A	254	ARG
1	A	279	LEU
1	A	288	LYS
1	A	291	LEU
1	A	294	LEU
1	A	325	LEU
1	A	326	VAL
1	A	344	VAL
1	A	347	VAL
1	A	350	ARG
1	A	359	VAL
1	A	366	LEU
1	A	373	MSE
1	A	377	MSE
1	A	383	GLN
1	A	390	THR
1	A	394	LEU
1	A	407	SER
1	A	425	LEU
1	A	429	THR
1	A	437	THR
1	A	438	CYS
1	A	442	GLU
1	A	445	ARG
1	A	450	VAL
1	A	453	LYS
1	A	454	LEU
1	A	457	THR
1	A	461	LEU
1	A	480	LEU
1	A	489	THR
1	A	504	ASP
1	A	510	PHE
1	A	515	ARG
1	A	519	SER
1	A	531	LEU
1	A	539	ARG
1	B	2	SER
1	B	3	GLN
1	B	4	LEU

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Mol	Chain	Res	Type
1	B	10	ASN
1	B	16	ASN
1	B	24	SER
1	B	28	SER
1	B	33	CYS
1	B	38	VAL
1	B	63	LEU
1	B	84	ARG
1	B	88	LEU
1	B	89	ASP
1	B	90	VAL
1	B	94	ILE
1	B	120	ASN
1	B	121	VAL
1	B	124	TYR
1	B	131	GLN
1	B	137	THR
1	B	141	ILE
1	B	153	LEU
1	B	154	LYS
1	B	161	ASP
1	B	167	PHE
1	B	170	SER
1	B	182	LEU
1	B	192	THR
1	B	204	ARG
1	B	212	GLN
1	B	220	GLN
1	B	225	TYR
1	B	227	GLU
1	B	246	LEU
1	B	254	ARG
1	B	279	LEU
1	B	288	LYS
1	B	291	LEU
1	B	294	LEU
1	B	297	GLU
1	B	300	ILE
1	B	325	LEU
1	B	326	VAL
1	B	344	VAL
1	B	347	VAL

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Mol	Chain	Res	Type
1	B	350	ARG
1	B	359	VAL
1	B	366	LEU
1	B	373	MSE
1	B	383	GLN
1	B	385	ASP
1	B	390	THR
1	B	394	LEU
1	B	407	SER
1	B	425	LEU
1	B	429	THR
1	B	435	ARG
1	B	437	THR
1	B	438	CYS
1	B	445	ARG
1	B	450	VAL
1	B	452	LEU
1	B	453	LYS
1	B	454	LEU
1	B	457	THR
1	B	461	LEU
1	B	480	LEU
1	B	489	THR
1	B	504	ASP
1	B	510	PHE
1	B	515	ARG
1	B	519	SER
1	B	531	LEU
1	B	539	ARG
1	C	2	SER
1	C	3	GLN
1	C	4	LEU
1	C	10	ASN
1	C	16	ASN
1	C	24	SER
1	C	28	SER
1	C	33	CYS
1	C	38	VAL
1	C	63	LEU
1	C	84	ARG
1	C	88	LEU
1	C	89	ASP

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Mol	Chain	Res	Type
1	C	94	ILE
1	C	120	ASN
1	C	121	VAL
1	C	124	TYR
1	C	131	GLN
1	C	137	THR
1	C	141	ILE
1	C	153	LEU
1	C	154	LYS
1	C	161	ASP
1	C	167	PHE
1	C	170	SER
1	C	182	LEU
1	C	192	THR
1	C	204	ARG
1	C	212	GLN
1	C	220	GLN
1	C	246	LEU
1	C	254	ARG
1	C	279	LEU
1	C	288	LYS
1	C	291	LEU
1	C	293	VAL
1	C	294	LEU
1	C	297	GLU
1	C	325	LEU
1	C	326	VAL
1	C	344	VAL
1	C	347	VAL
1	C	350	ARG
1	C	359	VAL
1	C	366	LEU
1	C	373	MSE
1	C	383	GLN
1	C	385	ASP
1	C	387	LEU
1	C	390	THR
1	C	394	LEU
1	C	407	SER
1	C	425	LEU
1	C	429	THR
1	C	437	THR

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Mol	Chain	Res	Type
1	C	438	CYS
1	C	445	ARG
1	C	450	VAL
1	C	453	LYS
1	C	454	LEU
1	C	457	THR
1	C	458	VAL
1	C	461	LEU
1	C	480	LEU
1	C	489	THR
1	C	504	ASP
1	C	510	PHE
1	C	515	ARG
1	C	519	SER
1	C	531	LEU
1	C	539	ARG
1	D	2	SER
1	D	3	GLN
1	D	4	LEU
1	D	5	VAL
1	D	10	ASN
1	D	16	ASN
1	D	24	SER
1	D	33	CYS
1	D	38	VAL
1	D	63	LEU
1	D	84	ARG
1	D	88	LEU
1	D	89	ASP
1	D	90	VAL
1	D	94	ILE
1	D	120	ASN
1	D	121	VAL
1	D	124	TYR
1	D	131	GLN
1	D	137	THR
1	D	141	ILE
1	D	153	LEU
1	D	154	LYS
1	D	161	ASP
1	D	167	PHE
1	D	170	SER

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Mol	Chain	Res	Type
1	D	182	LEU
1	D	192	THR
1	D	204	ARG
1	D	212	GLN
1	D	220	GLN
1	D	225	TYR
1	D	227	GLU
1	D	246	LEU
1	D	254	ARG
1	D	279	LEU
1	D	288	LYS
1	D	289	GLU
1	D	291	LEU
1	D	294	LEU
1	D	325	LEU
1	D	326	VAL
1	D	344	VAL
1	D	347	VAL
1	D	350	ARG
1	D	359	VAL
1	D	366	LEU
1	D	373	MSE
1	D	377	MSE
1	D	383	GLN
1	D	390	THR
1	D	394	LEU
1	D	407	SER
1	D	425	LEU
1	D	429	THR
1	D	437	THR
1	D	438	CYS
1	D	445	ARG
1	D	450	VAL
1	D	453	LYS
1	D	454	LEU
1	D	457	THR
1	D	461	LEU
1	D	475	SER
1	D	480	LEU
1	D	489	THR
1	D	504	ASP
1	D	510	PHE

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Mol	Chain	Res	Type
1	D	515	ARG
1	D	519	SER
1	D	531	LEU
1	D	539	ARG

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

Mol	Chain	Res	Type
1	A	25	GLN
1	A	29	GLN
1	A	78	HIS
1	A	82	HIS
1	A	131	GLN
1	A	202	ASN
1	A	247	HIS
1	A	261	ASN
1	A	386	HIS
1	A	428	ASN
1	A	466	GLN
1	A	481	GLN
1	A	528	GLN
1	B	25	GLN
1	B	29	GLN
1	B	78	HIS
1	B	82	HIS
1	B	131	GLN
1	B	202	ASN
1	B	247	HIS
1	B	261	ASN
1	B	386	HIS
1	B	428	ASN
1	B	466	GLN
1	B	481	GLN
1	B	528	GLN
1	C	25	GLN
1	C	29	GLN
1	C	78	HIS
1	C	82	HIS
1	C	131	GLN
1	C	202	ASN
1	C	261	ASN
1	C	386	HIS

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Mol	Chain	Res	Type
1	C	428	ASN
1	C	466	GLN
1	C	481	GLN
1	C	528	GLN
1	D	25	GLN
1	D	29	GLN
1	D	78	HIS
1	D	82	HIS
1	D	131	GLN
1	D	202	ASN
1	D	247	HIS
1	D	261	ASN
1	D	386	HIS
1	D	428	ASN
1	D	466	GLN
1	D	481	GLN
1	D	528	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	532/541 (98%)	0.46	51 (9%)	10 11	29, 53, 164, 213	0
1	B	532/541 (98%)	0.36	44 (8%)	14 14	30, 53, 158, 222	0
1	C	532/541 (98%)	0.43	52 (9%)	10 10	31, 60, 149, 194	0
1	D	532/541 (98%)	0.49	66 (12%)	5 6	33, 60, 159, 199	0
All	All	2128/2164 (98%)	0.44	213 (10%)	9 10	29, 56, 157, 222	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	PRO	10.1
1	C	166	SER	9.9
1	D	122	PRO	7.6
1	B	166	SER	7.0
1	A	115	LEU	6.6
1	D	115	LEU	6.2
1	B	121	VAL	6.2
1	C	121	VAL	5.9
1	C	174	THR	5.9
1	A	121	VAL	5.7
1	A	147	GLU	5.4
1	A	120	ASN	5.4
1	A	146	TYR	5.4
1	C	149	LEU	5.3
1	C	10	ASN	5.2
1	C	86	GLY	4.9
1	D	124	TYR	4.7
1	A	158	TRP	4.7
1	B	171	TRP	4.7
1	B	149	LEU	4.6
1	D	147	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	87	ALA	4.4
1	A	65	ALA	4.2
1	A	90	VAL	4.2
1	C	171	TRP	4.2
1	D	69	ALA	4.2
1	A	124	TYR	4.1
1	D	90	VAL	4.1
1	B	174	THR	4.1
1	A	149	LEU	4.1
1	D	171	TRP	4.0
1	B	138	LEU	4.0
1	D	165	SER	3.9
1	D	157	GLU	3.9
1	A	87	ALA	3.9
1	A	171	TRP	3.9
1	C	91	CYS	3.9
1	A	14	GLY	3.8
1	B	79	LYS	3.8
1	C	47	THR	3.8
1	C	176	THR	3.7
1	D	160	PRO	3.7
1	C	87	ALA	3.7
1	D	149	LEU	3.7
1	B	47	THR	3.7
1	D	120	ASN	3.7
1	D	34	VAL	3.7
1	A	172	GLY	3.6
1	C	11	PHE	3.6
1	B	11	PHE	3.6
1	B	86	GLY	3.6
1	D	6	GLU	3.6
1	D	146	TYR	3.6
1	C	79	LYS	3.5
1	A	119	LEU	3.4
1	C	88	LEU	3.4
1	C	138	LEU	3.4
1	A	69	ALA	3.4
1	A	89	ASP	3.4
1	D	121	VAL	3.4
1	B	78	HIS	3.4
1	D	87	ALA	3.4
1	C	153	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	62	ALA	3.3
1	A	166	SER	3.3
1	A	34	VAL	3.3
1	C	170	SER	3.2
1	A	163	GLY	3.2
1	A	66	ALA	3.2
1	A	71	GLN	3.2
1	D	508	ASP	3.2
1	B	428	ASN	3.2
1	C	73	ILE	3.2
1	A	174	THR	3.1
1	D	158	TRP	3.1
1	A	35	LEU	3.1
1	D	138	LEU	3.1
1	D	89	ASP	3.1
1	A	157	GLU	3.1
1	D	163	GLY	3.1
1	B	154	LYS	3.1
1	A	173	ALA	3.1
1	A	178	ALA	3.0
1	D	174	THR	3.0
1	B	150	PRO	3.0
1	D	72	LEU	3.0
1	D	172	GLY	3.0
1	D	49	TYR	3.0
1	D	35	LEU	3.0
1	D	74	ASP	2.9
1	D	62	ALA	2.9
1	D	164	PRO	2.9
1	C	175	VAL	2.9
1	A	508	ASP	2.9
1	A	33	CYS	2.9
1	C	74	ASP	2.9
1	C	150	PRO	2.9
1	D	178	ALA	2.9
1	B	126	TYR	2.8
1	D	93	PHE	2.8
1	D	123	VAL	2.8
1	B	10	ASN	2.8
1	A	93	PHE	2.8
1	C	36	LEU	2.8
1	D	65	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	66	ALA	2.8
1	D	173	ALA	2.8
1	C	428	ASN	2.8
1	B	178	ALA	2.8
1	C	506	THR	2.8
1	C	90	VAL	2.8
1	B	158	TRP	2.7
1	C	80	GLY	2.7
1	D	119	LEU	2.7
1	A	74	ASP	2.7
1	C	12	SER	2.7
1	D	166	SER	2.7
1	D	237	ASN	2.7
1	C	71	GLN	2.7
1	C	172	GLY	2.7
1	B	164	PRO	2.7
1	A	151	GLU	2.7
1	A	150	PRO	2.7
1	A	164	PRO	2.7
1	B	77	LYS	2.7
1	C	78	HIS	2.7
1	B	91	CYS	2.6
1	C	93	PHE	2.6
1	B	73	ILE	2.6
1	B	170	SER	2.6
1	B	175	VAL	2.6
1	C	143	ALA	2.6
1	C	236	THR	2.6
1	C	126	TYR	2.6
1	C	158	TRP	2.6
1	B	147	GLU	2.6
1	A	91	CYS	2.5
1	A	77	LYS	2.5
1	D	77	LYS	2.5
1	A	165	SER	2.5
1	D	136	GLN	2.5
1	D	10	ASN	2.5
1	D	116	ALA	2.5
1	B	36	LEU	2.5
1	B	153	LEU	2.5
1	B	88	LEU	2.5
1	D	99	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLY	2.4
1	B	113	GLN	2.4
1	D	86	GLY	2.4
1	D	150	PRO	2.4
1	C	5	VAL	2.4
1	B	176	THR	2.4
1	B	71	GLN	2.4
1	C	168	VAL	2.4
1	C	165	SER	2.4
1	A	116	ALA	2.3
1	B	141	ILE	2.3
1	D	82	HIS	2.3
1	B	13	GLU	2.3
1	B	122	PRO	2.3
1	D	68	THR	2.3
1	D	79	LYS	2.3
1	B	172	GLY	2.3
1	D	126	TYR	2.3
1	D	33	CYS	2.3
1	D	111	PHE	2.3
1	D	148	ALA	2.3
1	D	208	ARG	2.3
1	C	122	PRO	2.3
1	D	88	LEU	2.3
1	C	173	ALA	2.3
1	B	139	PRO	2.3
1	C	147	GLU	2.3
1	A	88	LEU	2.3
1	A	175	VAL	2.3
1	B	14	GLY	2.3
1	C	6	GLU	2.2
1	B	72	LEU	2.2
1	C	4	LEU	2.2
1	C	72	LEU	2.2
1	D	273	VAL	2.2
1	B	74	ASP	2.2
1	D	139	PRO	2.2
1	D	71	GLN	2.2
1	B	6	GLU	2.2
1	B	541	GLU	2.2
1	D	14	GLY	2.2
1	D	274	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	89	ASP	2.2
1	A	139	PRO	2.2
1	C	189	LEU	2.2
1	A	6	GLU	2.1
1	D	325	LEU	2.1
1	A	10	ASN	2.1
1	D	162	PHE	2.1
1	A	123	VAL	2.1
1	A	86	GLY	2.1
1	B	12	SER	2.1
1	B	89	ASP	2.1
1	C	16	ASN	2.1
1	D	153	LEU	2.1
1	A	152	LYS	2.0
1	C	13	GLU	2.0
1	A	179	ARG	2.0
1	C	424	LYS	2.0
1	C	48	VAL	2.0
1	C	77	LYS	2.0
1	D	51	PHE	2.0
1	A	160	PRO	2.0
1	D	73	ILE	2.0
1	C	141	ILE	2.0
1	D	20	ILE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.