



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:06 PM UTC

PDB ID : 7JSR / pdb_00007jsr
Title : Crystal structure of the large glutamate dehydrogenase composed of 180 kDa subunits from Mycobacterium smegmatis
Authors : Lazaro, M.; Melero, R.; Huet, C.; Lopez-Alonso, J.P.; Delgado, S.; Dodu, A.; Bruch, E.M.; Abriata, L.A.; Alzari, P.M.; Valle, M.; Lisa, M.N.
Deposited on : 2020-08-15
Resolution : 6.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

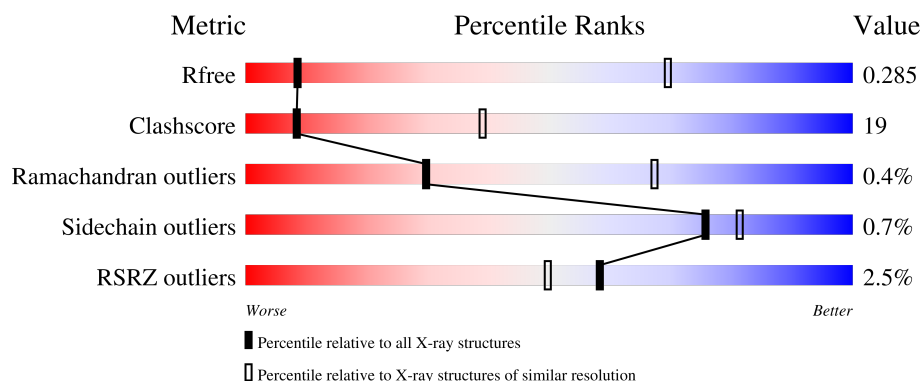
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

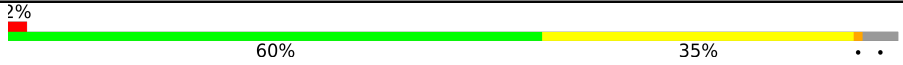
The reported resolution of this entry is 6.27 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1154 (8.50-4.00)
Clashscore	190562	1015 (8.50-4.02)
Ramachandran outliers	187476	1042 (8.50-4.00)
Sidechain outliers	187428	1007 (8.50-4.00)
RSRZ outliers	180081	1147 (8.50-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	1611	
1	B	1611	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24096 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 NAD-specific glutamate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1554	Total	C	N	O	S	Se	0	0	0
			12015	7553	2149	2279	7	27			
1	B	1564	Total	C	N	O	S	Se	0	0	0
			12081	7590	2162	2295	7	27			

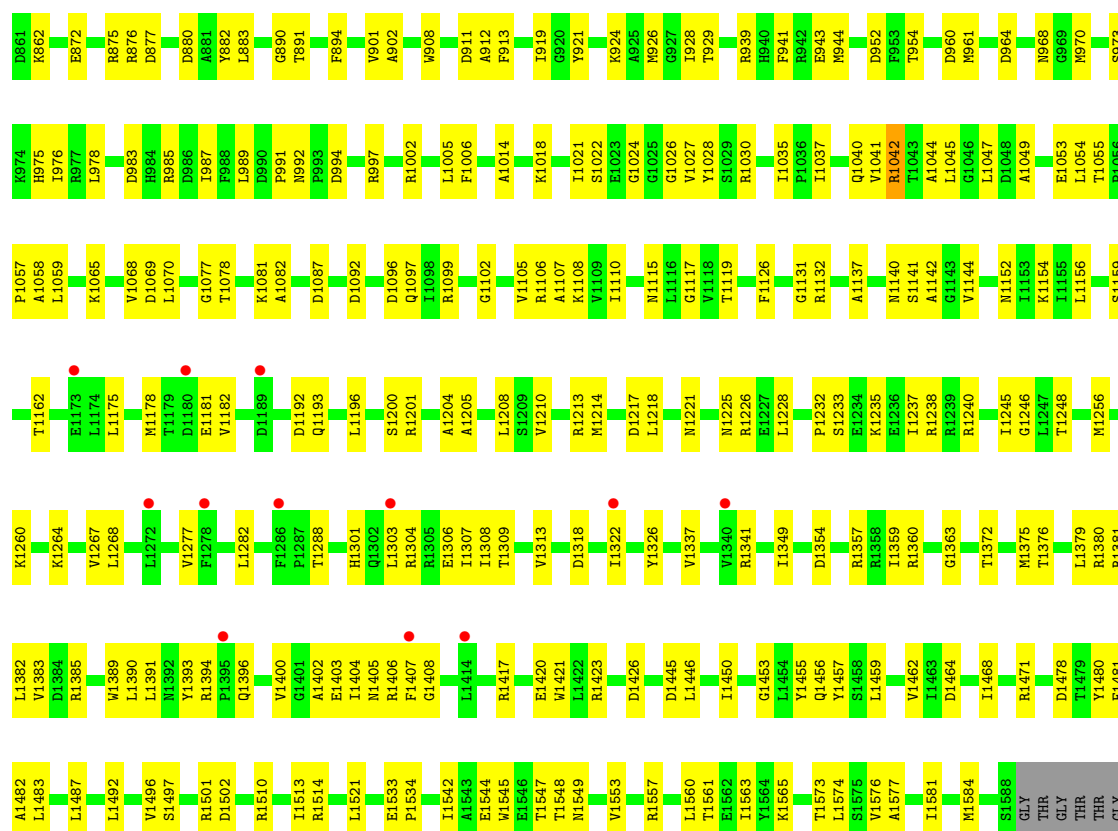
There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MSE	-	initiating methionine	UNP A0R1C2
A	-15	HIS	-	expression tag	UNP A0R1C2
A	-14	HIS	-	expression tag	UNP A0R1C2
A	-13	HIS	-	expression tag	UNP A0R1C2
A	-12	HIS	-	expression tag	UNP A0R1C2
A	-11	HIS	-	expression tag	UNP A0R1C2
A	-10	HIS	-	expression tag	UNP A0R1C2
A	-9	GLU	-	expression tag	UNP A0R1C2
A	-8	ASN	-	expression tag	UNP A0R1C2
A	-7	LEU	-	expression tag	UNP A0R1C2
A	-6	TYR	-	expression tag	UNP A0R1C2
A	-5	PHE	-	expression tag	UNP A0R1C2
A	-4	GLN	-	expression tag	UNP A0R1C2
A	-3	GLY	-	expression tag	UNP A0R1C2
A	-2	ALA	-	expression tag	UNP A0R1C2
A	-1	ALA	-	expression tag	UNP A0R1C2
A	0	SER	-	expression tag	UNP A0R1C2
B	-16	MSE	-	initiating methionine	UNP A0R1C2
B	-15	HIS	-	expression tag	UNP A0R1C2
B	-14	HIS	-	expression tag	UNP A0R1C2
B	-13	HIS	-	expression tag	UNP A0R1C2
B	-12	HIS	-	expression tag	UNP A0R1C2
B	-11	HIS	-	expression tag	UNP A0R1C2
B	-10	HIS	-	expression tag	UNP A0R1C2
B	-9	GLU	-	expression tag	UNP A0R1C2

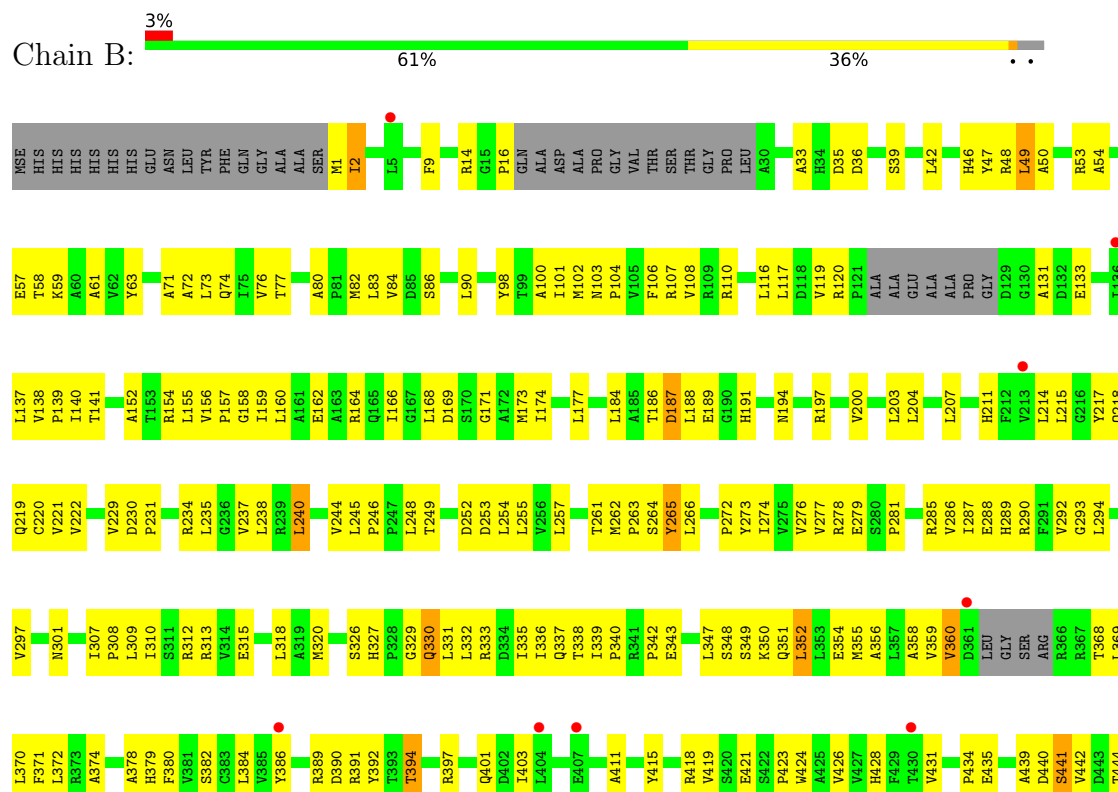
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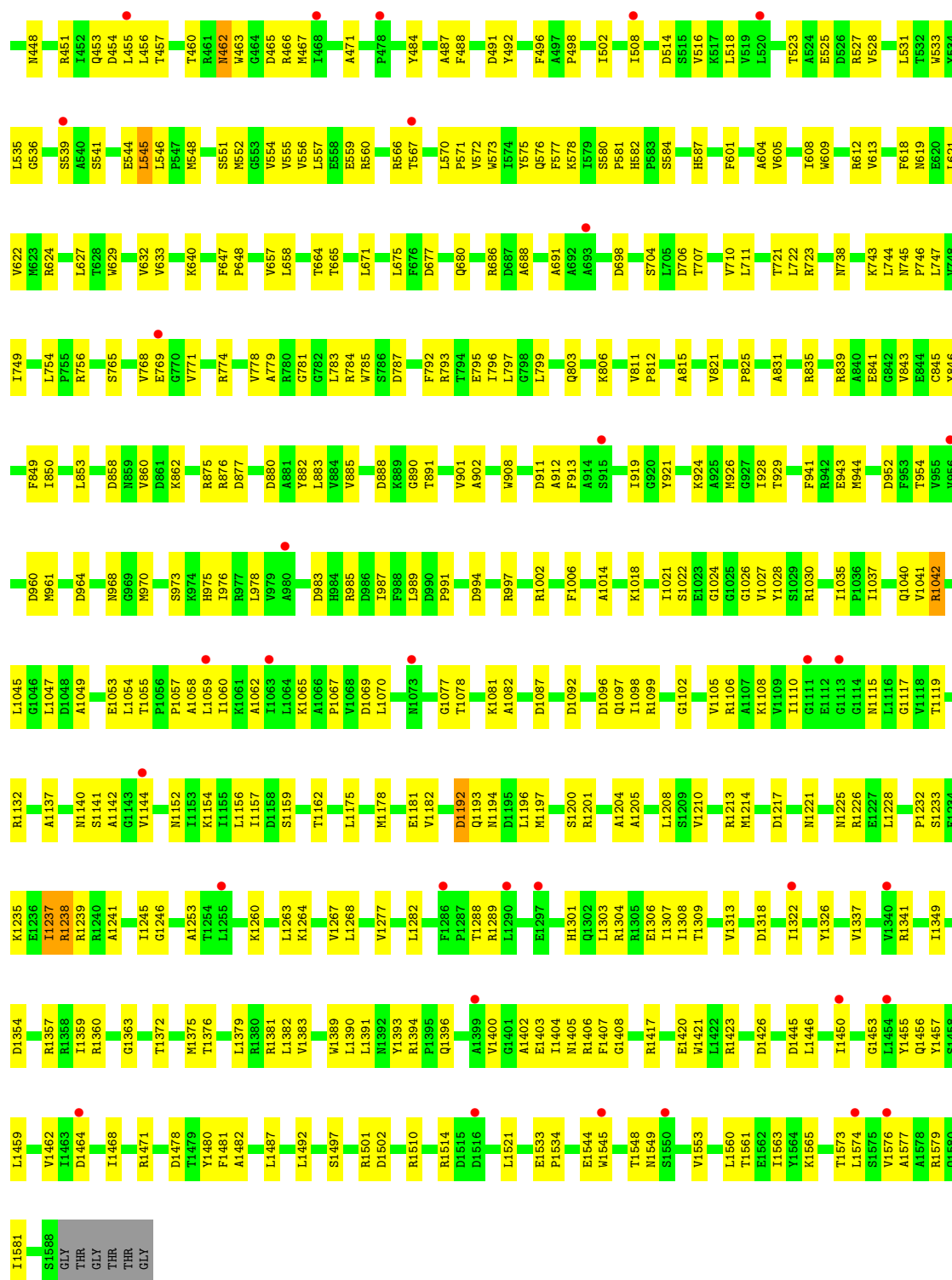
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASN	-	expression tag	UNP A0R1C2
B	-7	LEU	-	expression tag	UNP A0R1C2
B	-6	TYR	-	expression tag	UNP A0R1C2
B	-5	PHE	-	expression tag	UNP A0R1C2
B	-4	GLN	-	expression tag	UNP A0R1C2
B	-3	GLY	-	expression tag	UNP A0R1C2
B	-2	ALA	-	expression tag	UNP A0R1C2
B	-1	ALA	-	expression tag	UNP A0R1C2
B	0	SER	-	expression tag	UNP A0R1C2



● Molecule 1: NAD-specific glutamate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	151.56Å 253.54Å 399.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 6.27 24.98 – 6.27	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.98-6.27) 84.9 (24.98-6.27)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 6.51Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.226 , 0.284 0.228 , 0.285	Depositor DCC
R_{free} test set	875 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	329.5	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 420.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.046 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.058 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24096	wwPDB-VP
Average B, all atoms (Å ²)	456.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/12213	0.64	5/16558 (0.0%)
1	B	0.33	0/12281	0.67	13/16652 (0.1%)
All	All	0.33	0/24494	0.66	18/33210 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1237	ILE	N-CA-C	9.75	119.78	110.42
1	B	49	LEU	N-CA-C	9.41	121.22	110.97
1	B	1239	ARG	N-CA-C	-8.06	102.45	111.07
1	B	1042	ARG	N-CA-C	7.72	119.69	111.28
1	B	1194	ASN	N-CA-C	6.30	119.12	111.82
1	A	1042	ARG	N-CA-C	6.22	118.06	111.28
1	B	360	VAL	CB-CA-C	-6.20	102.22	112.26
1	B	47	TYR	N-CA-C	-6.08	104.21	111.69
1	B	360	VAL	N-CA-C	6.06	118.66	111.09
1	B	48	ARG	N-CA-C	5.83	117.64	111.28
1	A	1044	ALA	N-CA-C	-5.76	106.25	113.28
1	B	358	ALA	N-CA-C	-5.59	105.09	111.07
1	B	1192	ASP	N-CA-C	-5.56	105.22	111.28
1	B	352	LEU	N-CA-C	-5.44	105.00	111.69
1	A	1044	ALA	N-CA-CB	5.34	118.85	110.46
1	A	456	LEU	N-CA-C	-5.12	107.16	113.41
1	B	1238	ARG	CA-C-O	5.10	125.25	119.18
1	A	458	GLU	N-CA-C	5.03	117.65	111.82

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	12015	0	11963	468	0
1	B	12081	0	12022	469	0
All	All	24096	0	23985	919	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 19.

All (919) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1483:LEU:HD23	1:A:1542:ILE:HG12	1.22	1.13
1:A:1483:LEU:CD2	1:A:1542:ILE:HG12	1.87	1.04
1:A:1226:ARG:HD3	1:A:1233:SER:HA	1.43	1.00
1:B:1226:ARG:HD3	1:B:1233:SER:HA	1.44	0.98
1:B:355:MSE:SE	1:B:371:PHE:CD2	2.68	0.96
1:B:335:ILE:HG23	1:B:359:VAL:HG11	1.48	0.94
1:A:1483:LEU:HD23	1:A:1542:ILE:CG1	1.98	0.92
1:B:484:TYR:HE1	1:B:567:THR:HB	1.33	0.91
1:A:484:TYR:HE1	1:A:567:THR:HB	1.35	0.89
1:A:991:PRO:HD2	1:A:1022:SER:HB2	1.55	0.88
1:B:991:PRO:HD2	1:B:1022:SER:HB2	1.56	0.87
1:A:50:ALA:HB2	1:A:76:VAL:HG21	1.59	0.84
1:B:1081:LYS:HB2	1:B:1099:ARG:HD3	1.57	0.83
1:B:1045:LEU:HD23	1:B:1047:LEU:HD11	1.59	0.83
1:B:50:ALA:HB2	1:B:76:VAL:HG21	1.59	0.82
1:B:403:ILE:HD13	1:B:455:LEU:HB3	1.64	0.80
1:A:1081:LYS:HB2	1:A:1099:ARG:HD3	1.62	0.80
1:B:928:ILE:HG13	1:B:1142:ALA:HB1	1.64	0.80
1:A:556:VAL:O	1:B:541:SER:HB3	1.82	0.79
1:A:584:SER:HB2	1:A:624:ARG:HH12	1.48	0.79
1:A:207:LEU:HA	1:A:211:HIS:HB2	1.65	0.79
1:A:332:LEU:HG	1:A:335:ILE:HD12	1.66	0.78
1:B:1193:GLN:HE22	1:B:1260:LYS:NZ	1.82	0.78
1:A:862:LYS:HD3	1:A:1162:THR:HB	1.66	0.77
1:B:222:VAL:HB	1:B:286:VAL:HB	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:H	1:A:42:LEU:HD12	1.48	0.77
1:A:203:LEU:HD13	1:A:308:PRO:HD2	1.66	0.77
1:B:215:LEU:HG	1:B:293:GLY:HA2	1.65	0.77
1:B:584:SER:HB2	1:B:624:ARG:HH12	1.49	0.77
1:A:215:LEU:HG	1:A:293:GLY:HA2	1.64	0.77
1:A:928:ILE:HG13	1:A:1142:ALA:HB1	1.65	0.77
1:B:332:LEU:HG	1:B:335:ILE:HD12	1.66	0.76
1:B:207:LEU:HA	1:B:211:HIS:HB2	1.67	0.76
1:A:222:VAL:HB	1:A:286:VAL:HB	1.67	0.76
1:B:39:SER:H	1:B:42:LEU:HD12	1.50	0.76
1:B:1037:ILE:HG13	1:B:1054:LEU:HD13	1.67	0.76
1:A:1037:ILE:HG13	1:A:1054:LEU:HD13	1.67	0.75
1:B:203:LEU:HD13	1:B:308:PRO:HD2	1.69	0.75
1:B:332:LEU:HD23	1:B:356:ALA:HB1	1.68	0.75
1:A:110:ARG:HG2	1:A:116:LEU:HA	1.69	0.75
1:A:80:ALA:HB3	1:A:83:LEU:HD21	1.69	0.74
1:A:1456:GLN:HA	1:A:1459:LEU:HD12	1.68	0.74
1:A:84:VAL:HG11	1:A:103:ASN:HD22	1.53	0.74
1:A:391:ARG:HH12	1:A:462:ASN:HB2	1.51	0.74
1:B:1065:LYS:O	1:B:1106:ARG:NH2	2.20	0.73
1:B:84:VAL:HG11	1:B:103:ASN:HD22	1.52	0.73
1:B:1282:LEU:HB2	1:B:1308:ILE:HD11	1.71	0.73
1:B:349:SER:HA	1:B:352:LEU:HB2	1.70	0.73
1:A:1193:GLN:OE1	1:A:1260:LYS:NZ	2.22	0.73
1:A:987:ILE:HD13	1:A:1059:LEU:HD23	1.69	0.73
1:B:110:ARG:HG2	1:B:116:LEU:HA	1.69	0.72
1:B:862:LYS:HD3	1:B:1162:THR:HB	1.71	0.72
1:A:330:GLN:HG2	1:B:297:VAL:HG22	1.71	0.72
1:A:484:TYR:CE1	1:A:567:THR:HB	2.22	0.72
1:A:1232:PRO:HB2	1:A:1237:ILE:HG13	1.72	0.72
1:B:484:TYR:CE1	1:B:567:THR:HB	2.21	0.72
1:A:1381:ARG:HH21	1:A:1514:ARG:NH2	1.88	0.72
1:B:1456:GLN:HA	1:B:1459:LEU:HD12	1.72	0.72
1:B:391:ARG:HH12	1:B:462:ASN:HB2	1.54	0.71
1:A:338:THR:N	1:A:418:ARG:HH21	1.88	0.71
1:A:462:ASN:OD1	1:A:463:TRP:N	2.24	0.71
1:B:721:THR:HA	1:B:744:LEU:HD23	1.72	0.71
1:A:1282:LEU:HB2	1:A:1308:ILE:HD11	1.72	0.71
1:B:987:ILE:HD13	1:B:1059:LEU:HD23	1.70	0.71
1:A:793:ARG:HH12	1:A:797:LEU:HD22	1.55	0.71
1:B:1232:PRO:HB2	1:B:1237:ILE:HG13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ILE:HD13	1:A:455:LEU:HB3	1.71	0.70
1:A:166:ILE:HD11	1:A:237:VAL:HG13	1.73	0.70
1:B:166:ILE:HD11	1:B:237:VAL:HG13	1.72	0.70
1:A:330:GLN:H	1:B:297:VAL:HG13	1.56	0.70
1:A:778:VAL:HG12	1:A:812:PRO:HB3	1.73	0.70
1:B:80:ALA:HB3	1:B:83:LEU:HD21	1.74	0.69
1:B:340:PRO:HD2	1:B:384:LEU:HD21	1.74	0.69
1:B:778:VAL:HG12	1:B:812:PRO:HB3	1.74	0.69
1:A:721:THR:HA	1:A:744:LEU:HD23	1.74	0.69
1:B:1014:ALA:HA	1:B:1027:VAL:HG11	1.73	0.69
1:A:882:TYR:O	1:A:883:LEU:HG	1.91	0.69
1:B:882:TYR:O	1:B:883:LEU:HG	1.92	0.69
1:A:754:LEU:HD13	1:A:756:ARG:HG2	1.73	0.69
1:B:1394:ARG:HH12	1:B:1406:ARG:HD2	1.58	0.69
1:A:723:ARG:HH12	1:A:858:ASP:CG	2.01	0.68
1:B:793:ARG:HH12	1:B:797:LEU:HD22	1.57	0.68
1:A:166:ILE:HG23	1:A:173:MSE:HE1	1.75	0.68
1:B:539:SER:HB2	1:B:573:TRP:CE2	2.28	0.68
1:B:1381:ARG:HH21	1:B:1514:ARG:NH2	1.90	0.68
1:A:1014:ALA:HA	1:A:1027:VAL:HG11	1.76	0.68
1:B:166:ILE:HG23	1:B:173:MSE:HE1	1.75	0.68
1:A:677:ASP:HB3	1:A:680:GLN:HG2	1.76	0.68
1:B:355:MSE:SE	1:B:371:PHE:CE2	2.97	0.67
1:B:359:VAL:HA	1:B:369:LEU:CD2	2.24	0.67
1:A:612:ARG:O	1:A:738:ASN:ND2	2.27	0.67
1:B:612:ARG:O	1:B:738:ASN:ND2	2.26	0.67
1:B:677:ASP:HB3	1:B:680:GLN:HG2	1.77	0.67
1:A:107:ARG:N	1:A:120:ARG:O	2.27	0.67
1:A:1268:LEU:HD11	1:A:1306:GLU:HG3	1.77	0.67
1:B:53:ARG:NH2	1:B:57:GLU:O	2.27	0.67
1:B:246:PRO:O	1:B:290:ARG:NH2	2.27	0.67
1:B:110:ARG:NH2	1:B:133:GLU:OE2	2.27	0.67
1:A:1394:ARG:HH12	1:A:1406:ARG:HD2	1.59	0.67
1:B:368:THR:HG21	1:B:456:LEU:HB2	1.75	0.67
1:B:711:LEU:N	1:B:711:LEU:HD12	2.10	0.67
1:A:330:GLN:HA	1:A:333:ARG:HB2	1.76	0.67
1:B:107:ARG:N	1:B:120:ARG:O	2.28	0.67
1:B:1045:LEU:HD21	1:B:1062:ALA:HB1	1.78	0.66
1:B:723:ARG:HH12	1:B:858:ASP:CG	2.03	0.66
1:A:1501:ARG:HG2	1:A:1510:ARG:HD3	1.77	0.66
1:B:1501:ARG:HG2	1:B:1510:ARG:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:TYR:HB3	1:A:926:MSE:SE	2.45	0.66
1:B:754:LEU:HD13	1:B:756:ARG:HG2	1.78	0.66
1:B:330:GLN:HA	1:B:333:ARG:HB2	1.77	0.66
1:A:334:ASP:OD1	1:B:301:ASN:ND2	2.29	0.66
1:A:539:SER:HB2	1:A:573:TRP:CE2	2.30	0.66
1:B:525:GLU:HG3	1:B:528:VAL:HB	1.77	0.66
1:A:80:ALA:H	1:A:83:LEU:HD11	1.61	0.65
1:A:347:LEU:HD21	1:A:352:LEU:HB2	1.76	0.65
1:A:710:VAL:HG12	1:A:711:LEU:HD12	1.78	0.65
1:B:545:LEU:HA	1:B:548:MSE:SE	2.46	0.65
1:B:1193:GLN:HE22	1:B:1260:LYS:HZ2	1.44	0.65
1:B:332:LEU:HD21	1:B:360:VAL:HG21	1.79	0.65
1:B:379:HIS:CD2	1:B:435:GLU:HA	2.31	0.65
1:B:382:SER:OG	1:B:428:HIS:NE2	2.27	0.65
1:A:110:ARG:NH2	1:A:133:GLU:OE2	2.30	0.65
1:B:462:ASN:OD1	1:B:463:TRP:N	2.27	0.65
1:B:1417:ARG:NH2	1:B:1420:GLU:OE1	2.29	0.65
1:A:657:VAL:CG1	1:A:711:LEU:HD11	2.27	0.65
1:B:351:GLN:HA	1:B:354:GLU:CD	2.23	0.64
1:B:710:VAL:HG12	1:B:711:LEU:HD12	1.79	0.64
1:B:1057:PRO:HB3	1:B:1097:GLN:OE1	1.97	0.64
1:A:101:ILE:HA	1:A:138:VAL:HG22	1.78	0.64
1:B:191:HIS:HB3	1:B:279:GLU:HG3	1.77	0.64
1:A:1175:LEU:HA	1:A:1178:MSE:HE2	1.80	0.64
1:B:53:ARG:HG2	1:B:54:ALA:H	1.63	0.64
1:A:315:GLU:HA	1:A:318:LEU:HB2	1.80	0.64
1:A:919:ILE:O	1:A:1154:LYS:NZ	2.26	0.64
1:A:1301:HIS:O	1:A:1304:ARG:NH1	2.28	0.64
1:A:941:PHE:HE2	1:A:1070:LEU:HD13	1.63	0.64
1:A:1217:ASP:OD1	1:A:1221:ASN:ND2	2.30	0.64
1:B:973:SER:HB3	1:B:976:ILE:HG13	1.80	0.64
1:A:1502:ASP:N	1:A:1502:ASP:OD1	2.31	0.64
1:A:317:ALA:HB1	1:A:352:LEU:HD22	1.80	0.63
1:B:221:VAL:HG22	1:B:287:ILE:HG12	1.78	0.63
1:A:53:ARG:HG2	1:A:54:ALA:H	1.64	0.63
1:A:221:VAL:HG22	1:A:287:ILE:HG12	1.79	0.63
1:B:657:VAL:HG12	1:B:711:LEU:HD11	1.81	0.63
1:B:1349:ILE:HG23	1:B:1408:GLY:HA2	1.81	0.63
1:A:191:HIS:HB3	1:A:279:GLU:HG3	1.79	0.63
1:A:382:SER:OG	1:A:428:HIS:NE2	2.27	0.63
1:B:545:LEU:HD12	1:B:548:MSE:SE	2.49	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:NH2	1:A:57:GLU:O	2.28	0.62
1:A:200:VAL:HG22	1:A:255:LEU:HD22	1.81	0.62
1:B:921:TYR:HB3	1:B:926:MSE:SE	2.50	0.62
1:B:1175:LEU:HA	1:B:1178:MSE:HE2	1.81	0.62
1:B:657:VAL:CG1	1:B:711:LEU:HD11	2.30	0.62
1:B:941:PHE:HE2	1:B:1070:LEU:HD13	1.64	0.62
1:B:347:LEU:HD11	1:B:352:LEU:HA	1.81	0.62
1:B:1181:GLU:OE2	1:B:1288:THR:N	2.31	0.62
1:B:1502:ASP:OD1	1:B:1502:ASP:N	2.32	0.62
1:A:369:LEU:HB2	1:A:386:TYR:HB2	1.81	0.62
1:A:657:VAL:HG12	1:A:711:LEU:HD11	1.80	0.62
1:A:1057:PRO:HB3	1:A:1097:GLN:OE1	1.98	0.62
1:A:723:ARG:NH1	1:A:858:ASP:OD1	2.33	0.62
1:B:1192:ASP:OD1	1:B:1360:ARG:NH1	2.33	0.62
1:B:1268:LEU:HD11	1:B:1306:GLU:HG3	1.80	0.62
1:A:1192:ASP:OD1	1:A:1360:ARG:NH1	2.33	0.62
1:A:525:GLU:HG3	1:A:528:VAL:HB	1.81	0.61
1:A:711:LEU:HD12	1:A:711:LEU:N	2.15	0.61
1:A:1483:LEU:HD23	1:A:1542:ILE:CD1	2.30	0.61
1:B:200:VAL:HG22	1:B:255:LEU:HD22	1.80	0.61
1:A:330:GLN:CG	1:B:297:VAL:HG22	2.30	0.61
1:A:973:SER:HB3	1:A:976:ILE:HG13	1.82	0.61
1:A:1417:ARG:NH2	1:A:1420:GLU:OE1	2.32	0.61
1:B:723:ARG:NH1	1:B:858:ASP:OD1	2.34	0.61
1:A:357:LEU:O	1:A:360:VAL:HG12	2.00	0.61
1:A:891:THR:O	1:A:891:THR:HG22	2.01	0.61
1:B:315:GLU:HA	1:B:318:LEU:HB2	1.82	0.61
1:B:779:ALA:HB1	1:B:815:ALA:HB2	1.82	0.61
1:A:246:PRO:O	1:A:290:ARG:NH2	2.33	0.61
1:B:1267:VAL:HB	1:B:1309:THR:HG23	1.83	0.61
1:A:1349:ILE:HG23	1:A:1408:GLY:HA2	1.81	0.61
1:B:54:ALA:HB3	1:B:57:GLU:HB2	1.83	0.60
1:A:1423:ARG:HD2	1:A:1482:ALA:HA	1.82	0.60
1:B:1115:ASN:OD1	1:B:1140:ASN:ND2	2.34	0.60
1:B:570:LEU:HD12	1:B:571:PRO:HD2	1.83	0.60
1:A:1115:ASN:OD1	1:A:1140:ASN:ND2	2.35	0.60
1:A:330:GLN:OE1	1:B:301:ASN:N	2.35	0.60
1:B:101:ILE:HA	1:B:138:VAL:HG22	1.84	0.60
1:A:523:THR:HG23	1:A:525:GLU:H	1.67	0.60
1:B:335:ILE:CG2	1:B:359:VAL:HG11	2.29	0.60
1:B:1055:THR:HG23	1:B:1058:ALA:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1359:ILE:HG21	1:B:1376:THR:HG23	1.84	0.59
1:B:1423:ARG:HD2	1:B:1482:ALA:HA	1.83	0.59
1:A:554:VAL:HA	1:A:581:PRO:HA	1.84	0.59
1:B:245:LEU:O	1:B:290:ARG:NH1	2.35	0.59
1:A:1225:ASN:HB3	1:A:1228:LEU:HB2	1.84	0.59
1:B:313:ARG:NH1	1:B:347:LEU:O	2.35	0.59
1:A:331:LEU:HD11	1:A:422:SER:HB2	1.85	0.59
1:B:379:HIS:NE2	1:B:435:GLU:HA	2.18	0.59
1:B:71:ALA:O	1:B:140:ILE:N	2.36	0.59
1:B:919:ILE:O	1:B:1154:LYS:NZ	2.25	0.59
1:B:440:ASP:OD1	1:B:441:SER:N	2.36	0.59
1:B:347:LEU:HD21	1:B:352:LEU:CB	2.32	0.58
1:B:1421:TRP:CD1	1:B:1481:PHE:HD2	2.21	0.58
1:A:332:LEU:HA	1:A:335:ILE:HD12	1.85	0.58
1:B:1225:ASN:HB3	1:B:1228:LEU:HB2	1.85	0.58
1:B:318:LEU:HD21	1:B:333:ARG:HE	1.68	0.58
1:B:347:LEU:HD21	1:B:352:LEU:HB2	1.84	0.58
1:A:657:VAL:CG1	1:A:711:LEU:CD1	2.82	0.58
1:B:80:ALA:H	1:B:83:LEU:HD11	1.69	0.58
1:B:369:LEU:HB2	1:B:386:TYR:HB2	1.86	0.58
1:A:229:VAL:HG23	1:A:244:VAL:HG13	1.86	0.58
1:A:349:SER:O	1:A:353:LEU:HG	2.04	0.58
1:B:1426:ASP:OD1	1:B:1455:TYR:OH	2.21	0.58
1:A:664:THR:HG23	1:A:698:ASP:HB3	1.86	0.58
1:A:1055:THR:HG23	1:A:1058:ALA:H	1.68	0.58
1:B:343:GLU:H	1:B:343:GLU:CD	2.11	0.58
1:B:1200:SER:HB3	1:B:1322:ILE:HD11	1.86	0.58
1:A:779:ALA:HB1	1:A:815:ALA:HB2	1.85	0.57
1:B:523:THR:HG23	1:B:525:GLU:H	1.69	0.57
1:A:1549:ASN:HB2	1:A:1553:VAL:HB	1.87	0.57
1:A:313:ARG:NH1	1:A:347:LEU:O	2.37	0.57
1:A:1421:TRP:CD1	1:A:1481:PHE:HD2	2.22	0.57
1:A:774:ARG:HH22	1:A:880:ASP:CG	2.12	0.57
1:A:318:LEU:HD21	1:A:333:ARG:HE	1.68	0.57
1:B:664:THR:HG23	1:B:698:ASP:HB3	1.87	0.57
1:A:1214:MSE:HG2	1:A:1326:TYR:CD2	2.40	0.57
1:A:784:ARG:HH11	1:A:799:LEU:HD11	1.70	0.57
1:A:1181:GLU:OE2	1:A:1288:THR:N	2.30	0.56
1:B:378:ALA:HB2	1:B:439:ALA:HA	1.87	0.56
1:A:419:VAL:HB	1:B:419:VAL:HB	1.87	0.56
1:B:774:ARG:HH22	1:B:880:ASP:CG	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:VAL:HG23	1:B:244:VAL:HG13	1.86	0.56
1:B:350:LYS:HG3	1:B:351:GLN:N	2.21	0.56
1:A:54:ALA:HB3	1:A:57:GLU:HB2	1.87	0.56
1:B:944:MSE:SE	1:B:1132:ARG:HE	2.38	0.56
1:B:559:GLU:HA	1:B:576:GLN:O	2.06	0.56
1:B:1217:ASP:OD1	1:B:1221:ASN:ND2	2.38	0.56
1:A:71:ALA:O	1:A:140:ILE:N	2.37	0.56
1:A:359:VAL:C	1:A:361:ASP:H	2.13	0.56
1:B:554:VAL:HA	1:B:581:PRO:HA	1.86	0.56
1:B:1193:GLN:NE2	1:B:1260:LYS:NZ	2.52	0.56
1:A:1267:VAL:HB	1:A:1309:THR:HG23	1.87	0.56
1:B:1400:VAL:HA	1:B:1403:GLU:OE2	2.06	0.56
1:A:220:CYS:O	1:A:288:GLU:N	2.26	0.56
1:A:259:GLN:HB3	1:A:377:LEU:HD22	1.87	0.56
1:A:1381:ARG:HH21	1:A:1514:ARG:HH22	1.52	0.56
1:B:1077:GLY:O	1:B:1117:GLY:HA2	2.05	0.56
1:A:1077:GLY:O	1:A:1117:GLY:HA2	2.06	0.56
1:A:989:LEU:HD13	1:A:1041:VAL:HG11	1.88	0.55
1:B:1105:VAL:HG11	1:B:1110:ILE:HD11	1.87	0.55
1:B:1549:ASN:HB2	1:B:1553:VAL:HB	1.87	0.55
1:A:514:ASP:N	1:A:536:GLY:O	2.40	0.55
1:A:415:TYR:OH	1:B:389:ARG:NH2	2.39	0.55
1:A:1081:LYS:HB2	1:A:1099:ARG:CD	2.35	0.55
1:A:1389:TRP:HB2	1:A:1457:TYR:HE1	1.72	0.55
1:B:140:ILE:HG22	1:B:141:THR:O	2.07	0.55
1:B:359:VAL:HA	1:B:369:LEU:HD23	1.88	0.55
1:A:793:ARG:NH1	1:A:797:LEU:HD22	2.21	0.55
1:A:397:ARG:NH1	1:A:415:TYR:OH	2.40	0.55
1:B:1210:VAL:O	1:B:1214:MSE:HG3	2.07	0.55
1:A:350:LYS:HG3	1:A:351:GLN:N	2.22	0.55
1:B:1381:ARG:HH21	1:B:1514:ARG:HH22	1.54	0.55
1:B:781:GLY:HA3	1:B:815:ALA:O	2.07	0.55
1:B:1372:THR:HA	1:B:1375:MSE:HE3	1.88	0.55
1:A:1200:SER:HB3	1:A:1322:ILE:HD11	1.89	0.55
1:A:1379:LEU:O	1:A:1383:VAL:HG13	2.06	0.55
1:B:1301:HIS:O	1:B:1304:ARG:NH1	2.35	0.55
1:A:781:GLY:HA3	1:A:815:ALA:O	2.07	0.54
1:B:989:LEU:HD13	1:B:1041:VAL:HG11	1.89	0.54
1:A:944:MSE:HE3	1:A:1108:LYS:HB3	1.89	0.54
1:A:1081:LYS:O	1:A:1102:GLY:N	2.39	0.54
1:A:1421:TRP:O	1:A:1423:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LEU:HD21	1:B:254:LEU:HD11	1.89	0.54
1:A:484:TYR:HA	1:A:487:ALA:HB3	1.89	0.54
1:B:1214:MSE:HG2	1:B:1326:TYR:CD2	2.42	0.54
1:A:391:ARG:NH1	1:A:462:ASN:HB2	2.20	0.54
1:B:110:ARG:NE	1:B:133:GLU:OE1	2.40	0.54
1:A:457:THR:O	1:A:460:THR:OG1	2.24	0.54
1:A:559:GLU:HA	1:A:576:GLN:O	2.07	0.54
1:B:110:ARG:HA	1:B:117:LEU:HG	1.90	0.54
1:B:657:VAL:CG1	1:B:711:LEU:CD1	2.85	0.54
1:A:570:LEU:HD12	1:A:571:PRO:HD2	1.90	0.54
1:B:1533:GLU:HG2	1:B:1534:PRO:HD2	1.89	0.54
1:A:187:ASP:HB3	1:A:197:ARG:HD2	1.90	0.54
1:A:245:LEU:O	1:A:290:ARG:NH1	2.37	0.54
1:B:944:MSE:HE3	1:B:1108:LYS:HB3	1.89	0.54
1:B:1081:LYS:O	1:B:1102:GLY:N	2.40	0.54
1:A:90:LEU:HD11	1:A:155:LEU:HD12	1.90	0.53
1:A:831:ALA:O	1:A:835:ARG:NE	2.40	0.53
1:B:264:SER:C	1:B:266:LEU:H	2.16	0.53
1:B:1196:LEU:HD22	1:B:1318:ASP:HA	1.90	0.53
1:B:1394:ARG:NH1	1:B:1406:ARG:HD2	2.23	0.53
1:A:944:MSE:SE	1:A:1132:ARG:HE	2.41	0.53
1:A:1400:VAL:HA	1:A:1403:GLU:OE2	2.08	0.53
1:B:187:ASP:HB3	1:B:197:ARG:HD2	1.90	0.53
1:B:546:LEU:HD11	1:B:556:VAL:HB	1.89	0.53
1:B:1081:LYS:HB2	1:B:1099:ARG:CD	2.31	0.53
1:A:463:TRP:O	1:A:467:MSE:HG3	2.08	0.53
1:B:1238:ARG:HA	1:B:1241:ALA:HB3	1.89	0.53
1:A:1359:ILE:HG21	1:A:1376:THR:HG23	1.89	0.53
1:B:162:GLU:HB3	1:B:237:VAL:HG12	1.91	0.53
1:B:463:TRP:O	1:B:467:MSE:HG3	2.08	0.53
1:A:110:ARG:HA	1:A:117:LEU:HG	1.91	0.53
1:A:217:TYR:O	1:A:234:ARG:HA	2.09	0.53
1:A:952:ASP:HA	1:A:975:HIS:HB3	1.91	0.53
1:B:276:VAL:HG22	1:B:290:ARG:HG2	1.91	0.53
1:A:1391:LEU:HA	1:A:1396:GLN:HE22	1.74	0.53
1:B:457:THR:O	1:B:460:THR:OG1	2.26	0.53
1:B:566:ARG:HD3	1:B:570:LEU:HB3	1.91	0.53
1:B:1379:LEU:O	1:B:1383:VAL:HG13	2.08	0.53
1:A:264:SER:C	1:A:266:LEU:H	2.17	0.53
1:A:604:ALA:O	1:A:608:ILE:HG13	2.09	0.53
1:A:621:LEU:HD22	1:A:665:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:THR:HA	1:A:1375:MSE:HE3	1.91	0.53
1:A:1533:GLU:HG2	1:A:1534:PRO:HD2	1.89	0.53
1:B:307:ILE:HG21	1:B:310:ILE:HG12	1.90	0.53
1:B:1337:VAL:O	1:B:1341:ARG:HG3	2.09	0.53
1:B:1391:LEU:HA	1:B:1396:GLN:HE22	1.74	0.53
1:A:162:GLU:HB3	1:A:237:VAL:HG12	1.90	0.53
1:B:952:ASP:HA	1:B:975:HIS:HB3	1.90	0.53
1:A:276:VAL:HG22	1:A:290:ARG:HG2	1.90	0.52
1:A:657:VAL:HG11	1:A:711:LEU:CD1	2.39	0.52
1:A:169:ASP:HB3	1:A:235:LEU:HB3	1.91	0.52
1:A:343:GLU:H	1:A:343:GLU:CD	2.16	0.52
1:B:793:ARG:NH1	1:B:797:LEU:HD22	2.23	0.52
1:B:1421:TRP:O	1:B:1423:ARG:NH1	2.41	0.52
1:B:1497:SER:HA	1:B:1510:ARG:HH21	1.75	0.52
1:B:200:VAL:O	1:B:204:LEU:HG	2.09	0.52
1:B:1045:LEU:O	1:B:1067:PRO:CD	2.57	0.52
1:A:257:LEU:HD11	1:A:273:TYR:HB3	1.89	0.52
1:A:1196:LEU:HD22	1:A:1318:ASP:HA	1.91	0.52
1:B:249:THR:HG21	1:B:278:ARG:HB2	1.92	0.52
1:B:604:ALA:O	1:B:608:ILE:HG13	2.08	0.52
1:A:107:ARG:HG3	1:A:120:ARG:HB2	1.91	0.52
1:A:184:LEU:HD21	1:A:254:LEU:HD11	1.91	0.52
1:A:723:ARG:HB2	1:A:743:LYS:HB3	1.89	0.52
1:A:860:VAL:HB	1:A:908:TRP:CG	2.44	0.52
1:A:184:LEU:HD13	1:A:200:VAL:HG12	1.90	0.52
1:A:850:ILE:HG13	1:A:901:VAL:HG11	1.92	0.52
1:B:220:CYS:O	1:B:288:GLU:N	2.26	0.52
1:B:1042:ARG:NH1	1:B:1047:LEU:O	2.43	0.52
1:B:1394:ARG:HH11	1:B:1407:PHE:HE2	1.58	0.52
1:A:546:LEU:HD11	1:A:556:VAL:HB	1.91	0.52
1:A:1497:SER:HA	1:A:1510:ARG:HH21	1.74	0.52
1:B:784:ARG:HH11	1:B:799:LEU:HD11	1.75	0.52
1:B:811:VAL:HG21	1:B:1307:ILE:HG12	1.91	0.52
1:B:831:ALA:O	1:B:835:ARG:NE	2.43	0.52
1:B:184:LEU:HD13	1:B:200:VAL:HG12	1.92	0.52
1:B:1421:TRP:HE3	1:B:1478:ASP:OD1	1.91	0.52
1:A:846:TYR:O	1:A:850:ILE:HG12	2.10	0.52
1:B:217:TYR:O	1:B:234:ARG:HA	2.09	0.52
1:B:397:ARG:NH1	1:B:415:TYR:OH	2.42	0.52
1:B:491:ASP:OD1	1:B:491:ASP:N	2.43	0.52
1:A:140:ILE:HG22	1:A:141:THR:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG21	1:A:278:ARG:HB2	1.92	0.52
1:A:675:LEU:HD22	1:A:876:ARG:HD2	1.91	0.52
1:A:162:GLU:HG2	1:A:240:LEU:HD21	1.92	0.51
1:A:1105:VAL:HG11	1:A:1110:ILE:HD11	1.91	0.51
1:A:1337:VAL:O	1:A:1341:ARG:HG3	2.10	0.51
1:B:42:LEU:HD23	1:B:63:TYR:CD2	2.45	0.51
1:A:785:TRP:HB3	1:A:890:GLY:HA3	1.91	0.51
1:A:1394:ARG:HH11	1:A:1407:PHE:HE2	1.58	0.51
1:A:1394:ARG:NH1	1:A:1406:ARG:HD2	2.24	0.51
1:A:1483:LEU:HD21	1:A:1542:ILE:HG12	1.86	0.51
1:B:846:TYR:O	1:B:850:ILE:HG12	2.10	0.51
1:B:1045:LEU:HG	1:B:1047:LEU:HD21	1.92	0.51
1:A:811:VAL:HG21	1:A:1307:ILE:HG12	1.92	0.51
1:A:970:MSE:HE2	1:A:978:LEU:HD22	1.93	0.51
1:A:1426:ASP:OD1	1:A:1455:TYR:OH	2.25	0.51
1:B:332:LEU:HA	1:B:335:ILE:HD12	1.91	0.51
1:B:875:ARG:HG3	1:B:875:ARG:O	2.08	0.51
1:A:491:ASP:N	1:A:491:ASP:OD1	2.43	0.51
1:A:1042:ARG:NH1	1:A:1047:LEU:O	2.44	0.51
1:B:514:ASP:N	1:B:536:GLY:O	2.44	0.51
1:A:338:THR:HG22	1:A:418:ARG:HE	1.75	0.51
1:A:561:PRO:HG2	1:B:560:ARG:NH1	2.26	0.51
1:A:875:ARG:O	1:A:875:ARG:HG3	2.11	0.51
1:A:1152:ASN:OD1	1:A:1303:LEU:HD22	2.11	0.51
1:A:1563:ILE:HG21	1:A:1577:ALA:HB2	1.93	0.51
1:B:379:HIS:HE2	1:B:435:GLU:HA	1.76	0.51
1:B:391:ARG:NH1	1:B:462:ASN:HB2	2.23	0.51
1:B:657:VAL:HG13	1:B:707:THR:HG23	1.92	0.51
1:B:675:LEU:HD22	1:B:876:ARG:HD2	1.91	0.51
1:A:259:GLN:HB2	1:A:377:LEU:HB2	1.92	0.51
1:A:723:ARG:HE	1:A:877:ASP:CG	2.19	0.51
1:B:107:ARG:HG3	1:B:120:ARG:HB2	1.93	0.51
1:B:671:LEU:HA	1:B:691:ALA:HB1	1.93	0.51
1:A:348:SER:HB2	1:A:350:LYS:HG2	1.92	0.50
1:A:516:VAL:HG12	1:A:535:LEU:HD23	1.93	0.50
1:B:970:MSE:HE2	1:B:978:LEU:HD22	1.93	0.50
1:A:110:ARG:NE	1:A:133:GLU:OE1	2.44	0.50
1:A:164:ARG:O	1:A:168:LEU:HG	2.11	0.50
1:B:46:HIS:HB3	1:B:74:GLN:HB3	1.93	0.50
1:B:90:LEU:HD11	1:B:155:LEU:HD12	1.92	0.50
1:B:622:VAL:HG23	1:B:632:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD23	1:A:63:TYR:CD2	2.47	0.50
1:A:784:ARG:NH2	1:A:795:GLU:OE2	2.44	0.50
1:B:954:THR:HG23	1:B:1069:ASP:H	1.76	0.50
1:B:169:ASP:HB3	1:B:235:LEU:HB3	1.94	0.50
1:A:1560:LEU:HD11	1:A:1581:ILE:HG12	1.92	0.50
1:B:629:TRP:CD1	1:B:629:TRP:H	2.29	0.50
1:B:711:LEU:N	1:B:711:LEU:CD1	2.74	0.50
1:B:723:ARG:HB2	1:B:743:LYS:HB3	1.94	0.50
1:B:1363:GLY:CA	1:B:1372:THR:HG21	2.41	0.50
1:A:331:LEU:O	1:A:335:ILE:HG13	2.12	0.50
1:A:784:ARG:NH1	1:A:799:LEU:HD11	2.26	0.50
1:A:1561:THR:O	1:A:1565:LYS:HG2	2.12	0.50
1:B:531:LEU:HB3	1:B:577:PHE:HB2	1.94	0.50
1:B:72:ALA:HB1	1:B:137:LEU:HD11	1.93	0.50
1:B:171:GLY:HA2	1:B:174:ILE:HD12	1.94	0.50
1:B:860:VAL:HB	1:B:908:TRP:CG	2.47	0.50
1:B:1389:TRP:HB2	1:B:1457:TYR:HE1	1.77	0.50
1:A:601:PHE:CE2	1:A:605:VAL:HG21	2.46	0.50
1:B:273:TYR:CE2	1:B:342:PRO:HB3	2.47	0.50
1:B:369:LEU:HA	1:B:453:GLN:NE2	2.27	0.50
1:B:785:TRP:HB3	1:B:890:GLY:HA3	1.93	0.50
1:A:1210:VAL:O	1:A:1214:MSE:HG3	2.11	0.50
1:B:442:VAL:HG12	1:B:444:THR:HG23	1.93	0.49
1:B:862:LYS:HD2	1:B:1159:SER:HA	1.94	0.49
1:A:252:ASP:OD1	1:A:253:ASP:N	2.45	0.49
1:B:162:GLU:HG2	1:B:240:LEU:HD21	1.94	0.49
1:B:164:ARG:O	1:B:168:LEU:HG	2.12	0.49
1:B:484:TYR:HB3	1:B:488:PHE:CZ	2.47	0.49
1:B:784:ARG:NH2	1:B:795:GLU:OE2	2.44	0.49
1:A:307:ILE:HG21	1:A:310:ILE:HG12	1.95	0.49
1:A:340:PRO:HG2	1:A:428:HIS:ND1	2.27	0.49
1:A:970:MSE:HE1	1:A:978:LEU:HB2	1.93	0.49
1:B:219:GLN:HE21	1:B:289:HIS:CD2	2.30	0.49
1:B:850:ILE:HG13	1:B:901:VAL:HG11	1.93	0.49
1:B:888:ASP:H	1:B:891:THR:HB	1.77	0.49
1:A:257:LEU:HD11	1:A:273:TYR:HD2	1.76	0.49
1:A:1381:ARG:NH2	1:A:1514:ARG:NH2	2.59	0.49
1:B:252:ASP:OD1	1:B:253:ASP:N	2.44	0.49
1:B:257:LEU:HD11	1:B:273:TYR:HB3	1.93	0.49
1:B:723:ARG:HE	1:B:877:ASP:CG	2.20	0.49
1:B:774:ARG:HD2	1:B:883:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB1	1:A:36:ASP:HB2	1.93	0.49
1:A:1042:ARG:CZ	1:A:1049:ALA:HA	2.42	0.49
1:B:307:ILE:HB	1:B:310:ILE:HB	1.94	0.49
1:A:976:ILE:O	1:A:1002:ARG:NH2	2.46	0.49
1:B:484:TYR:HA	1:B:487:ALA:HB3	1.95	0.49
1:B:601:PHE:CE2	1:B:605:VAL:HG21	2.46	0.49
1:B:1382:LEU:HD13	1:B:1453:GLY:O	2.13	0.49
1:A:1421:TRP:HE3	1:A:1478:ASP:OD1	1.95	0.49
1:B:309:LEU:HD23	1:B:310:ILE:HD13	1.94	0.49
1:B:523:THR:HG22	1:B:528:VAL:O	2.12	0.49
1:A:392:TYR:CE1	1:A:397:ARG:HB2	2.48	0.49
1:A:671:LEU:HA	1:A:691:ALA:HB1	1.95	0.49
1:A:839:ARG:O	1:A:843:VAL:HG23	2.13	0.49
1:A:960:ASP:OD2	1:A:985:ARG:NH2	2.29	0.49
1:A:1208:LEU:HD22	1:A:1245:ILE:O	2.13	0.49
1:A:72:ALA:HB1	1:A:137:LEU:HD11	1.94	0.49
1:A:189:GLU:HB3	1:A:191:HIS:CE1	2.48	0.49
1:A:219:GLN:HE21	1:A:289:HIS:CD2	2.31	0.49
1:A:274:ILE:HG23	1:A:292:VAL:HG22	1.94	0.49
1:A:309:LEU:HD23	1:A:310:ILE:HD13	1.95	0.49
1:A:415:TYR:OH	1:B:389:ARG:CZ	2.61	0.49
1:A:1096:ASP:HA	1:A:1099:ARG:NH1	2.28	0.49
1:B:839:ARG:O	1:B:843:VAL:HG23	2.12	0.49
1:B:1042:ARG:CZ	1:B:1049:ALA:HA	2.43	0.49
1:A:330:GLN:OE1	1:B:301:ASN:HB2	2.13	0.49
1:A:629:TRP:H	1:A:629:TRP:CD1	2.30	0.49
1:B:1545:TRP:HA	1:B:1548:THR:HG22	1.95	0.49
1:A:162:GLU:HG2	1:A:240:LEU:HD11	1.94	0.48
1:A:557:LEU:HB2	1:A:578:LYS:O	2.13	0.48
1:B:108:VAL:HG21	1:B:133:GLU:CD	2.37	0.48
1:B:943:GLU:OE1	1:B:1201:ARG:NH1	2.46	0.48
1:B:1096:ASP:HA	1:B:1099:ARG:NH1	2.28	0.48
1:B:274:ILE:HG23	1:B:292:VAL:HG22	1.94	0.48
1:B:621:LEU:HD22	1:B:665:THR:HG21	1.94	0.48
1:B:970:MSE:HE1	1:B:978:LEU:HB2	1.95	0.48
1:A:557:LEU:O	1:B:541:SER:HA	2.14	0.48
1:A:912:ALA:HB2	1:A:1154:LYS:CB	2.44	0.48
1:A:961:MSE:HE3	1:A:1006:PHE:HB2	1.94	0.48
1:B:327:HIS:H	1:B:327:HIS:HD1	1.60	0.48
1:B:657:VAL:HG11	1:B:711:LEU:CD1	2.43	0.48
1:B:976:ILE:O	1:B:1002:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1152:ASN:OD1	1:B:1303:LEU:HD22	2.13	0.48
1:A:261:THR:HA	1:A:377:LEU:HD11	1.94	0.48
1:A:747:LEU:HD23	1:A:756:ARG:HB2	1.95	0.48
1:A:200:VAL:O	1:A:204:LEU:HG	2.13	0.48
1:A:862:LYS:HD2	1:A:1159:SER:HA	1.94	0.48
1:A:1105:VAL:HG12	1:A:1107:ALA:H	1.78	0.48
1:A:1363:GLY:CA	1:A:1372:THR:HG21	2.43	0.48
1:B:194:ASN:O	1:B:197:ARG:HG3	2.14	0.48
1:B:257:LEU:HD11	1:B:273:TYR:HD2	1.77	0.48
1:B:309:LEU:HD21	1:B:313:ARG:CZ	2.44	0.48
1:A:309:LEU:HD21	1:A:313:ARG:CZ	2.43	0.48
1:A:992:ASN:O	1:A:1022:SER:OG	2.31	0.48
1:A:46:HIS:HB3	1:A:74:GLN:HB3	1.95	0.48
1:A:392:TYR:HE1	1:A:397:ARG:HB2	1.77	0.48
1:A:484:TYR:HB3	1:A:488:PHE:CZ	2.48	0.48
1:A:1382:LEU:HD13	1:A:1453:GLY:O	2.14	0.48
1:B:1560:LEU:HD11	1:B:1581:ILE:HG12	1.95	0.48
1:A:954:THR:HG23	1:A:1069:ASP:H	1.78	0.48
1:A:1045:LEU:HG	1:A:1047:LEU:HD21	1.96	0.48
1:B:533:TRP:CH2	1:B:545:LEU:HG	2.48	0.48
1:B:1208:LEU:HD22	1:B:1245:ILE:O	2.13	0.48
1:B:912:ALA:HB2	1:B:1154:LYS:CB	2.44	0.48
1:B:1205:ALA:HA	1:B:1246:GLY:N	2.28	0.48
1:A:1092:ASP:HB3	1:A:1099:ARG:NH2	2.29	0.48
1:A:704:SER:OG	1:A:706:ASP:OD1	2.29	0.47
1:A:785:TRP:CD1	1:A:785:TRP:C	2.92	0.47
1:B:747:LEU:HD23	1:B:756:ARG:HB2	1.95	0.47
1:B:152:ALA:O	1:B:156:VAL:HG23	2.14	0.47
1:B:516:VAL:HG12	1:B:535:LEU:HD23	1.96	0.47
1:A:368:THR:HA	1:A:386:TYR:O	2.13	0.47
1:B:1081:LYS:NZ	1:B:1082:ALA:O	2.31	0.47
1:A:73:LEU:O	1:A:137:LEU:HA	2.15	0.47
1:A:1480:TYR:OH	1:A:1521:LEU:HD23	2.14	0.47
1:B:784:ARG:NH1	1:B:799:LEU:HD11	2.29	0.47
1:B:1563:ILE:HG21	1:B:1577:ALA:HB2	1.96	0.47
1:A:1545:TRP:HA	1:A:1548:THR:HG22	1.96	0.47
1:A:49:LEU:HD13	1:A:61:ALA:HB2	1.97	0.47
1:B:33:ALA:HB1	1:B:36:ASP:HB2	1.96	0.47
1:B:374:ALA:N	1:B:444:THR:HG21	2.29	0.47
1:B:961:MSE:HE3	1:B:1006:PHE:HB2	1.97	0.47
1:B:1137:ALA:O	1:B:1141:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1354:ASP:O	1:B:1357:ARG:HG2	2.14	0.47
1:A:158:GLY:O	1:A:162:GLU:HG3	2.15	0.47
1:A:262:MSE:O	1:A:272:PRO:HD2	2.14	0.47
1:A:273:TYR:CE2	1:A:342:PRO:HB3	2.48	0.47
1:A:531:LEU:HB3	1:A:577:PHE:HB2	1.96	0.47
1:B:783:LEU:O	1:B:891:THR:OG1	2.20	0.47
1:B:1078:THR:HG21	1:B:1119:THR:HG23	1.96	0.47
1:A:352:LEU:C	1:A:352:LEU:HD23	2.40	0.47
1:A:417:ALA:H	1:B:421:GLU:HG2	1.79	0.47
1:A:711:LEU:N	1:A:711:LEU:CD1	2.77	0.47
1:B:369:LEU:HA	1:B:453:GLN:HE21	1.79	0.47
1:B:991:PRO:HB2	1:B:1040:GLN:HB3	1.97	0.47
1:B:1561:THR:O	1:B:1565:LYS:HG2	2.14	0.47
1:A:100:ALA:HB3	1:A:139:PRO:HD2	1.97	0.47
1:A:353:LEU:HA	1:A:356:ALA:HB3	1.96	0.47
1:B:49:LEU:HD13	1:B:61:ALA:HB2	1.96	0.47
1:B:924:LYS:HA	1:B:964:ASP:CG	2.40	0.47
1:A:348:SER:O	1:A:351:GLN:N	2.47	0.47
1:A:1402:ALA:HA	1:A:1405:ASN:ND2	2.30	0.47
1:B:332:LEU:HD21	1:B:360:VAL:CG2	2.43	0.47
1:B:1092:ASP:HB3	1:B:1099:ARG:NH2	2.30	0.47
1:A:1204:ALA:O	1:A:1246:GLY:HA3	2.15	0.46
1:A:1471:ARG:NH1	1:A:1534:PRO:HG3	2.30	0.46
1:B:108:VAL:N	1:B:131:ALA:O	2.33	0.46
1:B:527:ARG:HH12	1:B:587:HIS:HA	1.80	0.46
1:B:647:PHE:HE2	1:B:710:VAL:HG22	1.80	0.46
1:B:960:ASP:OD2	1:B:985:ARG:NH2	2.29	0.46
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.77	0.46
1:A:352:LEU:O	1:A:355:MSE:N	2.48	0.46
1:A:471:ALA:HB2	1:A:502:ILE:HD12	1.97	0.46
1:A:647:PHE:HE2	1:A:710:VAL:HG22	1.81	0.46
1:A:1078:THR:HG21	1:A:1119:THR:HG23	1.97	0.46
1:A:1081:LYS:NZ	1:A:1082:ALA:O	2.32	0.46
1:A:1205:ALA:HA	1:A:1246:GLY:N	2.29	0.46
1:B:983:ASP:OD2	1:B:985:ARG:NH2	2.49	0.46
1:A:1137:ALA:O	1:A:1141:SER:HB2	2.15	0.46
1:B:162:GLU:HG2	1:B:240:LEU:HD11	1.96	0.46
1:B:360:VAL:O	1:B:360:VAL:HG12	2.15	0.46
1:B:557:LEU:HB2	1:B:578:LYS:O	2.15	0.46
1:A:9:PHE:CG	1:A:104:PRO:HG3	2.50	0.46
1:B:392:TYR:HE1	1:B:397:ARG:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ILE:CG2	1:B:566:ARG:HG2	2.46	0.46
1:B:1181:GLU:CD	1:B:1288:THR:H	2.21	0.46
1:B:1381:ARG:NH2	1:B:1514:ARG:NH2	2.61	0.46
1:A:774:ARG:HD2	1:A:883:LEU:HD21	1.97	0.46
1:A:1264:LYS:HG3	1:A:1313:VAL:HG21	1.97	0.46
1:B:73:LEU:O	1:B:137:LEU:HA	2.16	0.46
1:B:336:ILE:O	1:B:339:ILE:N	2.42	0.46
1:A:35:ASP:OD1	1:A:35:ASP:N	2.42	0.46
1:A:104:PRO:HB2	1:A:106:PHE:CE1	2.51	0.46
1:A:664:THR:HG23	1:A:698:ASP:CB	2.46	0.46
1:A:722:LEU:N	1:A:743:LYS:O	2.40	0.46
1:A:1181:GLU:CD	1:A:1288:THR:H	2.20	0.46
1:B:159:ILE:HG21	1:B:265:TYR:HB2	1.98	0.46
1:B:331:LEU:O	1:B:335:ILE:HG13	2.15	0.46
1:A:1393:TYR:O	1:A:1394:ARG:HD2	2.15	0.46
1:B:35:ASP:OD1	1:B:35:ASP:N	2.41	0.46
1:B:104:PRO:HB2	1:B:106:PHE:CE1	2.51	0.46
1:B:1028:TYR:CD1	1:B:1035:ILE:HG23	2.50	0.46
1:B:1277:VAL:HG11	1:B:1400:VAL:HB	1.98	0.46
1:A:622:VAL:HG23	1:A:632:VAL:HG21	1.97	0.46
1:B:622:VAL:HG13	1:B:627:LEU:O	2.16	0.46
1:A:203:LEU:HD13	1:A:307:ILE:HG23	1.97	0.46
1:A:749:ILE:O	1:A:756:ARG:NH1	2.49	0.46
1:B:335:ILE:HG23	1:B:359:VAL:CG1	2.34	0.46
1:B:704:SER:OG	1:B:706:ASP:OD1	2.30	0.46
1:B:1018:LYS:O	1:B:1021:ILE:HG22	2.17	0.46
1:A:307:ILE:HB	1:A:310:ILE:HB	1.98	0.45
1:A:1018:LYS:O	1:A:1021:ILE:HG22	2.16	0.45
1:B:545:LEU:HD11	1:B:609:TRP:CZ3	2.51	0.45
1:B:779:ALA:CB	1:B:815:ALA:HB2	2.46	0.45
1:B:792:PHE:O	1:B:796:ILE:HG12	2.16	0.45
1:A:657:VAL:HG13	1:A:707:THR:HG23	1.97	0.45
1:A:983:ASP:OD2	1:A:985:ARG:NH2	2.49	0.45
1:A:1213:ARG:HB3	1:A:1326:TYR:OH	2.15	0.45
1:A:1354:ASP:O	1:A:1357:ARG:HG2	2.16	0.45
1:B:552:MSE:HE2	1:B:601:PHE:CD1	2.51	0.45
1:B:749:ILE:O	1:B:756:ARG:NH1	2.49	0.45
1:B:806:LYS:HD3	1:B:1144:VAL:HG21	1.97	0.45
1:A:84:VAL:HG11	1:A:103:ASN:ND2	2.27	0.45
1:A:523:THR:HG22	1:A:528:VAL:O	2.16	0.45
1:A:647:PHE:CD1	1:A:648:PRO:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASP:HA	1:B:231:PRO:HD3	1.81	0.45
1:B:1464:ASP:O	1:B:1468:ILE:HG12	2.17	0.45
1:B:1544:GLU:O	1:B:1548:THR:HG22	2.17	0.45
1:A:350:LYS:HG3	1:A:351:GLN:H	1.82	0.45
1:B:9:PHE:CG	1:B:104:PRO:HG3	2.52	0.45
1:A:640:LYS:HB3	1:A:769:GLU:OE2	2.17	0.45
1:A:902:ALA:HB2	1:A:913:PHE:CD2	2.51	0.45
1:A:1380:ARG:O	1:A:1383:VAL:HG22	2.17	0.45
1:A:1464:ASP:O	1:A:1468:ILE:HG12	2.16	0.45
1:B:964:ASP:OD1	1:B:968:ASN:ND2	2.49	0.45
1:A:9:PHE:CD2	1:A:104:PRO:HG3	2.51	0.45
1:A:943:GLU:OE1	1:A:1201:ARG:NH1	2.50	0.45
1:B:1573:THR:O	1:B:1576:VAL:HG12	2.17	0.45
1:A:194:ASN:O	1:A:197:ARG:HG3	2.17	0.45
1:B:16:PRO:HB3	1:B:98:TYR:CZ	2.52	0.45
1:B:262:MSE:O	1:B:272:PRO:HD2	2.16	0.45
1:B:350:LYS:HG3	1:B:351:GLN:H	1.81	0.45
1:B:392:TYR:CE1	1:B:397:ARG:HB2	2.51	0.45
1:B:411:ALA:HB2	1:B:434:PRO:HG3	1.99	0.45
1:B:1200:SER:CB	1:B:1322:ILE:HD11	2.47	0.45
1:B:1480:TYR:OH	1:B:1521:LEU:HD23	2.17	0.45
1:A:442:VAL:HG12	1:A:444:THR:HG23	1.99	0.45
1:A:912:ALA:HB2	1:A:1154:LYS:HB3	1.99	0.45
1:A:1028:TYR:CD1	1:A:1035:ILE:HG23	2.52	0.45
1:A:1240:ARG:NH1	1:A:1248:THR:HG23	2.32	0.45
1:B:154:ARG:O	1:B:157:PRO:HD2	2.17	0.45
1:B:1021:ILE:HG12	1:B:1026:GLY:N	2.31	0.45
1:B:1445:ASP:OD1	1:B:1446:LEU:N	2.50	0.45
1:A:49:LEU:HD11	1:A:59:LYS:HB3	1.99	0.45
1:A:1480:TYR:CZ	1:A:1521:LEU:HD23	2.52	0.45
1:B:307:ILE:CG2	1:B:310:ILE:HG12	2.47	0.45
1:B:356:ALA:O	1:B:360:VAL:HG23	2.17	0.45
1:B:403:ILE:HG21	1:B:455:LEU:HB3	1.99	0.45
1:A:108:VAL:HG21	1:A:133:GLU:CD	2.42	0.45
1:A:261:THR:HA	1:A:377:LEU:CD1	2.47	0.45
1:A:281:PRO:HG2	1:A:285:ARG:HD3	1.98	0.45
1:A:508:ILE:CG2	1:A:566:ARG:HG2	2.46	0.45
1:A:1065:LYS:O	1:A:1106:ARG:NH2	2.49	0.45
1:B:348:SER:O	1:B:351:GLN:N	2.50	0.45
1:B:390:ASP:N	1:B:390:ASP:OD1	2.49	0.45
1:B:1204:ALA:O	1:B:1246:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1390:LEU:HD23	1:B:1390:LEU:HA	1.77	0.45
1:B:1471:ARG:NH1	1:B:1534:PRO:HG3	2.32	0.45
1:A:390:ASP:OD1	1:A:390:ASP:N	2.49	0.44
1:B:49:LEU:HD11	1:B:59:LYS:HB3	1.98	0.44
1:B:86:SER:OG	1:B:266:LEU:HA	2.17	0.44
1:B:173:MSE:HB3	1:B:214:LEU:HD13	1.98	0.44
1:B:911:ASP:OD1	1:B:911:ASP:N	2.48	0.44
1:A:152:ALA:O	1:A:156:VAL:HG23	2.17	0.44
1:A:518:LEU:HD11	1:A:533:TRP:CE2	2.53	0.44
1:A:555:VAL:N	1:A:580:SER:O	2.49	0.44
1:A:644:GLN:HB3	1:A:793:ARG:HB2	1.99	0.44
1:B:1421:TRP:HD1	1:B:1481:PHE:HD2	1.62	0.44
1:B:1579:ARG:O	1:B:1579:ARG:HG2	2.16	0.44
1:A:492:TYR:O	1:A:496:PHE:HB2	2.18	0.44
1:A:1218:LEU:HD23	1:A:1218:LEU:HA	1.77	0.44
1:B:166:ILE:HD13	1:B:215:LEU:HA	1.98	0.44
1:B:177:LEU:HD12	1:B:177:LEU:HA	1.76	0.44
1:A:61:ALA:O	1:A:73:LEU:HD12	2.17	0.44
1:A:334:ASP:O	1:A:418:ARG:NE	2.50	0.44
1:A:806:LYS:HD3	1:A:1144:VAL:HG21	2.00	0.44
1:B:912:ALA:HB2	1:B:1154:LYS:HB3	2.00	0.44
1:B:1081:LYS:HB3	1:B:1081:LYS:HE3	1.67	0.44
1:A:159:ILE:HG21	1:A:265:TYR:HB2	1.98	0.44
1:A:317:ALA:CB	1:A:352:LEU:HD22	2.46	0.44
1:A:330:GLN:OE1	1:B:297:VAL:O	2.35	0.44
1:A:779:ALA:HA	1:A:813:VAL:O	2.17	0.44
1:A:1156:LEU:HD12	1:A:1301:HIS:HD2	1.82	0.44
1:B:293:GLY:O	1:B:294:LEU:HG	2.18	0.44
1:B:471:ALA:HB2	1:B:502:ILE:HD12	1.99	0.44
1:B:686:ARG:HG3	1:B:688:ALA:HB2	2.00	0.44
1:B:1480:TYR:CZ	1:B:1521:LEU:HD23	2.53	0.44
1:A:911:ASP:OD1	1:A:911:ASP:N	2.50	0.44
1:A:1256:MSE:HE2	1:A:1256:MSE:HB3	1.87	0.44
1:B:158:GLY:O	1:B:162:GLU:HG3	2.18	0.44
1:B:189:GLU:HB3	1:B:191:HIS:CE1	2.52	0.44
1:B:924:LYS:HA	1:B:964:ASP:OD1	2.18	0.44
1:A:332:LEU:O	1:A:335:ILE:HB	2.18	0.44
1:A:527:ARG:HH12	1:A:587:HIS:HA	1.82	0.44
1:A:1544:GLU:O	1:A:1548:THR:HG22	2.17	0.44
1:A:86:SER:OG	1:A:266:LEU:HA	2.18	0.44
1:A:262:MSE:HE2	1:A:262:MSE:HB3	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:SER:O	1:A:453:GLN:HB3	2.18	0.44
1:B:100:ALA:HB3	1:B:139:PRO:HD2	1.99	0.44
1:B:1213:ARG:HB3	1:B:1326:TYR:OH	2.18	0.44
1:B:262:MSE:HE2	1:B:262:MSE:HB3	1.65	0.44
1:B:989:LEU:HD12	1:B:1028:TYR:CE2	2.53	0.44
1:A:566:ARG:HD3	1:A:570:LEU:HB3	1.99	0.43
1:B:722:LEU:HD21	1:B:745:ASN:HB2	2.00	0.43
1:B:1087:ASP:HB3	1:B:1096:ASP:OD1	2.18	0.43
1:B:1471:ARG:HD3	1:B:1534:PRO:HG3	2.00	0.43
1:A:921:TYR:HE2	1:A:1182:VAL:HG11	1.83	0.43
1:A:991:PRO:HB2	1:A:1040:GLN:HB3	1.99	0.43
1:A:331:LEU:HD23	1:A:332:LEU:HD12	2.00	0.43
1:A:454:ASP:O	1:A:457:THR:N	2.51	0.43
1:A:779:ALA:CB	1:A:815:ALA:HB2	2.47	0.43
1:A:1021:ILE:HG12	1:A:1026:GLY:N	2.32	0.43
1:A:1087:ASP:HB3	1:A:1096:ASP:OD1	2.18	0.43
1:B:423:PRO:HG2	1:B:424:TRP:CD1	2.53	0.43
1:B:781:GLY:HA2	1:B:803:GLN:NE2	2.33	0.43
1:A:1394:ARG:NH1	1:A:1407:PHE:HE2	2.16	0.43
1:B:186:THR:O	1:B:188:LEU:N	2.52	0.43
1:B:825:PRO:HD3	1:B:841:GLU:HG2	2.00	0.43
1:A:309:LEU:O	1:A:312:ARG:HB3	2.17	0.43
1:A:394:THR:O	1:A:397:ARG:HB3	2.18	0.43
1:A:484:TYR:HD2	1:A:488:PHE:CE1	2.37	0.43
1:A:924:LYS:HA	1:A:964:ASP:CG	2.44	0.43
1:A:1053:GLU:O	1:A:1054:LEU:HD12	2.17	0.43
1:A:1081:LYS:HB3	1:A:1081:LYS:HE3	1.69	0.43
1:B:9:PHE:CD2	1:B:104:PRO:HG3	2.53	0.43
1:B:332:LEU:O	1:B:335:ILE:HB	2.17	0.43
1:B:640:LYS:HB3	1:B:769:GLU:OE2	2.19	0.43
1:B:908:TRP:H	1:B:908:TRP:CD1	2.37	0.43
1:A:862:LYS:HD3	1:A:1162:THR:CB	2.43	0.43
1:A:1471:ARG:HD3	1:A:1534:PRO:HG3	2.00	0.43
1:B:1459:LEU:HA	1:B:1462:VAL:HB	2.00	0.43
1:A:619:ASN:HA	1:A:632:VAL:HG11	2.01	0.43
1:B:61:ALA:O	1:B:73:LEU:HD12	2.18	0.43
1:B:255:LEU:CD1	1:B:277:VAL:HG22	2.48	0.43
1:B:281:PRO:HG2	1:B:285:ARG:HD3	2.00	0.43
1:B:806:LYS:CD	1:B:1144:VAL:HG21	2.47	0.43
1:B:921:TYR:HE2	1:B:1182:VAL:HG11	1.84	0.43
1:B:1030:ARG:HE	1:B:1030:ARG:HB3	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ARG:HG3	1:A:688:ALA:HB2	2.00	0.43
1:A:929:THR:HA	1:A:1142:ALA:HB3	2.01	0.43
1:A:994:ASP:OD2	1:A:997:ARG:HD3	2.18	0.43
1:B:518:LEU:HD11	1:B:533:TRP:CE2	2.54	0.43
1:B:746:PRO:HA	1:B:749:ILE:HD12	1.99	0.43
1:B:787:ASP:OD1	1:B:787:ASP:N	2.52	0.43
1:B:994:ASP:OD2	1:B:997:ARG:HD3	2.19	0.43
1:B:1393:TYR:O	1:B:1394:ARG:HD2	2.19	0.43
1:A:446:LEU:HA	1:A:449:GLU:HB2	2.01	0.43
1:A:630:GLN:H	1:A:630:GLN:HG3	1.62	0.43
1:B:309:LEU:O	1:B:312:ARG:HB3	2.18	0.43
1:B:370:LEU:HD11	1:B:372:LEU:HD21	2.01	0.43
1:B:647:PHE:CD1	1:B:648:PRO:HD2	2.53	0.43
1:B:778:VAL:HA	1:B:882:TYR:CD2	2.53	0.43
1:A:806:LYS:CD	1:A:1144:VAL:HG21	2.49	0.43
1:A:1423:ARG:CZ	1:A:1482:ALA:HB2	2.49	0.43
1:A:1445:ASP:OD1	1:A:1446:LEU:N	2.51	0.43
1:B:440:ASP:C	1:B:442:VAL:H	2.26	0.43
1:B:1423:ARG:CZ	1:B:1482:ALA:HB2	2.49	0.43
1:A:380:PHE:HA	1:A:431:VAL:O	2.20	0.42
1:A:467:MSE:HE2	1:A:467:MSE:HB2	1.82	0.42
1:A:491:ASP:O	1:A:494:GLN:HG3	2.19	0.42
1:A:1092:ASP:HB3	1:A:1099:ARG:HH22	1.84	0.42
1:A:1359:ILE:HD11	1:A:1450:ILE:HD11	2.01	0.42
1:A:1390:LEU:HA	1:A:1390:LEU:HD23	1.75	0.42
1:A:1560:LEU:HD12	1:A:1584:MSE:HE1	2.01	0.42
1:B:664:THR:HG23	1:B:698:ASP:CB	2.48	0.42
1:B:785:TRP:CD1	1:B:785:TRP:C	2.95	0.42
1:B:902:ALA:HB2	1:B:913:PHE:CD2	2.54	0.42
1:B:1394:ARG:NH1	1:B:1407:PHE:HE2	2.17	0.42
1:A:307:ILE:CG2	1:A:310:ILE:HG12	2.49	0.42
1:A:546:LEU:HD23	1:A:550:GLN:HB2	2.01	0.42
1:A:1277:VAL:HG11	1:A:1400:VAL:HB	2.01	0.42
1:A:104:PRO:HB2	1:A:106:PHE:CZ	2.54	0.42
1:A:154:ARG:O	1:A:157:PRO:HD2	2.18	0.42
1:A:727:PHE:O	1:A:872:GLU:HB3	2.19	0.42
1:A:1030:ARG:HE	1:A:1030:ARG:HB3	1.61	0.42
1:B:454:ASP:C	1:B:456:LEU:N	2.77	0.42
1:B:535:LEU:HD12	1:B:575:TYR:HE1	1.84	0.42
1:B:891:THR:HG22	1:B:891:THR:O	2.18	0.42
1:B:1053:GLU:O	1:B:1054:LEU:HD12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:SER:HB3	1:B:14:ARG:NH1	2.34	0.42
1:A:369:LEU:HA	1:A:453:GLN:HE21	1.85	0.42
1:A:397:ARG:HG2	1:A:401:GLN:OE1	2.19	0.42
1:B:331:LEU:HD23	1:B:332:LEU:HD12	2.01	0.42
1:B:394:THR:O	1:B:397:ARG:HB3	2.20	0.42
1:B:1045:LEU:CD2	1:B:1047:LEU:HD11	2.38	0.42
1:B:1193:GLN:HE22	1:B:1260:LYS:HZ3	1.60	0.42
1:A:1400:VAL:HG12	1:A:1404:ILE:HD12	2.01	0.42
1:B:82:MSE:H	1:B:82:MSE:HE2	1.83	0.42
1:B:320:MSE:H	1:B:320:MSE:HG2	1.68	0.42
1:B:849:PHE:O	1:B:853:LEU:HG	2.20	0.42
1:A:101:ILE:C	1:A:102:MSE:HG3	2.45	0.42
1:A:369:LEU:HA	1:A:453:GLN:NE2	2.35	0.42
1:A:1459:LEU:HA	1:A:1462:VAL:HB	2.01	0.42
1:B:418:ARG:HB3	1:B:426:VAL:O	2.20	0.42
1:B:582:HIS:ND1	1:B:584:SER:OG	2.39	0.42
1:B:821:VAL:HG12	1:B:845:CYS:SG	2.59	0.42
1:B:862:LYS:HD3	1:B:1162:THR:CB	2.47	0.42
1:A:518:LEU:HD23	1:A:531:LEU:HD21	2.02	0.42
1:A:1200:SER:CB	1:A:1322:ILE:HD11	2.49	0.42
1:A:1421:TRP:HD1	1:A:1481:PHE:HD2	1.64	0.42
1:B:466:ARG:HG3	1:B:498:PRO:HB2	2.01	0.42
1:B:492:TYR:O	1:B:496:PHE:HB2	2.18	0.42
1:B:1308:ILE:HD13	1:B:1308:ILE:HA	1.87	0.42
1:A:53:ARG:NH2	1:A:77:THR:HA	2.34	0.42
1:A:393:THR:OG1	1:A:395:ALA:HB3	2.19	0.42
1:A:535:LEU:HD12	1:A:575:TYR:HE1	1.85	0.42
1:A:722:LEU:HD21	1:A:745:ASN:HB2	2.01	0.42
1:A:1487:LEU:HA	1:A:1487:LEU:HD23	1.77	0.42
1:B:104:PRO:HB2	1:B:106:PHE:CZ	2.55	0.42
1:B:548:MSE:O	1:B:551:SER:OG	2.33	0.42
1:B:744:LEU:O	1:B:746:PRO:HD3	2.20	0.42
1:B:1238:ARG:HA	1:B:1241:ALA:CB	2.49	0.42
1:A:98:TYR:HA	1:A:140:ILE:HD13	2.02	0.42
1:A:100:ALA:O	1:A:138:VAL:HG13	2.20	0.42
1:A:392:TYR:OH	1:A:397:ARG:HD3	2.19	0.42
1:A:744:LEU:O	1:A:746:PRO:HD3	2.20	0.42
1:A:778:VAL:HA	1:A:882:TYR:CD2	2.55	0.42
1:B:1024:GLY:HA3	1:B:1040:GLN:OE1	2.19	0.42
1:B:1157:ILE:HD12	1:B:1175:LEU:CD1	2.50	0.42
1:B:1400:VAL:HG12	1:B:1404:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:N	1:A:131:ALA:O	2.36	0.42
1:A:166:ILE:HD13	1:A:215:LEU:HA	2.02	0.42
1:A:171:GLY:HA2	1:A:174:ILE:HD12	2.02	0.42
1:A:230:ASP:HA	1:A:231:PRO:HD3	1.83	0.42
1:A:330:GLN:HB2	1:B:301:ASN:HB2	2.02	0.42
1:A:592:GLU:HA	1:A:595:ARG:NH1	2.34	0.42
1:A:939:ARG:HA	1:A:939:ARG:HD2	1.96	0.42
1:A:1560:LEU:HD11	1:A:1581:ILE:CG1	2.50	0.42
1:B:354:GLU:H	1:B:354:GLU:HG3	1.49	0.42
1:B:448:ASN:OD1	1:B:451:ARG:NH2	2.47	0.42
1:B:1060:ILE:HG21	1:B:1098:ILE:HD12	2.02	0.42
1:A:552:MSE:O	1:A:623:MSE:HG3	2.20	0.41
1:B:53:ARG:NH2	1:B:77:THR:HA	2.35	0.41
1:A:248:LEU:HD12	1:A:276:VAL:HG21	2.02	0.41
1:A:533:TRP:CH2	1:A:545:LEU:HG	2.54	0.41
1:A:1024:GLY:HA3	1:A:1040:GLN:OE1	2.20	0.41
1:A:1178:MSE:HE3	1:A:1178:MSE:HB2	1.98	0.41
1:A:1544:GLU:HA	1:A:1547:THR:HB	2.03	0.41
1:B:264:SER:HB3	1:B:272:PRO:HG3	2.02	0.41
1:B:397:ARG:HG2	1:B:401:GLN:OE1	2.20	0.41
1:B:536:GLY:HA2	1:B:572:VAL:HG12	2.02	0.41
1:A:325:PRO:HG2	1:B:14:ARG:HH22	1.85	0.41
1:A:411:ALA:HB2	1:A:434:PRO:HG3	2.02	0.41
1:A:1045:LEU:HD23	1:A:1047:LEU:HD11	2.03	0.41
1:B:203:LEU:HD13	1:B:307:ILE:HG23	2.00	0.41
1:B:1235:LYS:HA	1:B:1238:ARG:NH1	2.35	0.41
1:B:1264:LYS:HG3	1:B:1313:VAL:HG21	2.01	0.41
1:A:186:THR:O	1:A:188:LEU:N	2.54	0.41
1:A:471:ALA:CB	1:A:481:LEU:HD21	2.51	0.41
1:A:545:LEU:HD12	1:A:548:MSE:SE	2.71	0.41
1:A:545:LEU:HD11	1:A:609:TRP:CZ3	2.54	0.41
1:A:908:TRP:CD1	1:A:908:TRP:H	2.38	0.41
1:A:1557:ARG:CZ	1:A:1557:ARG:HB3	2.51	0.41
1:B:467:MSE:HE2	1:B:467:MSE:HB2	1.89	0.41
1:B:1263:LEU:HD23	1:B:1263:LEU:HA	1.91	0.41
1:A:781:GLY:HA2	1:A:803:GLN:NE2	2.35	0.41
1:A:964:ASP:OD1	1:A:968:ASN:ND2	2.53	0.41
1:A:1492:LEU:HD23	1:A:1574:LEU:HD22	2.03	0.41
1:B:765:SER:HB3	1:B:768:VAL:HG12	2.01	0.41
1:B:929:THR:HA	1:B:1142:ALA:HB3	2.02	0.41
1:B:1301:HIS:O	1:B:1304:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HE	1:A:287:ILE:HD11	1.85	0.41
1:A:313:ARG:HA	1:A:316:GLU:OE2	2.21	0.41
1:A:843:VAL:HG22	1:A:894:PHE:CE1	2.55	0.41
1:A:1379:LEU:HD12	1:A:1379:LEU:HA	1.94	0.41
1:B:619:ASN:HA	1:B:632:VAL:HG11	2.01	0.41
1:A:332:LEU:HA	1:A:335:ILE:CG1	2.51	0.41
1:A:1573:THR:O	1:A:1576:VAL:HG12	2.21	0.41
1:B:465:ASP:OD1	1:B:466:ARG:N	2.54	0.41
1:B:613:VAL:HG12	1:B:633:VAL:CG2	2.51	0.41
1:B:1492:LEU:HD23	1:B:1574:LEU:HD22	2.02	0.41
1:A:46:HIS:HB3	1:A:74:GLN:CB	2.50	0.41
1:A:404:LEU:O	1:A:408:LEU:HB2	2.21	0.41
1:A:1391:LEU:O	1:A:1396:GLN:NE2	2.54	0.41
1:A:1510:ARG:O	1:A:1513:ILE:HG22	2.21	0.41
1:B:58:THR:HG21	1:B:160:LEU:HB2	2.02	0.41
1:B:101:ILE:C	1:B:102:MSE:HG3	2.46	0.41
1:B:1359:ILE:HD11	1:B:1450:ILE:HD11	2.01	0.41
1:A:82:MSE:HE2	1:A:82:MSE:H	1.85	0.41
1:A:88:THR:O	1:A:91:LEU:HB2	2.20	0.41
1:A:257:LEU:HD11	1:A:273:TYR:CD2	2.55	0.41
1:A:264:SER:C	1:A:266:LEU:N	2.79	0.41
1:A:320:MSE:HG3	1:A:353:LEU:HD11	2.02	0.41
1:A:644:GLN:OE1	1:A:791:ASP:HA	2.21	0.41
1:A:954:THR:HG23	1:A:1068:VAL:HG13	2.02	0.41
1:A:1301:HIS:O	1:A:1304:ARG:HG2	2.20	0.41
1:A:1385:ARG:NE	1:A:1514:ARG:CZ	2.84	0.41
1:B:46:HIS:HB3	1:B:74:GLN:CB	2.50	0.41
1:B:218:GLN:OE1	1:B:238:LEU:HD22	2.21	0.41
1:B:1178:MSE:HG2	1:B:1289:ARG:HH21	1.86	0.41
1:B:1487:LEU:HD23	1:B:1487:LEU:HA	1.76	0.41
1:A:173:MSE:HB3	1:A:214:LEU:HD13	2.03	0.41
1:A:416:SER:HA	1:B:421:GLU:HG2	2.02	0.41
1:A:825:PRO:HD3	1:A:841:GLU:HG2	2.02	0.41
1:B:2:ILE:H	1:B:2:ILE:HG13	1.63	0.41
1:B:332:LEU:HA	1:B:335:ILE:CG1	2.51	0.41
1:B:555:VAL:N	1:B:580:SER:O	2.53	0.41
1:B:1197:MSE:SE	1:B:1253:ALA:HB2	2.71	0.41
1:B:1402:ALA:HA	1:B:1405:ASN:ND2	2.35	0.41
1:A:418:ARG:HB3	1:A:426:VAL:O	2.21	0.40
1:A:849:PHE:O	1:A:853:LEU:HG	2.21	0.40
1:A:1235:LYS:O	1:A:1238:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PHE:HA	1:B:431:VAL:O	2.21	0.40
1:B:484:TYR:HD2	1:B:488:PHE:CE1	2.39	0.40
1:B:771:VAL:HG13	1:B:792:PHE:HE1	1.87	0.40
1:A:400:MSE:HG2	1:A:456:LEU:HD22	2.03	0.40
1:A:458:GLU:HA	1:A:461:ARG:HG3	2.03	0.40
1:A:754:LEU:CD1	1:A:756:ARG:HG2	2.47	0.40
1:A:203:LEU:CD1	1:A:307:ILE:HG23	2.50	0.40
1:A:293:GLY:O	1:A:294:LEU:HG	2.21	0.40
1:A:374:ALA:N	1:A:444:THR:HG21	2.36	0.40
1:A:686:ARG:CG	1:A:688:ALA:HB2	2.51	0.40
1:A:792:PHE:O	1:A:796:ILE:HG12	2.21	0.40
1:A:924:LYS:HA	1:A:964:ASP:OD1	2.21	0.40
1:A:1126:PHE:CZ	1:A:1131:GLY:HA3	2.57	0.40
1:B:336:ILE:O	1:B:337:GLN:C	2.65	0.40
1:B:722:LEU:N	1:B:743:LYS:O	2.43	0.40
1:B:783:LEU:HD13	1:B:885:VAL:HG13	2.02	0.40
1:B:926:MSE:HE2	1:B:926:MSE:HB3	1.98	0.40
1:B:961:MSE:HE2	1:B:1002:ARG:O	2.21	0.40
1:B:1156:LEU:HD12	1:B:1301:HIS:HD2	1.86	0.40
1:A:324:ASP:OD1	1:A:326:SER:OG	2.39	0.40
1:A:338:THR:HG23	1:A:339:ILE:N	2.36	0.40
1:A:754:LEU:HD13	1:A:754:LEU:HA	1.97	0.40
1:A:1005:LEU:HD23	1:A:1005:LEU:HA	1.84	0.40
1:A:1496:VAL:HG13	1:A:1513:ILE:HG23	2.04	0.40
1:B:246:PRO:O	1:B:248:LEU:HG	2.20	0.40
1:B:261:THR:HA	1:B:380:PHE:HZ	1.86	0.40
1:B:262:MSE:HA	1:B:263:PRO:HD3	1.90	0.40
1:B:541:SER:HB2	1:B:544:GLU:OE1	2.21	0.40
1:B:707:THR:O	1:B:711:LEU:HD13	2.21	0.40
1:B:1228:LEU:HD23	1:B:1228:LEU:HA	1.91	0.40
1:A:554:VAL:HG12	1:A:581:PRO:HA	2.04	0.40
1:B:343:GLU:OE2	1:B:428:HIS:CD2	2.74	0.40
1:B:618:PHE:HE1	1:B:658:LEU:HD12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1544/1611 (96%)	1488 (96%)	50 (3%)	6 (0%)	30	67
1	B	1556/1611 (97%)	1499 (96%)	52 (3%)	5 (0%)	36	72
All	All	3100/3222 (96%)	2987 (96%)	102 (3%)	11 (0%)	30	67

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	ASN
1	B	462	ASN
1	A	187	ASP
1	B	187	ASP
1	B	326	SER
1	A	265	TYR
1	A	326	SER
1	B	265	TYR
1	A	329	GLY
1	A	360	VAL
1	B	329	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1257/1266 (99%)	1249 (99%)	8 (1%)	78	83
1	B	1263/1266 (100%)	1254 (99%)	9 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2520/2532 (100%)	2503 (99%)	17 (1%)	76	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	ILE
1	A	119	VAL
1	A	330	GLN
1	A	338	THR
1	A	348	SER
1	A	394	THR
1	A	545	LEU
1	B	1	MSE
1	B	2	ILE
1	B	119	VAL
1	B	240	LEU
1	B	330	GLN
1	B	338	THR
1	B	394	THR
1	B	441	SER
1	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	219	GLN
1	A	322	HIS
1	A	499	GLN
1	A	803	GLN
1	A	968	ASN
1	A	1190	ASN
1	A	1225	ASN
1	B	79	GLN
1	B	103	ASN
1	B	219	GLN
1	B	322	HIS
1	B	499	GLN
1	B	803	GLN
1	B	968	ASN

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Mol	Chain	Res	Type
1	B	1193	GLN
1	B	1225	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1527/1611 (94%)	0.04	35 (2%) 61 52	366, 451, 525, 581	0
1	B	1537/1611 (95%)	0.06	41 (2%) 56 48	364, 455, 529, 592	0
All	All	3064/3222 (95%)	0.05	76 (2%) 58 50	364, 453, 527, 592	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1286	PHE	5.8
1	A	381	VAL	5.2
1	A	64	PRO	4.0
1	B	1297	GLU	3.8
1	A	423	PRO	3.7
1	B	1113	GLY	3.6
1	A	372	LEU	3.6
1	A	408	LEU	3.5
1	A	383	CYS	3.4
1	B	5	LEU	3.4
1	B	404	LEU	3.3
1	B	915	SER	3.3
1	B	567	THR	3.2
1	B	1073	ASN	3.2
1	A	333	ARG	3.0
1	B	1111	GLY	3.0
1	A	1286	PHE	3.0
1	B	1545	TRP	2.9
1	B	980	ALA	2.9
1	A	261	THR	2.8
1	A	452	ILE	2.8
1	B	1322	ILE	2.8
1	B	956	VAL	2.8
1	B	1516	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1278	PHE	2.7
1	A	742	PHE	2.7
1	B	1464	ASP	2.7
1	B	213	VAL	2.7
1	B	1063	ILE	2.7
1	A	1414	LEU	2.7
1	B	430	THR	2.7
1	A	158	GLY	2.7
1	A	434	PRO	2.6
1	A	488	PHE	2.6
1	A	450	SER	2.6
1	A	1395	PRO	2.6
1	B	693	ALA	2.5
1	A	1340	VAL	2.5
1	A	392	TYR	2.5
1	B	468	ILE	2.5
1	B	1144	VAL	2.5
1	B	508	ILE	2.4
1	B	520	LEU	2.4
1	B	1454	LEU	2.4
1	B	1340	VAL	2.4
1	A	1322	ILE	2.4
1	B	386	TYR	2.4
1	A	387	LEU	2.4
1	B	1399	ALA	2.4
1	A	73	LEU	2.4
1	A	695	VAL	2.3
1	A	152	ALA	2.3
1	B	1576	VAL	2.3
1	A	47	TYR	2.3
1	A	1303	LEU	2.3
1	A	388	PRO	2.3
1	B	361	ASP	2.3
1	B	1059	LEU	2.3
1	B	539	SER	2.3
1	B	1255	LEU	2.2
1	A	1189	ASP	2.2
1	B	407	GLU	2.2
1	B	478	PRO	2.2
1	B	1450	ILE	2.2
1	B	1290	LEU	2.2
1	A	1407	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	136	ILE	2.1
1	B	769	GLU	2.1
1	A	1272	LEU	2.1
1	A	1180	ASP	2.1
1	B	1550	SER	2.1
1	A	370	LEU	2.0
1	A	382	SER	2.0
1	B	1574	LEU	2.0
1	B	455	LEU	2.0
1	A	1173	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.