Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 09:25 AM GMT

PDB ID	:	3IBV
Title	:	Karyopherin cytosolic state
Authors	:	Cook, A.G.; Fukuhara, N.; Jinek, M.; Conti, E.
Deposited on	:	2009-07-17
Resolution	:	3.10 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:

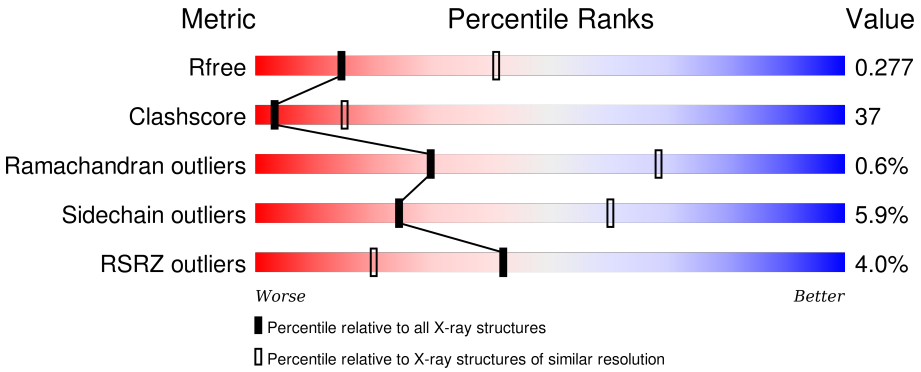
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	980	4% 52% 38% • 6%
1	B	980	3% 50% 38% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12876 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 Exportin-T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	0	0
			6515	4164	1087	1241	23			
1	B	902	Total	C	N	O	S	0	0	0
			6357	4067	1053	1212	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP O94258
A	0	PRO	-	EXPRESSION TAG	UNP O94258
B	-1	GLY	-	EXPRESSION TAG	UNP O94258
B	0	PRO	-	EXPRESSION TAG	UNP O94258

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

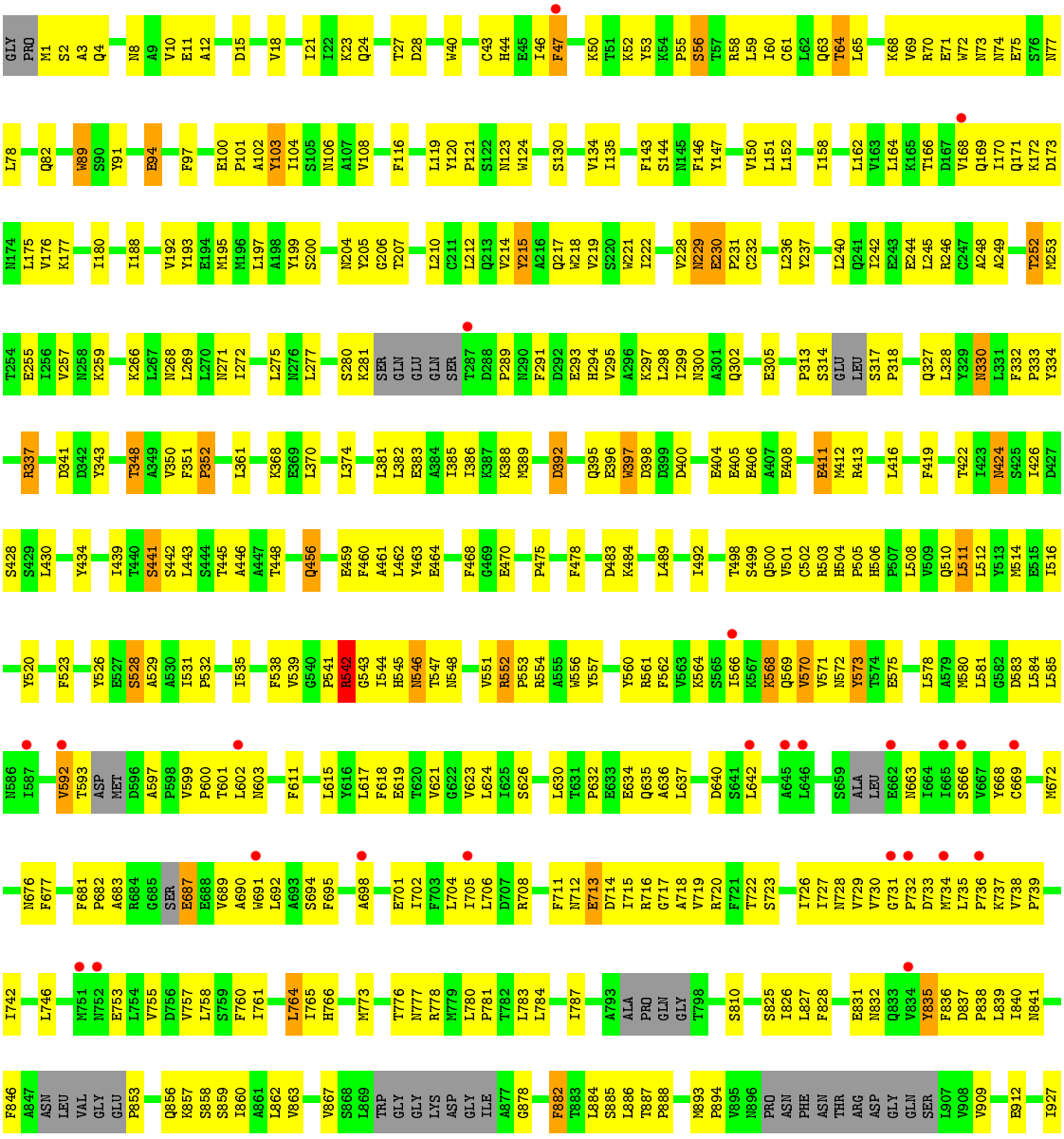
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

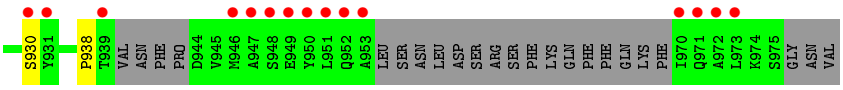
3 Residue-property plots (i)

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: Exportin-T

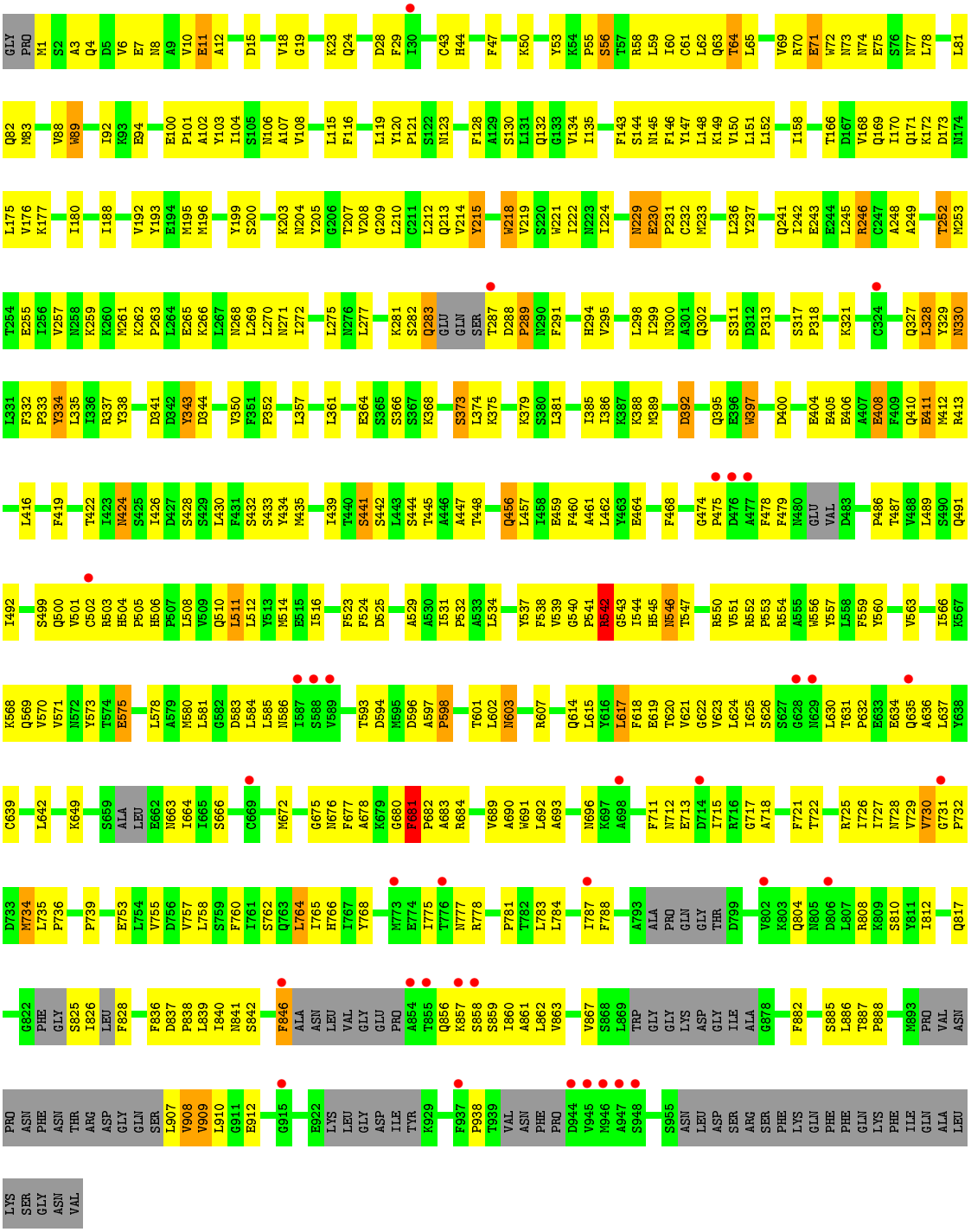
Chain A:





- Molecule 1: Exportin-T

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	119.90Å 130.10Å 173.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.10 49.36 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.90-3.10) 97.8 (49.36-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.313 0.278 , 0.277	Depositor DCC
R_{free} test set	2496 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	88.3	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 104.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 48907 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12876	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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

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

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	0.66	13/6629 (0.2%)	0.73	6/9047 (0.1%)
1	B	0.72	22/6470 (0.3%)	1.06	17/8844 (0.2%)
All	All	0.69	35/13099 (0.3%)	0.91	23/17891 (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	6	0
1	B	8	1
All	All	14	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	681	PHE	CG-CD1	-15.08	1.16	1.38
1	A	552	ARG	NE-CZ	13.02	1.50	1.33
1	B	552	ARG	NE-CZ	12.97	1.50	1.33
1	A	542	ARG	NE-CZ	12.87	1.49	1.33
1	B	70	ARG	NE-CZ	12.31	1.49	1.33
1	A	70	ARG	NE-CZ	12.16	1.48	1.33
1	B	542	ARG	NE-CZ	12.09	1.48	1.33
1	B	681	PHE	CG-CD2	9.42	1.52	1.38
1	B	909	VAL	CA-C	7.91	1.73	1.52
1	B	909	VAL	C-O	7.57	1.37	1.23
1	B	681	PHE	CA-CB	7.35	1.70	1.53
1	B	910	LEU	N-CA	7.27	1.60	1.46
1	B	681	PHE	CA-C	6.51	1.69	1.52
1	B	681	PHE	N-CA	-6.41	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	TYR	CB-CG	-5.91	1.42	1.51
1	A	846	PHE	CB-CG	-5.79	1.41	1.51
1	A	71	GLU	CB-CG	-5.64	1.41	1.52
1	A	230	GLU	CB-CG	-5.63	1.41	1.52
1	A	882	PHE	CB-CG	-5.60	1.41	1.51
1	B	411	GLU	CB-CG	-5.53	1.41	1.52
1	B	882	PHE	CB-CG	-5.50	1.42	1.51
1	B	11	GLU	CB-CG	-5.45	1.41	1.52
1	B	713	GLU	CB-CG	-5.45	1.41	1.52
1	A	411	GLU	CB-CG	-5.39	1.42	1.52
1	B	846	PHE	CB-CG	-5.37	1.42	1.51
1	A	713	GLU	CB-CG	-5.35	1.42	1.52
1	A	75	GLU	CB-CG	-5.30	1.42	1.52
1	B	230	GLU	CB-CG	-5.30	1.42	1.52
1	B	218	TRP	NE1-CE2	5.29	1.44	1.37
1	B	71	GLU	CB-CG	-5.28	1.42	1.52
1	B	575	GLU	CB-CG	-5.26	1.42	1.52
1	B	75	GLU	CB-CG	-5.25	1.42	1.52
1	A	575	GLU	CB-CG	-5.22	1.42	1.52
1	A	11	GLU	CB-CG	-5.20	1.42	1.52
1	B	908	VAL	CA-C	-5.14	1.39	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	681	PHE	CB-CG-CD2	-59.01	79.50	120.80
1	B	681	PHE	CB-CG-CD1	32.74	143.72	120.80
1	B	681	PHE	CB-CA-C	-13.53	83.34	110.40
1	B	908	VAL	CA-C-O	11.99	145.27	120.10
1	B	552	ARG	CD-NE-CZ	-8.88	111.17	123.60
1	B	681	PHE	CG-CD2-CE2	-8.62	111.32	120.80
1	A	542	ARG	CD-NE-CZ	-8.55	111.64	123.60
1	B	542	ARG	CD-NE-CZ	-8.31	111.97	123.60
1	A	70	ARG	CD-NE-CZ	-8.19	112.14	123.60
1	B	681	PHE	N-CA-CB	8.11	125.20	110.60
1	A	552	ARG	CD-NE-CZ	-8.07	112.30	123.60
1	B	908	VAL	O-C-N	-7.95	109.97	122.70
1	B	70	ARG	CD-NE-CZ	-7.80	112.69	123.60
1	B	598	PRO	N-CA-CB	6.15	110.68	103.30
1	A	630	LEU	N-CA-C	-6.01	94.76	111.00
1	B	908	VAL	CA-C-N	-5.95	104.10	117.20
1	A	853	PRO	N-CA-CB	5.86	110.33	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	681	PHE	CD1-CG-CD2	5.81	125.85	118.30
1	B	938	PRO	N-CA-CB	5.76	110.21	103.30
1	B	94	GLU	N-CA-C	-5.61	95.87	111.00
1	B	908	VAL	C-N-CA	-5.57	107.77	121.70
1	A	938	PRO	N-CA-CB	5.54	109.95	103.30
1	B	474	GLY	N-CA-C	-5.23	100.02	113.10

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	46	ILE	CB
1	A	158	ILE	CB
1	A	674	ILE	CB
1	A	761	ILE	CB
1	A	767	ILE	CB
1	A	840	ILE	CB
1	B	46	ILE	CB
1	B	158	ILE	CB
1	B	674	ILE	CB
1	B	726	ILE	CB
1	B	727	ILE	CB
1	B	761	ILE	CB
1	B	787	ILE	CB
1	B	840	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	681	PHE	Sidechain

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	6515	0	5799	454	0
1	B	6357	0	5573	467	1
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
All	All	12876	0	11372	908	1

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 (908) 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:101:PRO:HB2	1:A:103:TYR:CE2	1.58	1.36
1:A:101:PRO:CB	1:A:103:TYR:HE2	1.47	1.27
1:B:683:ALA:HB1	1:B:728:ASN:C	1.52	1.27
1:A:204:ASN:HD22	1:B:204:ASN:CB	1.45	1.26
1:A:204:ASN:ND2	1:B:204:ASN:HB3	1.50	1.26
1:A:716:ARG:O	1:A:720:ARG:HG3	1.43	1.18
1:A:101:PRO:CB	1:A:103:TYR:CE2	2.24	1.16
1:B:205:TYR:HE2	1:B:242:ILE:HD13	1.03	1.16
1:B:683:ALA:CB	1:B:729:VAL:HA	1.77	1.14
1:A:248:ALA:O	1:A:252:THR:HG22	1.46	1.13
1:B:683:ALA:CA	1:B:729:VAL:HA	1.77	1.13
1:A:370:LEU:HD22	1:A:374:LEU:HD23	1.22	1.12
1:B:856:GLN:CG	1:B:909:VAL:HG11	1.80	1.12
1:B:229:ASN:HD22	1:B:229:ASN:C	1.50	1.12
1:A:716:ARG:HB2	1:A:720:ARG:HH21	1.03	1.10
1:B:683:ALA:HB1	1:B:729:VAL:N	1.65	1.09
1:A:511:LEU:HG	1:A:551:VAL:HG13	1.31	1.09
1:A:59:LEU:HD22	1:A:103:TYR:HD1	1.10	1.07
1:B:78:LEU:HG	1:B:82:GLN:NE2	1.69	1.07
1:B:692:LEU:HD22	1:B:730:VAL:HG22	1.35	1.06
1:A:568:LYS:HD2	1:A:568:LYS:H	1.11	1.06
1:A:59:LEU:HD22	1:A:103:TYR:CD1	1.91	1.06
1:B:78:LEU:HG	1:B:82:GLN:HE21	1.15	1.06
1:A:229:ASN:HD22	1:A:229:ASN:C	1.52	1.05
1:A:78:LEU:HG	1:A:82:GLN:HE21	1.20	1.04
1:B:683:ALA:HA	1:B:729:VAL:HA	1.35	1.03
1:B:205:TYR:CE2	1:B:242:ILE:HD13	1.94	1.02
1:B:783:LEU:O	1:B:787:ILE:HG23	1.58	1.02
1:B:229:ASN:HD21	1:B:232:CYS:H	1.04	1.02
1:A:370:LEU:CD2	1:A:374:LEU:HD23	1.89	1.01
1:A:632:PRO:HA	1:A:635:GLN:HG2	1.42	1.01
1:B:692:LEU:HD22	1:B:730:VAL:CG2	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ILE:O	1:A:746:LEU:HG	1.62	0.99
1:A:716:ARG:HB2	1:A:720:ARG:NH2	1.76	0.98
1:A:204:ASN:HD22	1:B:204:ASN:HB3	0.86	0.98
1:A:300:ASN:HD22	1:A:350:VAL:HA	1.29	0.98
1:B:152:LEU:HD13	1:B:214:VAL:HG22	1.43	0.97
1:A:101:PRO:HB2	1:A:103:TYR:CD2	1.99	0.97
1:A:593:THR:HG21	1:A:597:ALA:O	1.64	0.97
1:A:73:ASN:H	1:A:77:ASN:HD22	1.05	0.96
1:A:405:GLU:O	1:A:408:GLU:HG2	1.65	0.96
1:A:878:GLY:O	1:A:882:PHE:CG	2.19	0.96
1:A:368:LYS:HD3	1:A:368:LYS:O	1.65	0.96
1:B:856:GLN:CG	1:B:909:VAL:CG1	2.42	0.96
1:B:300:ASN:HD22	1:B:350:VAL:HA	1.30	0.96
1:A:783:LEU:O	1:A:787:ILE:HG13	1.65	0.95
1:B:837:ASP:HB3	1:B:841:ASN:HD21	1.31	0.95
1:A:758:LEU:HD12	1:A:810:SER:OG	1.65	0.95
1:B:784:LEU:HD22	1:B:839:LEU:HD21	1.49	0.94
1:A:538:PHE:O	1:A:544:ILE:HG13	1.66	0.94
1:A:293:GLU:HG2	1:A:297:LYS:HE3	1.46	0.94
1:B:60:ILE:O	1:B:64:THR:HG22	1.68	0.93
1:B:639:CYS:HG	1:B:681:PHE:HZ	1.06	0.93
1:B:318:PRO:HA	1:B:321:LYS:HB3	1.50	0.93
1:A:229:ASN:HD21	1:A:232:CYS:H	1.01	0.93
1:B:368:LYS:HD3	1:B:368:LYS:O	1.68	0.93
1:A:716:ARG:C	1:A:720:ARG:HE	1.72	0.92
1:A:68:LYS:HE2	1:A:68:LYS:HA	1.49	0.92
1:B:777:ASN:HD21	1:B:826:ILE:CB	1.83	0.92
1:A:78:LEU:HG	1:A:82:GLN:NE2	1.82	0.92
1:B:683:ALA:CB	1:B:729:VAL:CA	2.48	0.91
1:B:683:ALA:HB1	1:B:729:VAL:CA	2.00	0.91
1:A:204:ASN:ND2	1:B:204:ASN:CB	2.20	0.91
1:B:683:ALA:HB1	1:B:728:ASN:O	1.71	0.90
1:B:73:ASN:H	1:B:77:ASN:ND2	1.70	0.90
1:B:248:ALA:O	1:B:252:THR:HG22	1.70	0.90
1:B:257:VAL:O	1:B:266:LYS:HE2	1.73	0.89
1:B:538:PHE:O	1:B:544:ILE:HG13	1.72	0.88
1:A:244:GLU:HB3	1:B:203:LYS:HZ2	1.38	0.88
1:B:104:ILE:O	1:B:108:VAL:HG23	1.72	0.88
1:B:405:GLU:O	1:B:408:GLU:HG3	1.72	0.88
1:B:73:ASN:H	1:B:77:ASN:HD22	0.90	0.88
1:A:568:LYS:CD	1:A:568:LYS:H	1.83	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:HD13	1:A:334:TYR:HB3	1.55	0.88
1:A:784:LEU:HD23	1:A:787:ILE:HD12	1.54	0.88
1:A:672:MET:HE1	1:A:718:ALA:HA	1.55	0.88
1:A:60:ILE:O	1:A:64:THR:HG22	1.73	0.87
1:A:504:HIS:HD2	1:A:506:HIS:H	1.22	0.87
1:A:55:PRO:HB2	1:A:103:TYR:OH	1.74	0.87
1:A:152:LEU:HD13	1:A:214:VAL:HG22	1.57	0.86
1:B:241:GLN:HE21	1:B:283:GLN:NE2	1.73	0.86
1:B:299:ILE:HD13	1:B:334:TYR:HB3	1.57	0.86
1:A:204:ASN:HA	1:B:204:ASN:HA	1.56	0.86
1:B:317:SER:HB2	1:B:318:PRO:HD2	1.56	0.86
1:B:375:LYS:HE2	1:B:379:LYS:NZ	1.90	0.86
1:A:74:ASN:O	1:A:78:LEU:HB2	1.76	0.85
1:B:739:PRO:HD3	1:B:775:ILE:HD13	1.58	0.85
1:A:3:ALA:HB1	1:A:53:TYR:HE2	1.42	0.85
1:B:241:GLN:NE2	1:B:283:GLN:NE2	2.24	0.84
1:B:288:ASP:OD1	1:B:289:PRO:HD2	1.77	0.84
1:B:199:TYR:CD1	1:B:207:THR:HG21	2.12	0.84
1:A:689:VAL:HG13	1:A:691:TRP:CE3	2.13	0.84
1:A:863:VAL:O	1:A:867:VAL:HG23	1.78	0.84
1:A:244:GLU:HB3	1:B:203:LYS:NZ	1.92	0.84
1:B:683:ALA:CB	1:B:729:VAL:N	2.41	0.83
1:B:229:ASN:ND2	1:B:229:ASN:C	2.28	0.83
1:B:416:LEU:HA	1:B:419:PHE:HD1	1.42	0.83
1:A:760:PHE:O	1:A:764:LEU:HB2	1.77	0.83
1:B:504:HIS:HD2	1:B:506:HIS:H	1.27	0.83
1:A:47:PHE:HA	1:A:58:ARG:HG2	1.58	0.83
1:A:229:ASN:C	1:A:229:ASN:ND2	2.30	0.83
1:B:836:PHE:O	1:B:840:ILE:HG23	1.79	0.83
1:B:199:TYR:CE1	1:B:207:THR:HG21	2.14	0.83
1:A:416:LEU:HA	1:A:419:PHE:HD1	1.44	0.83
1:B:205:TYR:CE2	1:B:242:ILE:HG21	2.14	0.82
1:A:738:VAL:N	1:A:739:PRO:HD2	1.94	0.82
1:A:672:MET:HE2	1:A:672:MET:HA	1.62	0.82
1:A:100:GLU:HB3	1:A:101:PRO:HD2	1.62	0.81
1:A:24:GLN:O	1:A:27:THR:HG22	1.80	0.81
1:A:1:MET:HG3	1:A:4:GLN:H	1.44	0.81
1:A:566:ILE:CG2	1:A:569:GLN:HB2	2.10	0.81
1:B:683:ALA:CB	1:B:728:ASN:C	2.45	0.81
1:A:528:SER:O	1:A:531:ILE:HG13	1.81	0.81
1:B:65:LEU:O	1:B:69:VAL:HG23	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PRO:CG	1:A:103:TYR:HE2	1.94	0.81
1:A:229:ASN:ND2	1:A:232:CYS:H	1.79	0.80
1:A:104:ILE:O	1:A:108:VAL:HG23	1.80	0.80
1:A:713:GLU:HA	1:A:716:ARG:HG3	1.63	0.80
1:A:215:TYR:O	1:A:219:VAL:HG23	1.81	0.80
1:B:59:LEU:HD22	1:B:103:TYR:CD1	2.16	0.80
1:A:640:ASP:OD1	1:A:694:SER:HB3	1.81	0.80
1:B:570:VAL:HG12	1:B:570:VAL:O	1.80	0.80
1:B:375:LYS:HG2	1:B:379:LYS:HE3	1.62	0.80
1:A:171:GLN:O	1:A:175:LEU:HG	1.82	0.79
1:B:681:PHE:HB3	1:B:682:PRO:HD2	1.65	0.79
1:A:859:SER:HA	1:A:862:LEU:HD12	1.65	0.78
1:B:683:ALA:HB1	1:B:729:VAL:HA	1.57	0.78
1:A:831:GLU:O	1:A:835:TYR:CE1	2.36	0.78
1:A:370:LEU:HD22	1:A:374:LEU:CD2	2.09	0.78
1:B:44:HIS:HE1	1:B:83:MET:HG2	1.48	0.78
1:B:166:THR:HG22	1:B:168:VAL:H	1.48	0.78
1:A:411:GLU:CG	1:A:412:MET:N	2.47	0.77
1:A:836:PHE:O	1:A:840:ILE:HG23	1.84	0.77
1:B:837:ASP:HB3	1:B:841:ASN:ND2	1.99	0.77
1:A:737:LYS:C	1:A:739:PRO:HD2	2.05	0.77
1:B:3:ALA:HB1	1:B:53:TYR:HE2	1.49	0.77
1:A:43:CYS:SG	1:A:64:THR:HG21	2.25	0.77
1:A:722:THR:HG22	1:A:726:ILE:HD12	1.67	0.77
1:A:716:ARG:O	1:A:720:ARG:CG	2.31	0.77
1:B:784:LEU:CD2	1:B:839:LEU:HD21	2.15	0.77
1:A:55:PRO:HB3	1:A:104:ILE:HD11	1.66	0.76
1:A:704:LEU:O	1:A:708:ARG:CG	2.33	0.76
1:A:55:PRO:CB	1:A:103:TYR:OH	2.34	0.76
1:A:593:THR:HG23	1:A:599:VAL:O	1.86	0.76
1:A:539:VAL:HG12	1:A:539:VAL:O	1.84	0.76
1:A:120:TYR:HA	1:A:124:TRP:HB3	1.66	0.76
1:A:856:GLN:O	1:A:860:ILE:HG23	1.86	0.76
1:B:246:ARG:HD3	1:B:291:PHE:CD1	2.21	0.75
1:A:733:ASP:O	1:A:736:PRO:HD2	1.87	0.75
1:A:570:VAL:O	1:A:570:VAL:HG12	1.87	0.75
1:B:300:ASN:HD21	1:B:352:PRO:HD2	1.52	0.75
1:B:539:VAL:HG12	1:B:539:VAL:O	1.86	0.74
1:A:885:SER:C	1:A:888:PRO:HD2	2.08	0.74
1:B:271:ASN:HA	1:B:327:GLN:NE2	2.02	0.74
1:B:229:ASN:ND2	1:B:232:CYS:H	1.82	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ILE:CD1	1:B:334:TYR:HB3	2.18	0.74
1:A:778:ARG:O	1:A:781:PRO:HD2	1.86	0.74
1:A:731:GLY:N	1:A:732:PRO:HD2	2.01	0.74
1:B:130:SER:O	1:B:134:VAL:HG23	1.86	0.74
1:A:632:PRO:HA	1:A:635:GLN:CG	2.17	0.74
1:B:625:ILE:HG21	1:B:639:CYS:SG	2.28	0.74
1:A:689:VAL:HG22	1:A:691:TRP:CH2	2.23	0.74
1:B:727:ILE:HG22	1:B:734:MET:HB3	1.70	0.74
1:A:73:ASN:H	1:A:77:ASN:ND2	1.83	0.74
1:A:229:ASN:HD21	1:A:232:CYS:N	1.84	0.73
1:B:73:ASN:N	1:B:77:ASN:HD22	1.76	0.73
1:A:230:GLU:N	1:A:231:PRO:HD2	2.02	0.73
1:B:171:GLN:O	1:B:175:LEU:HG	1.89	0.73
1:B:636:ALA:HB2	1:B:690:ALA:HB1	1.69	0.73
1:A:777:ASN:HD21	1:A:826:ILE:CB	2.01	0.73
1:B:722:THR:O	1:B:726:ILE:HG23	1.88	0.73
1:B:500:GLN:CD	1:B:500:GLN:H	1.92	0.73
1:B:58:ARG:NH1	1:B:100:GLU:OE1	2.21	0.72
1:A:566:ILE:HG22	1:A:569:GLN:HB2	1.70	0.72
1:B:329:TYR:CE1	1:B:373:SER:OG	2.41	0.72
1:B:860:ILE:CD1	1:B:912:GLU:CB	2.68	0.72
1:B:762:SER:HA	1:B:817:GLN:HE22	1.54	0.72
1:A:672:MET:CE	1:A:672:MET:HA	2.20	0.72
1:B:860:ILE:HD11	1:B:912:GLU:CB	2.20	0.71
1:B:61:CYS:O	1:B:64:THR:HG23	1.90	0.71
1:A:257:VAL:O	1:A:266:LYS:HE2	1.91	0.71
1:B:626:SER:HB2	1:B:682:PRO:CD	2.21	0.71
1:B:568:LYS:O	1:B:571:VAL:HG23	1.90	0.71
1:A:389:MET:CE	1:A:413:ARG:HG2	2.21	0.71
1:B:544:ILE:HG23	1:B:556:TRP:CD1	2.26	0.71
1:B:50:LYS:HA	1:B:58:ARG:NH2	2.06	0.71
1:A:173:ASP:O	1:A:177:LYS:HG3	1.92	0.70
1:B:329:TYR:HE1	1:B:373:SER:HG	1.39	0.70
1:A:511:LEU:HG	1:A:551:VAL:CG1	2.17	0.70
1:A:386:ILE:HG23	1:A:460:PHE:CZ	2.26	0.70
1:A:169:GLN:NE2	1:A:173:ASP:OD2	2.25	0.70
1:B:259:LYS:HB3	1:B:261:MET:CE	2.22	0.70
1:A:682:PRO:O	1:A:729:VAL:HG22	1.92	0.70
1:B:257:VAL:O	1:B:266:LYS:CE	2.39	0.69
1:A:702:ILE:O	1:A:706:LEU:N	2.25	0.69
1:B:50:LYS:O	1:B:58:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ILE:HA	1:B:718:ALA:HB3	1.73	0.69
1:B:885:SER:O	1:B:888:PRO:HD2	1.92	0.69
1:A:59:LEU:O	1:A:63:GLN:HG3	1.92	0.69
1:A:271:ASN:HA	1:A:327:GLN:NE2	2.07	0.68
1:A:130:SER:O	1:A:134:VAL:HG23	1.93	0.68
1:A:546:ASN:HD22	1:A:547:THR:N	1.91	0.68
1:A:717:GLY:N	1:A:720:ARG:HE	1.92	0.68
1:B:375:LYS:HE2	1:B:379:LYS:HZ1	1.57	0.68
1:B:731:GLY:N	1:B:732:PRO:HD2	2.08	0.68
1:A:727:ILE:HG23	1:A:734:MET:CB	2.23	0.68
1:A:293:GLU:O	1:A:297:LYS:HG3	1.93	0.68
1:A:177:LYS:HE2	1:A:221:TRP:HB3	1.76	0.68
1:A:503:ARG:HA	1:A:542:ARG:CZ	2.22	0.68
1:A:3:ALA:HB1	1:A:53:TYR:CE2	2.28	0.68
1:B:299:ILE:HD13	1:B:334:TYR:CB	2.24	0.67
1:B:683:ALA:O	1:B:684:ARG:C	2.30	0.67
1:B:836:PHE:CE2	1:B:840:ILE:HG21	2.29	0.67
1:B:546:ASN:HD22	1:B:547:THR:N	1.92	0.67
1:B:215:TYR:O	1:B:219:VAL:HG23	1.94	0.67
1:A:504:HIS:CD2	1:A:506:HIS:H	2.11	0.67
1:A:104:ILE:HG22	1:A:104:ILE:O	1.94	0.67
1:A:1:MET:HB3	1:A:4:GLN:HB2	1.76	0.66
1:A:300:ASN:HD21	1:A:352:PRO:HD2	1.60	0.66
1:A:102:ALA:O	1:A:106:ASN:ND2	2.28	0.66
1:B:188:ILE:O	1:B:192:VAL:HG23	1.94	0.66
1:A:44:HIS:CD2	1:A:44:HIS:O	2.48	0.66
1:A:101:PRO:HB3	1:A:103:TYR:CE2	2.27	0.66
1:A:389:MET:HE3	1:A:413:ARG:HG2	1.78	0.66
1:A:299:ILE:CD1	1:A:334:TYR:HB3	2.24	0.66
1:B:731:GLY:HA3	1:B:768:TYR:CE2	2.30	0.66
1:B:177:LYS:HE2	1:B:221:TRP:HB3	1.77	0.66
1:A:405:GLU:HB2	1:A:408:GLU:OE2	1.96	0.66
1:B:885:SER:O	1:B:888:PRO:CD	2.44	0.66
1:A:689:VAL:HG13	1:A:691:TRP:CD2	2.31	0.66
1:B:506:HIS:O	1:B:510:GLN:HG3	1.96	0.65
1:A:119:LEU:HB3	1:A:123:ASN:HB2	1.78	0.65
1:A:713:GLU:CA	1:A:716:ARG:HG3	2.26	0.65
1:A:68:LYS:HE2	1:A:68:LYS:CA	2.24	0.65
1:A:831:GLU:O	1:A:835:TYR:HE1	1.78	0.65
1:B:411:GLU:CG	1:B:412:MET:N	2.59	0.65
1:B:44:HIS:CD2	1:B:44:HIS:O	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:LEU:HD22	1:A:676:ASN:HD22	1.60	0.65
1:A:408:GLU:O	1:A:411:GLU:CG	2.44	0.65
1:B:836:PHE:CZ	1:B:840:ILE:HG21	2.31	0.65
1:A:753:GLU:O	1:A:757:VAL:HG23	1.97	0.65
1:A:683:ALA:HB1	1:A:728:ASN:OD1	1.97	0.65
1:B:229:ASN:HD21	1:B:232:CYS:N	1.85	0.65
1:A:758:LEU:HD12	1:A:810:SER:CB	2.27	0.64
1:B:886:LEU:C	1:B:888:PRO:HD2	2.17	0.64
1:A:773:MET:HE2	1:A:773:MET:HA	1.79	0.64
1:B:230:GLU:N	1:B:231:PRO:HD2	2.12	0.64
1:B:288:ASP:OD1	1:B:289:PRO:CD	2.46	0.64
1:A:204:ASN:HD22	1:B:204:ASN:HB2	1.53	0.64
1:A:44:HIS:HD2	1:A:44:HIS:O	1.79	0.64
1:B:50:LYS:HA	1:B:58:ARG:CZ	2.27	0.64
1:B:672:MET:HE2	1:B:672:MET:HA	1.79	0.64
1:B:566:ILE:HG22	1:B:569:GLN:HG3	1.79	0.64
1:B:408:GLU:O	1:B:411:GLU:CG	2.46	0.64
1:A:689:VAL:CG1	1:A:691:TRP:CD2	2.80	0.64
1:A:611:PHE:CZ	1:A:669:CYS:HB2	2.32	0.64
1:A:237:TYR:OH	1:A:277:LEU:HD23	1.98	0.64
1:B:856:GLN:HB3	1:B:909:VAL:HG21	1.80	0.64
1:A:695:PHE:O	1:A:698:ALA:HB3	1.98	0.64
1:A:299:ILE:HD13	1:A:334:TYR:CB	2.27	0.63
1:B:218:TRP:O	1:B:222:ILE:HG13	1.98	0.63
1:B:74:ASN:O	1:B:78:LEU:HB2	1.98	0.63
1:B:758:LEU:HD12	1:B:810:SER:CB	2.28	0.63
1:A:825:SER:HA	1:A:828:PHE:CD1	2.33	0.63
1:B:100:GLU:HB3	1:B:101:PRO:HD2	1.79	0.63
1:A:400:ASP:HB3	1:A:404:GLU:HB2	1.81	0.63
1:B:311:SER:O	1:B:313:PRO:HD3	1.98	0.63
1:A:58:ARG:HH12	1:A:100:GLU:CD	2.02	0.63
1:A:204:ASN:ND2	1:B:204:ASN:HB2	2.11	0.63
1:A:780:LEU:HB2	1:A:781:PRO:HD3	1.80	0.63
1:A:780:LEU:O	1:A:784:LEU:HG	1.97	0.63
1:B:152:LEU:HD13	1:B:214:VAL:CG2	2.25	0.63
1:B:784:LEU:HB3	1:B:788:PHE:HE1	1.62	0.63
1:B:784:LEU:O	1:B:788:PHE:HD1	1.82	0.63
1:A:294:HIS:HA	1:A:297:LYS:HD2	1.80	0.63
1:B:173:ASP:O	1:B:177:LYS:HG3	1.98	0.63
1:A:687:GLU:OE1	1:A:687:GLU:N	2.32	0.63
1:A:47:PHE:O	1:A:58:ARG:HD3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASN:ND2	1:B:352:PRO:HD2	2.14	0.62
1:B:44:HIS:O	1:B:44:HIS:HD2	1.80	0.62
1:B:837:ASP:HB2	1:B:838:PRO:CD	2.28	0.62
1:B:734:MET:HA	1:B:734:MET:CE	2.30	0.62
1:B:43:CYS:SG	1:B:64:THR:HG21	2.40	0.62
1:B:681:PHE:HB3	1:B:682:PRO:CD	2.28	0.62
1:A:566:ILE:O	1:A:566:ILE:HG22	1.99	0.62
1:A:528:SER:HB2	1:A:531:ILE:HD11	1.80	0.62
1:A:722:THR:HG22	1:A:726:ILE:CD1	2.29	0.62
1:B:784:LEU:O	1:B:788:PHE:CD1	2.53	0.62
1:A:385:ILE:HG23	1:A:416:LEU:HD22	1.82	0.62
1:A:601:THR:HG22	1:A:602:LEU:N	2.15	0.62
1:A:101:PRO:CB	1:A:103:TYR:CD2	2.70	0.62
1:A:742:ILE:O	1:A:746:LEU:CG	2.42	0.62
1:A:570:VAL:HG22	1:A:573:TYR:HB2	1.81	0.62
1:A:544:ILE:HG23	1:A:556:TRP:CD1	2.35	0.62
1:B:241:GLN:HE21	1:B:283:GLN:HE21	1.48	0.62
1:A:689:VAL:CG1	1:A:690:ALA:N	2.63	0.62
1:B:570:VAL:HA	1:B:573:TYR:HD1	1.64	0.62
1:B:730:VAL:HG12	1:B:730:VAL:O	2.00	0.61
1:A:177:LYS:HE2	1:A:221:TRP:CB	2.30	0.61
1:B:762:SER:HA	1:B:817:GLN:NE2	2.16	0.61
1:A:546:ASN:HD22	1:A:547:THR:H	1.47	0.61
1:A:119:LEU:CB	1:A:123:ASN:HB2	2.31	0.61
1:A:370:LEU:CD2	1:A:374:LEU:CD2	2.74	0.61
1:A:568:LYS:HD2	1:A:568:LYS:N	1.97	0.61
1:B:3:ALA:HB1	1:B:53:TYR:CE2	2.34	0.61
1:A:52:LYS:HD2	1:A:53:TYR:HE1	1.65	0.61
1:A:411:GLU:CG	1:A:412:MET:H	2.14	0.60
1:A:500:GLN:HB2	1:A:503:ARG:HE	1.66	0.60
1:B:566:ILE:CG2	1:B:569:GLN:HG3	2.31	0.60
1:B:632:PRO:HA	1:B:635:GLN:HG2	1.82	0.60
1:B:753:GLU:O	1:B:757:VAL:HG23	2.01	0.60
1:B:777:ASN:ND2	1:B:826:ILE:CB	2.61	0.60
1:A:636:ALA:HB2	1:A:690:ALA:HB1	1.83	0.60
1:A:50:LYS:HA	1:A:58:ARG:NH2	2.17	0.60
1:A:204:ASN:HA	1:B:204:ASN:CA	2.28	0.60
1:A:689:VAL:HG12	1:A:692:LEU:H	1.67	0.60
1:B:241:GLN:NE2	1:B:283:GLN:HE21	1.99	0.60
1:A:27:THR:HG23	1:A:28:ASP:N	2.16	0.60
1:A:386:ILE:HD12	1:A:434:TYR:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:PHE:HB3	1:A:682:PRO:HD2	1.84	0.60
1:B:406:GLU:O	1:B:410:GLN:HG2	2.01	0.60
1:A:100:GLU:HB3	1:A:101:PRO:CD	2.30	0.60
1:A:738:VAL:N	1:A:739:PRO:CD	2.65	0.60
1:B:837:ASP:O	1:B:841:ASN:N	2.30	0.60
1:B:400:ASP:O	1:B:404:GLU:CB	2.50	0.60
1:A:784:LEU:HA	1:A:787:ILE:HD12	1.84	0.59
1:A:68:LYS:HA	1:A:68:LYS:CE	2.28	0.59
1:A:602:LEU:HD22	1:A:714:ASP:OD2	2.02	0.59
1:A:835:TYR:O	1:A:838:PRO:HG2	2.02	0.59
1:B:259:LYS:HB3	1:B:261:MET:HE2	1.85	0.59
1:B:546:ASN:HD22	1:B:547:THR:H	1.49	0.59
1:A:499:SER:HB2	1:A:501:VAL:HG23	1.83	0.59
1:A:229:ASN:HD22	1:A:230:GLU:N	2.00	0.59
1:B:649:LYS:HE2	1:B:666:SER:OG	2.02	0.59
1:B:271:ASN:CA	1:B:327:GLN:NE2	2.66	0.59
1:B:147:TYR:CZ	1:B:151:LEU:HD11	2.38	0.59
1:A:61:CYS:O	1:A:64:THR:HG23	2.03	0.59
1:B:731:GLY:HA3	1:B:768:TYR:CZ	2.38	0.58
1:A:592:VAL:HG12	1:A:593:THR:N	2.18	0.58
1:B:570:VAL:CG1	1:B:570:VAL:O	2.49	0.58
1:A:176:VAL:O	1:A:180:ILE:HG13	2.03	0.58
1:A:687:GLU:N	1:A:687:GLU:CD	2.56	0.58
1:A:506:HIS:O	1:A:510:GLN:HG3	2.03	0.58
1:B:689:VAL:HG12	1:B:691:TRP:H	1.67	0.58
1:A:249:ALA:O	1:A:253:MET:HG3	2.03	0.58
1:B:672:MET:HE1	1:B:718:ALA:HA	1.86	0.58
1:B:15:ASP:HB3	1:B:18:VAL:HG23	1.85	0.58
1:A:249:ALA:O	1:A:252:THR:HG23	2.04	0.58
1:B:229:ASN:HD22	1:B:230:GLU:N	2.02	0.58
1:A:837:ASP:O	1:A:841:ASN:ND2	2.36	0.58
1:A:397:TRP:HE3	1:A:406:GLU:OE2	1.85	0.58
1:B:199:TYR:CD1	1:B:207:THR:CG2	2.86	0.58
1:B:575:GLU:CG	1:B:630:LEU:HD21	2.33	0.58
1:B:615:LEU:HD22	1:B:676:ASN:HD22	1.68	0.58
1:B:462:LEU:HD11	1:B:501:VAL:CG1	2.33	0.58
1:B:860:ILE:HD12	1:B:912:GLU:CB	2.34	0.58
1:A:727:ILE:O	1:A:731:GLY:HA2	2.04	0.58
1:B:158:ILE:CG1	1:B:177:LYS:HG2	2.34	0.58
1:B:489:LEU:O	1:B:492:ILE:HB	2.04	0.57
1:A:689:VAL:HG12	1:A:690:ALA:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:GLU:O	1:A:705:ILE:N	2.37	0.57
1:B:361:LEU:HB3	1:B:426:ILE:HD13	1.85	0.57
1:A:640:ASP:OD1	1:A:694:SER:CB	2.51	0.57
1:B:636:ALA:HB2	1:B:690:ALA:CB	2.35	0.57
1:A:857:LYS:O	1:A:860:ILE:HG12	2.04	0.57
1:B:456:GLN:H	1:B:456:GLN:NE2	2.02	0.57
1:A:337:ARG:O	1:A:337:ARG:HD2	2.03	0.57
1:A:592:VAL:HG12	1:A:593:THR:H	1.68	0.57
1:B:783:LEU:C	1:B:787:ILE:HG23	2.25	0.57
1:A:731:GLY:N	1:A:732:PRO:CD	2.68	0.57
1:B:825:SER:HA	1:B:828:PHE:CD1	2.38	0.57
1:A:300:ASN:ND2	1:A:350:VAL:HA	2.10	0.57
1:B:566:ILE:HG21	1:B:569:GLN:CD	2.24	0.57
1:B:120:TYR:OH	1:B:180:ILE:HA	2.05	0.57
1:A:317:SER:HB2	1:A:318:PRO:HD2	1.87	0.57
1:A:103:TYR:HD2	1:A:103:TYR:H	1.53	0.57
1:A:884:LEU:O	1:A:887:THR:HB	2.04	0.57
1:A:277:LEU:HD11	1:A:302:GLN:HE22	1.69	0.57
1:B:177:LYS:HE2	1:B:221:TRP:CB	2.34	0.57
1:B:385:ILE:HG23	1:B:416:LEU:HD22	1.87	0.56
1:A:212:LEU:HD22	1:A:252:THR:HG21	1.86	0.56
1:B:504:HIS:CD2	1:B:506:HIS:H	2.15	0.56
1:A:884:LEU:O	1:A:888:PRO:HD3	2.04	0.56
1:A:885:SER:O	1:A:888:PRO:HD2	2.04	0.56
1:B:683:ALA:HA	1:B:729:VAL:CA	2.24	0.56
1:A:735:LEU:N	1:A:736:PRO:CD	2.68	0.56
1:B:499:SER:HB3	1:B:501:VAL:HG23	1.87	0.56
1:B:424:ASN:HD22	1:B:428:SER:HA	1.71	0.56
1:B:544:ILE:HG23	1:B:556:TRP:HD1	1.70	0.56
1:B:329:TYR:HE1	1:B:373:SER:OG	1.83	0.56
1:A:271:ASN:CA	1:A:327:GLN:NE2	2.69	0.56
1:A:619:GLU:O	1:A:623:VAL:HG23	2.05	0.56
1:B:619:GLU:O	1:B:623:VAL:HG23	2.05	0.56
1:B:145:ASN:O	1:B:149:LYS:HG3	2.05	0.56
1:A:784:LEU:HD13	1:A:839:LEU:HD11	1.88	0.56
1:A:416:LEU:HA	1:A:419:PHE:CD1	2.34	0.56
1:A:835:TYR:N	1:A:835:TYR:CD1	2.74	0.56
1:A:835:TYR:O	1:A:839:LEU:HG	2.06	0.56
1:A:120:TYR:N	1:A:121:PRO:HD2	2.20	0.56
1:A:634:GLU:O	1:A:637:LEU:N	2.38	0.56
1:A:778:ARG:C	1:A:781:PRO:HD2	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:ILE:O	1:A:731:GLY:CA	2.54	0.56
1:B:559:PHE:O	1:B:563:VAL:HG23	2.06	0.56
1:B:405:GLU:O	1:B:408:GLU:CG	2.52	0.56
1:B:762:SER:CA	1:B:817:GLN:HE22	2.19	0.56
1:B:601:THR:HG22	1:B:603:ASN:H	1.70	0.56
1:A:361:LEU:HB3	1:A:426:ILE:HD13	1.87	0.56
1:B:856:GLN:HB3	1:B:909:VAL:CG2	2.35	0.55
1:A:230:GLU:H	1:A:231:PRO:HD2	1.70	0.55
1:A:717:GLY:N	1:A:720:ARG:NE	2.54	0.55
1:B:241:GLN:NE2	1:B:283:GLN:HE22	2.04	0.55
1:B:462:LEU:HD11	1:B:501:VAL:HG11	1.87	0.55
1:A:498:THR:O	1:A:498:THR:HG22	2.06	0.55
1:B:856:GLN:CG	1:B:909:VAL:HG13	2.31	0.55
1:B:241:GLN:HE21	1:B:283:GLN:HE22	1.53	0.55
1:B:195:MET:CE	1:B:199:TYR:HE1	2.19	0.55
1:A:566:ILE:HG23	1:A:569:GLN:HB2	1.89	0.55
1:B:219:VAL:O	1:B:259:LYS:HE2	2.06	0.55
1:B:424:ASN:ND2	1:B:428:SER:HA	2.22	0.55
1:A:269:LEU:HA	1:A:272:ILE:HD12	1.89	0.55
1:B:295:VAL:HG11	1:B:338:TYR:OH	2.07	0.55
1:A:430:LEU:O	1:A:430:LEU:HD12	2.07	0.55
1:B:330:ASN:HD22	1:B:330:ASN:N	2.05	0.55
1:A:511:LEU:HD21	1:A:554:ARG:HG2	1.89	0.55
1:B:389:MET:CE	1:B:413:ARG:HG2	2.37	0.55
1:B:335:LEU:HD12	1:B:350:VAL:HG11	1.88	0.55
1:A:293:GLU:HG2	1:A:297:LYS:CE	2.28	0.55
1:B:634:GLU:O	1:B:637:LEU:N	2.39	0.55
1:B:334:TYR:CD1	1:B:334:TYR:N	2.75	0.54
1:A:570:VAL:CG1	1:A:570:VAL:O	2.54	0.54
1:B:259:LYS:HB3	1:B:261:MET:HE3	1.89	0.54
1:B:812:ILE:CB	1:B:862:LEU:HD11	2.37	0.54
1:B:55:PRO:HB3	1:B:104:ILE:HD11	1.89	0.54
1:A:578:LEU:HD21	1:A:624:LEU:HB2	1.90	0.54
1:A:412:MET:HG2	1:A:412:MET:O	2.06	0.54
1:A:887:THR:N	1:A:888:PRO:HD2	2.23	0.54
1:A:445:THR:O	1:A:448:THR:HB	2.08	0.54
1:B:622:GLY:C	1:B:680:GLY:O	2.46	0.54
1:B:511:LEU:HD21	1:B:554:ARG:HG2	1.89	0.54
1:A:158:ILE:CG1	1:A:177:LYS:HG2	2.38	0.54
1:B:539:VAL:CG1	1:B:539:VAL:O	2.55	0.54
1:B:541:PRO:O	1:B:546:ASN:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TRP:O	1:A:222:ILE:HG13	2.08	0.54
1:B:416:LEU:HA	1:B:419:PHE:CD1	2.32	0.54
1:A:330:ASN:HD22	1:A:330:ASN:N	2.05	0.54
1:B:626:SER:CB	1:B:682:PRO:HD3	2.38	0.54
1:A:172:LYS:O	1:A:176:VAL:HG23	2.07	0.54
1:B:626:SER:CB	1:B:682:PRO:CD	2.85	0.54
1:B:50:LYS:CA	1:B:58:ARG:NH2	2.71	0.54
1:B:271:ASN:CA	1:B:327:GLN:HE22	2.21	0.54
1:B:525:ASP:OD1	1:B:566:ILE:HG12	2.07	0.54
1:B:727:ILE:O	1:B:731:GLY:N	2.41	0.53
1:A:94:GLU:OE1	1:A:94:GLU:HA	2.08	0.53
1:B:158:ILE:CG1	1:B:177:LYS:HE3	2.37	0.53
1:B:88:VAL:O	1:B:92:ILE:HG13	2.09	0.53
1:B:541:PRO:HA	1:B:545:HIS:HB2	1.91	0.53
1:B:858:SER:O	1:B:861:ALA:HB3	2.08	0.53
1:B:503:ARG:HA	1:B:542:ARG:CZ	2.38	0.53
1:B:531:ILE:HD12	1:B:569:GLN:OE1	2.09	0.53
1:B:116:PHE:CE1	1:B:120:TYR:CD1	2.97	0.53
1:B:804:GLN:O	1:B:808:ARG:N	2.39	0.53
1:B:255:GLU:OE1	1:B:255:GLU:HA	2.08	0.53
1:A:58:ARG:NH1	1:A:100:GLU:OE1	2.39	0.53
1:A:300:ASN:ND2	1:A:352:PRO:HD2	2.21	0.53
1:A:271:ASN:CA	1:A:327:GLN:HE22	2.22	0.53
1:B:859:SER:HA	1:B:862:LEU:HD12	1.91	0.53
1:A:197:LEU:O	1:A:200:SER:HB3	2.09	0.53
1:A:557:TYR:O	1:A:560:TYR:HB3	2.09	0.53
1:A:773:MET:O	1:A:776:THR:HB	2.09	0.53
1:A:237:TYR:O	1:A:240:LEU:HB2	2.09	0.53
1:A:593:THR:CG2	1:A:597:ALA:O	2.48	0.53
1:B:102:ALA:O	1:B:106:ASN:ND2	2.42	0.53
1:A:499:SER:CB	1:A:501:VAL:HG23	2.38	0.52
1:B:412:MET:HG2	1:B:412:MET:O	2.08	0.52
1:B:479:PHE:HA	1:B:486:PRO:HA	1.91	0.52
1:A:734:MET:C	1:A:736:PRO:HD2	2.29	0.52
1:B:448:THR:HG22	1:B:448:THR:O	2.09	0.52
1:B:135:ILE:HG12	1:B:143:PHE:HD2	1.75	0.52
1:A:689:VAL:HG12	1:A:691:TRP:N	2.25	0.52
1:B:386:ILE:HD12	1:B:434:TYR:HE2	1.74	0.52
1:B:386:ILE:HG23	1:B:460:PHE:CZ	2.44	0.52
1:A:219:VAL:O	1:A:259:LYS:HE2	2.09	0.52
1:A:860:ILE:HD11	1:A:912:GLU:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:O	1:B:176:VAL:HG23	2.10	0.52
1:B:392:ASP:O	1:B:395:GLN:O	2.28	0.52
1:B:846:PHE:CG	1:B:846:PHE:O	2.61	0.52
1:A:737:LYS:C	1:A:739:PRO:CD	2.78	0.52
1:A:24:GLN:O	1:A:27:THR:CG2	2.55	0.52
1:B:887:THR:N	1:B:888:PRO:CD	2.73	0.52
1:A:489:LEU:O	1:A:492:ILE:HB	2.10	0.52
1:A:242:ILE:O	1:A:246:ARG:HB3	2.09	0.52
1:B:783:LEU:O	1:B:787:ILE:CG2	2.45	0.52
1:A:478:PHE:CE2	1:A:523:PHE:HB2	2.44	0.52
1:B:578:LEU:HD21	1:B:624:LEU:HB2	1.92	0.52
1:A:65:LEU:O	1:A:69:VAL:HG23	2.08	0.52
1:B:249:ALA:O	1:B:252:THR:HG23	2.09	0.52
1:B:593:THR:HG22	1:B:594:ASP:N	2.25	0.52
1:A:101:PRO:HG2	1:A:103:TYR:HE2	1.73	0.52
1:A:716:ARG:CB	1:A:720:ARG:NH2	2.63	0.52
1:B:712:ASN:CB	1:B:715:ILE:HD12	2.40	0.52
1:A:162:LEU:HG	1:A:164:LEU:H	1.75	0.52
1:B:193:TYR:CD2	1:B:193:TYR:C	2.83	0.52
1:A:712:ASN:O	1:A:716:ARG:HG3	2.10	0.51
1:A:544:ILE:CG2	1:A:584:LEU:HD13	2.40	0.51
1:A:734:MET:C	1:A:736:PRO:CD	2.78	0.51
1:B:422:THR:O	1:B:426:ILE:HG13	2.09	0.51
1:B:445:THR:O	1:B:448:THR:HB	2.10	0.51
1:A:341:ASP:O	1:A:388:LYS:HE3	2.11	0.51
1:A:389:MET:HE2	1:A:413:ARG:HG2	1.90	0.51
1:B:69:VAL:HG11	1:B:115:LEU:HD23	1.92	0.51
1:A:398:ASP:OD2	1:A:404:GLU:OE2	2.29	0.51
1:A:514:MET:CE	1:A:543:GLY:HA2	2.40	0.51
1:B:166:THR:O	1:B:170:ILE:HG13	2.11	0.51
1:A:15:ASP:HB3	1:A:18:VAL:HG23	1.93	0.51
1:B:119:LEU:HB3	1:B:123:ASN:HB2	1.93	0.51
1:B:570:VAL:HA	1:B:573:TYR:CD1	2.46	0.51
1:B:731:GLY:N	1:B:732:PRO:CD	2.73	0.51
1:A:146:PHE:O	1:A:150:VAL:HG23	2.11	0.51
1:B:838:PRO:O	1:B:842:SER:CB	2.59	0.51
1:B:550:ARG:O	1:B:553:PRO:HD2	2.11	0.51
1:B:58:ARG:HH12	1:B:100:GLU:CD	2.14	0.51
1:A:193:TYR:C	1:A:193:TYR:CD2	2.84	0.51
1:B:72:TRP:HE3	1:B:81:LEU:HD23	1.76	0.51
1:A:147:TYR:CZ	1:A:151:LEU:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:O	1:B:180:ILE:HG13	2.11	0.51
1:A:672:MET:CE	1:A:718:ALA:HA	2.36	0.50
1:B:147:TYR:CE2	1:B:151:LEU:HD11	2.47	0.50
1:A:825:SER:HA	1:A:828:PHE:HD1	1.73	0.50
1:B:514:MET:CE	1:B:543:GLY:HA2	2.41	0.50
1:A:672:MET:CA	1:A:672:MET:CE	2.90	0.50
1:A:689:VAL:CG1	1:A:691:TRP:H	2.25	0.50
1:B:350:VAL:HG12	1:B:350:VAL:O	2.11	0.50
1:A:636:ALA:O	1:A:640:ASP:CG	2.50	0.50
1:A:615:LEU:HD13	1:A:676:ASN:HD21	1.76	0.50
1:B:462:LEU:O	1:B:516:ILE:HD11	2.11	0.50
1:A:188:ILE:O	1:A:192:VAL:HG23	2.10	0.50
1:A:413:ARG:NH2	1:A:459:GLU:OE1	2.43	0.50
1:B:389:MET:HE2	1:B:413:ARG:HG2	1.94	0.50
1:A:514:MET:HE3	1:A:543:GLY:HA2	1.94	0.50
1:A:268:ASN:O	1:A:272:ILE:HG13	2.11	0.50
1:B:857:LYS:HA	1:B:860:ILE:HD11	1.92	0.50
1:A:531:ILE:O	1:A:535:ILE:HD12	2.12	0.50
1:A:230:GLU:N	1:A:231:PRO:CD	2.74	0.50
1:A:334:TYR:CD1	1:A:334:TYR:N	2.79	0.50
1:A:689:VAL:HG11	1:A:691:TRP:CD2	2.44	0.50
1:B:546:ASN:OD1	1:B:551:VAL:HG11	2.12	0.50
1:B:663:ASN:HA	1:B:666:SER:HB3	1.93	0.50
1:A:4:GLN:O	1:A:8:ASN:ND2	2.45	0.50
1:B:116:PHE:CD1	1:B:120:TYR:HB2	2.47	0.50
1:A:398:ASP:OD2	1:A:404:GLU:CD	2.50	0.50
1:A:475:PRO:HB3	1:A:526:TYR:OH	2.11	0.50
1:B:277:LEU:CD1	1:B:302:GLN:HE22	2.25	0.49
1:B:300:ASN:HD22	1:B:350:VAL:CA	2.14	0.49
1:A:626:SER:HB3	1:A:681:PHE:CD2	2.46	0.49
1:A:539:VAL:HG11	1:A:580:MET:HG3	1.93	0.49
1:A:462:LEU:O	1:A:516:ILE:HD11	2.12	0.49
1:A:827:LEU:O	1:A:832:ASN:CB	2.60	0.49
1:B:725:ARG:HD2	1:B:728:ASN:ND2	2.26	0.49
1:B:249:ALA:O	1:B:253:MET:HG3	2.12	0.49
1:A:89:TRP:CE3	1:A:89:TRP:HA	2.48	0.49
1:A:456:GLN:NE2	1:A:456:GLN:H	2.10	0.49
1:B:212:LEU:HD22	1:B:252:THR:HG21	1.93	0.49
1:B:626:SER:OG	1:B:682:PRO:HD3	2.12	0.49
1:A:539:VAL:O	1:A:539:VAL:CG1	2.54	0.49
1:A:205:TYR:CD2	1:A:245:LEU:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PRO:O	1:B:56:SER:C	2.51	0.49
1:B:544:ILE:CG2	1:B:584:LEU:HD13	2.43	0.49
1:B:210:LEU:O	1:B:214:VAL:HG23	2.13	0.49
1:B:837:ASP:HB2	1:B:838:PRO:HD3	1.93	0.49
1:A:733:ASP:O	1:A:736:PRO:CD	2.58	0.49
1:A:611:PHE:CE1	1:A:669:CYS:HB2	2.48	0.49
1:B:341:ASP:O	1:B:388:LYS:HE3	2.12	0.49
1:B:585:LEU:HD22	1:B:618:PHE:CD2	2.47	0.49
1:B:237:TYR:OH	1:B:277:LEU:HD23	2.13	0.48
1:A:777:ASN:ND2	1:A:826:ILE:CB	2.75	0.48
1:B:626:SER:HB2	1:B:682:PRO:HD3	1.95	0.48
1:B:89:TRP:HH2	1:B:134:VAL:HG21	1.77	0.48
1:B:397:TRP:CH2	1:B:508:LEU:HD13	2.48	0.48
1:A:599:VAL:HG13	1:A:600:PRO:HD2	1.94	0.48
1:B:318:PRO:HA	1:B:321:LYS:CB	2.34	0.48
1:A:506:HIS:CD2	1:A:508:LEU:HB2	2.49	0.48
1:A:448:THR:HG22	1:A:448:THR:O	2.13	0.48
1:B:837:ASP:C	1:B:841:ASN:HD22	2.16	0.48
1:B:100:GLU:HB3	1:B:101:PRO:CD	2.42	0.48
1:A:642:LEU:HD23	1:A:677:PHE:CD2	2.48	0.48
1:A:135:ILE:HG12	1:A:143:PHE:HD2	1.79	0.48
1:A:40:TRP:CB	1:A:68:LYS:HG3	2.43	0.48
1:B:725:ARG:HA	1:B:728:ASN:ND2	2.28	0.48
1:B:631:THR:CG2	1:B:632:PRO:HD2	2.44	0.48
1:A:229:ASN:ND2	1:A:231:PRO:HG2	2.28	0.48
1:A:761:ILE:O	1:A:765:ILE:N	2.44	0.48
1:A:541:PRO:HA	1:A:545:HIS:HB2	1.96	0.48
1:B:837:ASP:C	1:B:841:ASN:ND2	2.67	0.48
1:B:649:LYS:CE	1:B:666:SER:OG	2.62	0.48
1:B:514:MET:HE3	1:B:543:GLY:HA2	1.96	0.48
1:B:152:LEU:CD1	1:B:214:VAL:HG22	2.29	0.48
1:A:777:ASN:O	1:A:781:PRO:CD	2.62	0.48
1:A:27:THR:CG2	1:A:28:ASP:N	2.76	0.48
1:B:145:ASN:ND2	1:B:210:LEU:HD12	2.29	0.47
1:A:887:THR:N	1:A:888:PRO:CD	2.77	0.47
1:B:689:VAL:HG12	1:B:690:ALA:N	2.28	0.47
1:A:152:LEU:HD12	1:A:217:GLN:OE1	2.14	0.47
1:B:825:SER:HA	1:B:828:PHE:HD1	1.78	0.47
1:B:116:PHE:CE1	1:B:120:TYR:HB2	2.49	0.47
1:A:348:THR:HA	1:A:351:PHE:CD1	2.49	0.47
1:B:693:ALA:O	1:B:696:ASN:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:CE1	1:A:120:TYR:CG	3.03	0.47
1:A:40:TRP:HB2	1:A:68:LYS:HG3	1.97	0.47
1:A:10:VAL:CG2	1:A:60:ILE:HD12	2.44	0.47
1:B:631:THR:HG23	1:B:632:PRO:HD2	1.95	0.47
1:B:856:GLN:O	1:B:860:ILE:HG23	2.15	0.47
1:A:755:VAL:HG13	1:A:810:SER:HB2	1.97	0.47
1:B:836:PHE:O	1:B:840:ILE:CG2	2.58	0.47
1:B:435:MET:O	1:B:439:ILE:HG13	2.15	0.47
1:B:681:PHE:CD2	1:B:682:PRO:HD2	2.50	0.47
1:B:375:LYS:HE2	1:B:379:LYS:HZ3	1.76	0.47
1:B:332:PHE:N	1:B:333:PRO:CD	2.78	0.47
1:B:626:SER:HB2	1:B:682:PRO:HD2	1.97	0.47
1:B:411:GLU:CG	1:B:412:MET:H	2.28	0.47
1:A:462:LEU:HD11	1:A:501:VAL:CG1	2.45	0.47
1:A:199:TYR:CE1	1:A:207:THR:HG21	2.49	0.47
1:A:104:ILE:CG2	1:A:104:ILE:O	2.62	0.46
1:A:776:THR:O	1:A:780:LEU:HG	2.15	0.46
1:A:89:TRP:HH2	1:A:134:VAL:HG21	1.79	0.46
1:B:295:VAL:O	1:B:298:LEU:HB3	2.15	0.46
1:B:50:LYS:C	1:B:58:ARG:NH2	2.68	0.46
1:B:736:PRO:HA	1:B:775:ILE:HD11	1.96	0.46
1:A:332:PHE:N	1:A:333:PRO:CD	2.78	0.46
1:A:464:GLU:OE1	1:A:464:GLU:HA	2.16	0.46
1:B:89:TRP:CE3	1:B:89:TRP:HA	2.50	0.46
1:B:169:GLN:O	1:B:173:ASP:HB2	2.14	0.46
1:A:529:ALA:O	1:A:532:PRO:HD2	2.15	0.46
1:B:838:PRO:O	1:B:842:SER:HB3	2.15	0.46
1:B:681:PHE:CB	1:B:682:PRO:CD	2.93	0.46
1:A:544:ILE:HG22	1:A:584:LEU:HD13	1.96	0.46
1:A:120:TYR:CD2	1:A:121:PRO:N	2.83	0.46
1:B:281:LYS:O	1:B:282:SER:OG	2.30	0.46
1:B:857:LYS:HA	1:B:860:ILE:CD1	2.46	0.46
1:B:277:LEU:HD11	1:B:302:GLN:HE22	1.80	0.46
1:A:350:VAL:O	1:A:350:VAL:HG12	2.15	0.46
1:B:544:ILE:HG22	1:B:584:LEU:HD13	1.98	0.46
1:A:24:GLN:HG3	1:A:28:ASP:OD2	2.15	0.46
1:A:116:PHE:CE1	1:A:120:TYR:CD1	3.04	0.46
1:B:89:TRP:HE3	1:B:89:TRP:HA	1.81	0.46
1:B:15:ASP:O	1:B:23:LYS:NZ	2.36	0.46
1:A:166:THR:O	1:A:170:ILE:HG13	2.16	0.46
1:B:642:LEU:HD23	1:B:677:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASP:HB2	1:A:395:GLN:CB	2.46	0.46
1:B:560:TYR:HB2	1:B:620:THR:OG1	2.15	0.46
1:A:581:LEU:O	1:A:585:LEU:HG	2.15	0.46
1:A:275:LEU:HA	1:A:275:LEU:HD12	1.71	0.46
1:B:778:ARG:O	1:B:781:PRO:HD2	2.15	0.46
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.76	0.46
1:B:224:ILE:HD13	1:B:261:MET:CB	2.45	0.46
1:A:89:TRP:HE3	1:A:89:TRP:HA	1.79	0.46
1:A:611:PHE:CZ	1:A:615:LEU:HD21	2.51	0.46
1:A:468:PHE:O	1:A:468:PHE:CD2	2.68	0.46
1:B:195:MET:HE2	1:B:199:TYR:HE1	1.80	0.46
1:A:858:SER:O	1:A:862:LEU:HG	2.16	0.46
1:B:762:SER:HA	1:B:817:GLN:OE1	2.16	0.46
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.76	0.46
1:A:236:LEU:HB2	1:A:253:MET:HE3	1.98	0.46
1:B:837:ASP:CB	1:B:841:ASN:ND2	2.74	0.46
1:A:636:ALA:O	1:A:640:ASP:OD2	2.33	0.46
1:B:329:TYR:CZ	1:B:373:SER:OG	2.63	0.46
1:B:328:LEU:HD22	1:B:332:PHE:HE1	1.81	0.46
1:B:71:GLU:O	1:B:71:GLU:CG	2.63	0.46
1:A:55:PRO:O	1:A:56:SER:C	2.55	0.45
1:B:283:GLN:C	1:B:283:GLN:CD	2.74	0.45
1:B:144:SER:HB3	1:B:195:MET:HE1	1.98	0.45
1:B:539:VAL:HG11	1:B:580:MET:HG3	1.97	0.45
1:A:886:LEU:C	1:A:888:PRO:HD2	2.37	0.45
1:B:615:LEU:HD13	1:B:676:ASN:HD21	1.81	0.45
1:A:295:VAL:O	1:A:298:LEU:HB3	2.16	0.45
1:A:663:ASN:HA	1:A:666:SER:HB3	1.97	0.45
1:A:632:PRO:CA	1:A:635:GLN:HG2	2.30	0.45
1:B:334:TYR:HD1	1:B:334:TYR:H	1.64	0.45
1:A:53:TYR:N	1:A:53:TYR:CD1	2.84	0.45
1:B:715:ILE:HG22	1:B:715:ILE:O	2.15	0.45
1:A:271:ASN:CB	1:A:327:GLN:NE2	2.80	0.45
1:B:717:GLY:O	1:B:721:PHE:HB3	2.17	0.45
1:B:10:VAL:HG22	1:B:60:ILE:CD1	2.47	0.45
1:B:268:ASN:O	1:B:272:ILE:HG13	2.17	0.45
1:B:232:CYS:O	1:B:236:LEU:HG	2.16	0.45
1:A:441:SER:O	1:A:442:SER:C	2.54	0.45
1:B:762:SER:CB	1:B:817:GLN:OE1	2.64	0.45
1:A:333:PRO:O	1:A:337:ARG:HB3	2.16	0.45
1:A:510:GLN:NE2	1:A:542:ARG:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:MET:HG3	1:B:208:VAL:CG1	2.46	0.45
1:A:361:LEU:HB3	1:A:426:ILE:CD1	2.47	0.45
1:A:382:LEU:O	1:A:383:GLU:C	2.54	0.45
1:B:683:ALA:CB	1:B:728:ASN:O	2.55	0.45
1:A:716:ARG:C	1:A:720:ARG:NE	2.56	0.45
1:A:548:ASN:HB3	1:A:551:VAL:HG23	1.99	0.45
1:A:10:VAL:HG22	1:A:60:ILE:CD1	2.46	0.45
1:B:556:TRP:CZ2	1:B:584:LEU:HD22	2.51	0.45
1:B:457:LEU:O	1:B:460:PHE:HB3	2.17	0.45
1:B:593:THR:CG2	1:B:594:ASP:N	2.80	0.45
1:B:788:PHE:HZ	1:B:839:LEU:CD2	2.29	0.45
1:A:689:VAL:CG2	1:A:691:TRP:CH2	2.97	0.45
1:B:566:ILE:HG22	1:B:566:ILE:O	2.17	0.45
1:A:715:ILE:O	1:A:719:VAL:HG23	2.17	0.45
1:B:478:PHE:CE2	1:B:523:PHE:HB2	2.51	0.45
1:A:424:ASN:ND2	1:A:424:ASN:O	2.49	0.45
1:A:424:ASN:ND2	1:A:428:SER:HA	2.32	0.45
1:B:375:LYS:HE2	1:B:379:LYS:CE	2.47	0.45
1:B:135:ILE:HD11	1:B:147:TYR:CB	2.47	0.45
1:A:544:ILE:HG22	1:A:584:LEU:CD1	2.46	0.44
1:B:246:ARG:HD3	1:B:291:PHE:CE1	2.50	0.44
1:B:53:TYR:CD1	1:B:53:TYR:N	2.85	0.44
1:B:439:ILE:HG23	1:B:461:ALA:HB1	1.99	0.44
1:B:464:GLU:HA	1:B:464:GLU:OE1	2.17	0.44
1:A:483:ASP:O	1:A:484:LYS:CB	2.65	0.44
1:A:10:VAL:HG22	1:A:60:ILE:HD12	1.98	0.44
1:A:52:LYS:HD2	1:A:53:TYR:CE1	2.48	0.44
1:A:601:THR:CG2	1:A:602:LEU:N	2.78	0.44
1:A:520:TYR:O	1:A:523:PHE:HB3	2.18	0.44
1:A:381:LEU:HA	1:A:381:LEU:HD12	1.81	0.44
1:A:462:LEU:HD11	1:A:501:VAL:HG11	1.99	0.44
1:A:166:THR:HG22	1:A:168:VAL:H	1.83	0.44
1:B:444:SER:O	1:B:447:ALA:HB3	2.17	0.44
1:B:236:LEU:HB2	1:B:253:MET:HE3	2.00	0.44
1:A:672:MET:HE3	1:A:718:ALA:HB1	1.98	0.44
1:A:500:GLN:CB	1:A:503:ARG:HH21	2.30	0.44
1:B:727:ILE:O	1:B:731:GLY:CA	2.65	0.44
1:B:617:LEU:O	1:B:621:VAL:HG23	2.17	0.44
1:A:313:PRO:O	1:A:314:SER:CB	2.66	0.44
1:A:52:LYS:HB2	1:A:53:TYR:CD1	2.53	0.44
1:A:689:VAL:HG21	1:A:691:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:HD22	1:A:428:SER:HA	1.82	0.44
1:B:524:PHE:CE2	1:B:534:LEU:HD11	2.53	0.44
1:A:702:ILE:HA	1:A:705:ILE:CB	2.48	0.44
1:A:91:TYR:CZ	1:A:97:PHE:HB3	2.53	0.44
1:B:230:GLU:H	1:B:231:PRO:HD2	1.78	0.44
1:A:511:LEU:O	1:A:512:LEU:C	2.56	0.44
1:B:672:MET:CE	1:B:718:ALA:HA	2.48	0.44
1:A:552:ARG:N	1:A:553:PRO:CD	2.81	0.44
1:A:422:THR:O	1:A:426:ILE:HG13	2.18	0.44
1:A:50:LYS:HA	1:A:58:ARG:HH21	1.81	0.43
1:B:784:LEU:HB3	1:B:788:PHE:CE1	2.48	0.43
1:B:61:CYS:O	1:B:64:THR:CG2	2.64	0.43
1:B:343:TYR:O	1:B:344:ASP:C	2.56	0.43
1:A:689:VAL:CG1	1:A:691:TRP:N	2.82	0.43
1:A:760:PHE:CE2	1:A:764:LEU:HD12	2.53	0.43
1:A:722:THR:CG2	1:A:726:ILE:CD1	2.96	0.43
1:B:4:GLN:O	1:B:8:ASN:ND2	2.51	0.43
1:B:430:LEU:O	1:B:430:LEU:HD12	2.17	0.43
1:A:572:ASN:N	1:A:572:ASN:HD22	2.14	0.43
1:B:53:TYR:O	1:B:58:ARG:NH2	2.51	0.43
1:B:762:SER:OG	1:B:817:GLN:OE1	2.35	0.43
1:B:856:GLN:CB	1:B:909:VAL:HG21	2.47	0.43
1:A:568:LYS:O	1:A:571:VAL:HG23	2.17	0.43
1:A:24:GLN:C	1:A:27:THR:HG22	2.38	0.43
1:B:601:THR:HG22	1:B:602:LEU:N	2.34	0.43
1:B:1:MET:CB	1:B:4:GLN:HB2	2.48	0.43
1:A:439:ILE:HG23	1:A:461:ALA:HB1	2.00	0.43
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.79	0.43
1:B:100:GLU:OE1	1:B:104:ILE:HD13	2.19	0.43
1:B:585:LEU:HD22	1:B:618:PHE:CE2	2.54	0.43
1:B:788:PHE:CZ	1:B:839:LEU:HD23	2.53	0.43
1:A:556:TRP:CZ2	1:A:584:LEU:HD22	2.53	0.43
1:B:735:LEU:O	1:B:775:ILE:CD1	2.66	0.43
1:A:885:SER:O	1:A:888:PRO:HG2	2.18	0.43
1:B:169:GLN:O	1:B:173:ASP:CB	2.66	0.43
1:A:727:ILE:HG12	1:A:734:MET:CB	2.49	0.43
1:B:464:GLU:O	1:B:468:PHE:HB2	2.19	0.43
1:B:243:GLU:C	1:B:243:GLU:CD	2.77	0.43
1:A:291:PHE:O	1:A:294:HIS:HB2	2.18	0.43
1:B:432:SER:O	1:B:433:SER:C	2.56	0.43
1:B:196:MET:HG3	1:B:208:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PHE:O	1:B:294:HIS:HB2	2.19	0.43
1:B:6:VAL:HA	1:B:29:PHE:HE2	1.84	0.43
1:A:255:GLU:HA	1:A:255:GLU:OE1	2.18	0.43
1:B:413:ARG:NH2	1:B:459:GLU:OE1	2.50	0.43
1:B:663:ASN:O	1:B:664:ILE:C	2.56	0.43
1:A:443:LEU:O	1:A:446:ALA:HB3	2.19	0.43
1:B:413:ARG:HH22	1:B:459:GLU:CD	2.21	0.42
1:A:210:LEU:O	1:A:214:VAL:HG23	2.19	0.42
1:A:735:LEU:N	1:A:736:PRO:HD3	2.33	0.42
1:A:169:GLN:OE1	1:A:172:LYS:HE2	2.18	0.42
1:B:116:PHE:HE1	1:B:120:TYR:CD1	2.35	0.42
1:A:144:SER:HB3	1:A:195:MET:HE1	2.01	0.42
1:B:205:TYR:HD2	1:B:245:LEU:CD1	2.32	0.42
1:B:10:VAL:CG2	1:B:60:ILE:HD12	2.49	0.42
1:A:206:GLY:N	1:B:203:LYS:O	2.52	0.42
1:B:381:LEU:O	1:B:385:ILE:HG13	2.19	0.42
1:A:277:LEU:CD1	1:A:302:GLN:HE22	2.31	0.42
1:B:512:LEU:HA	1:B:512:LEU:HD12	1.78	0.42
1:B:675:GLY:O	1:B:678:ALA:HB3	2.19	0.42
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.72	0.42
1:B:540:GLY:C	1:B:542:ARG:H	2.23	0.42
1:B:116:PHE:CE1	1:B:120:TYR:CG	3.08	0.42
1:A:599:VAL:CG1	1:A:600:PRO:N	2.82	0.42
1:A:413:ARG:HH22	1:A:459:GLU:CD	2.22	0.42
1:B:300:ASN:ND2	1:B:350:VAL:HA	2.14	0.42
1:B:857:LYS:O	1:B:860:ILE:HG12	2.19	0.42
1:B:230:GLU:O	1:B:233:MET:N	2.53	0.42
1:A:689:VAL:CG2	1:A:691:TRP:CZ2	3.02	0.42
1:B:859:SER:O	1:B:862:LEU:HB2	2.19	0.42
1:A:585:LEU:HD22	1:A:618:PHE:CE2	2.55	0.42
1:B:243:GLU:O	1:B:243:GLU:CD	2.57	0.42
1:B:146:PHE:O	1:B:150:VAL:HG23	2.19	0.42
1:B:257:VAL:HG13	1:B:270:LEU:HD21	2.01	0.42
1:A:562:PHE:CZ	1:A:566:ILE:HD12	2.54	0.42
1:B:89:TRP:CH2	1:B:134:VAL:HG21	2.53	0.42
1:A:271:ASN:CB	1:A:327:GLN:HE22	2.33	0.42
1:A:302:GLN:O	1:A:305:GLU:HB2	2.20	0.42
1:A:147:TYR:CE2	1:A:151:LEU:HD11	2.55	0.42
1:B:642:LEU:HD23	1:B:677:PHE:CE2	2.55	0.42
1:A:780:LEU:O	1:A:784:LEU:CG	2.68	0.42
1:A:544:ILE:CG2	1:A:584:LEU:CD1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:CB	1:B:208:VAL:HG22	2.50	0.42
1:B:169:GLN:O	1:B:173:ASP:CG	2.58	0.42
1:B:441:SER:O	1:B:442:SER:C	2.58	0.42
1:B:24:GLN:HG3	1:B:28:ASP:OD2	2.20	0.42
1:B:10:VAL:HG22	1:B:60:ILE:HD13	2.01	0.42
1:B:271:ASN:CB	1:B:327:GLN:NE2	2.83	0.42
1:A:144:SER:HB3	1:A:195:MET:CE	2.50	0.42
1:A:837:ASP:N	1:A:838:PRO:HD2	2.35	0.42
1:A:504:HIS:CD2	1:A:505:PRO:HD2	2.55	0.42
1:B:502:CYS:HB2	1:B:537:TYR:CD1	2.55	0.42
1:A:835:TYR:O	1:A:838:PRO:HD2	2.20	0.42
1:A:500:GLN:CD	1:A:500:GLN:H	2.23	0.42
1:B:59:LEU:O	1:B:63:GLN:HG3	2.19	0.42
1:B:765:ILE:CB	1:B:817:GLN:NE2	2.83	0.42
1:A:757:VAL:O	1:A:761:ILE:HG23	2.20	0.42
1:B:364:GLU:O	1:B:366:SER:N	2.47	0.42
1:B:508:LEU:HA	1:B:508:LEU:HD12	1.82	0.41
1:A:101:PRO:HG2	1:A:103:TYR:CE2	2.54	0.41
1:B:344:ASP:OD1	1:B:388:LYS:NZ	2.53	0.41
1:B:557:TYR:O	1:B:560:TYR:HB3	2.20	0.41
1:B:581:LEU:HD22	1:B:617:LEU:HD21	2.03	0.41
1:A:351:PHE:N	1:A:352:PRO:CD	2.83	0.41
1:B:762:SER:C	1:B:817:GLN:HE22	2.23	0.41
1:A:546:ASN:O	1:A:552:ARG:HG3	2.21	0.41
1:B:209:GLY:O	1:B:213:GLN:HG2	2.20	0.41
1:B:148:LEU:HD13	1:B:210:LEU:HB3	2.03	0.41
1:B:389:MET:HE3	1:B:413:ARG:HG2	2.02	0.41
1:B:500:GLN:CB	1:B:503:ARG:HH21	2.34	0.41
1:B:224:ILE:HD13	1:B:261:MET:HB3	2.02	0.41
1:B:755:VAL:HG13	1:B:810:SER:CB	2.50	0.41
1:A:578:LEU:HD21	1:A:624:LEU:CB	2.51	0.41
1:B:504:HIS:CD2	1:B:505:PRO:HD2	2.54	0.41
1:B:271:ASN:O	1:B:275:LEU:HB2	2.20	0.41
1:B:381:LEU:HA	1:B:381:LEU:HD12	1.90	0.41
1:B:62:LEU:HA	1:B:62:LEU:HD23	1.78	0.41
1:B:237:TYR:N	1:B:253:MET:HE3	2.35	0.41
1:A:689:VAL:HG12	1:A:692:LEU:N	2.32	0.41
1:B:762:SER:O	1:B:817:GLN:NE2	2.50	0.41
1:B:132:GLN:HE22	1:B:188:ILE:HA	1.85	0.41
1:B:120:TYR:CE1	1:B:128:PHE:HE1	2.38	0.41
1:B:120:TYR:CE1	1:B:128:PHE:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:O	1:A:23:LYS:HE3	2.21	0.41
1:B:262:LYS:O	1:B:265:GLU:N	2.51	0.41
1:A:103:TYR:CD2	1:A:103:TYR:N	2.88	0.41
1:B:205:TYR:CD2	1:B:242:ILE:HG21	2.53	0.41
1:A:463:TYR:CA	1:A:512:LEU:HD21	2.51	0.41
1:B:837:ASP:O	1:B:838:PRO:C	2.59	0.41
1:A:668:TYR:O	1:A:672:MET:HG2	2.21	0.41
1:B:135:ILE:HD13	1:B:144:SER:HA	2.02	0.41
1:A:24:GLN:HA	1:A:27:THR:HG22	2.03	0.41
1:B:12:ALA:O	1:B:23:LYS:HE3	2.21	0.41
1:B:357:LEU:O	1:B:361:LEU:HD13	2.21	0.41
1:B:119:LEU:HD22	1:B:123:ASN:ND2	2.36	0.41
1:A:581:LEU:HD12	1:A:621:VAL:HG22	2.03	0.41
1:B:7:GLU:O	1:B:11:GLU:HB2	2.21	0.41
1:B:863:VAL:O	1:B:867:VAL:HG23	2.21	0.41
1:B:909:VAL:HG12	1:B:909:VAL:O	2.21	0.41
1:A:244:GLU:HB3	1:B:203:LYS:HZ3	1.82	0.41
1:B:287:THR:O	1:B:288:ASP:HB2	2.21	0.41
1:B:103:TYR:O	1:B:107:ALA:HB2	2.21	0.41
1:A:280:SER:O	1:A:281:LYS:C	2.58	0.41
1:A:300:ASN:HD22	1:A:350:VAL:CA	2.15	0.40
1:B:681:PHE:HD2	1:B:682:PRO:HD2	1.86	0.40
1:B:69:VAL:CG1	1:B:115:LEU:HD23	2.51	0.40
1:B:531:ILE:CD1	1:B:569:GLN:OE1	2.69	0.40
1:B:120:TYR:N	1:B:121:PRO:CD	2.83	0.40
1:B:553:PRO:HD2	1:B:554:ARG:H	1.86	0.40
1:B:269:LEU:HA	1:B:272:ILE:HD12	2.03	0.40
1:A:470:GLU:O	1:A:470:GLU:HG2	2.21	0.40
1:B:586:ASN:O	1:B:614:GLN:NE2	2.48	0.40
1:B:907:LEU:C	1:B:909:VAL:H	2.24	0.40
1:A:72:TRP:HB3	1:A:77:ASN:HB2	2.03	0.40
1:B:411:GLU:C	1:B:413:ARG:N	2.74	0.40
1:A:884:LEU:O	1:A:888:PRO:CD	2.69	0.40
1:A:615:LEU:HD13	1:A:676:ASN:ND2	2.36	0.40
1:B:19:GLY:O	1:B:23:LYS:HB2	2.22	0.40
1:A:560:TYR:CZ	1:A:564:LYS:HD2	2.56	0.40
1:A:927:ILE:O	1:A:930:SER:N	2.54	0.40
1:A:100:GLU:OE2	1:A:104:ILE:HD13	2.21	0.40
1:A:244:GLU:CB	1:B:203:LYS:NZ	2.73	0.40
1:A:397:TRP:CH2	1:A:508:LEU:HD13	2.57	0.40
1:A:856:GLN:CG	1:A:909:VAL:CG2	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:VAL:C	1:A:732:PRO:HD2	2.42	0.40
1:B:424:ASN:O	1:B:424:ASN:ND2	2.54	0.40
1:A:617:LEU:O	1:A:621:VAL:HG23	2.21	0.40
1:B:529:ALA:O	1:B:532:PRO:HD2	2.21	0.40
1:B:487:THR:O	1:B:491:GLN:HG3	2.22	0.40
1:A:510:GLN:O	1:A:514:MET:HG3	2.22	0.40
1:A:21:ILE:O	1:A:24:GLN:HB3	2.20	0.40
1:B:578:LEU:HD21	1:B:624:LEU:CB	2.52	0.40
1:B:760:PHE:O	1:B:764:LEU:HB2	2.21	0.40
1:A:228:VAL:O	1:A:229:ASN:C	2.60	0.40
1:A:411:GLU:C	1:A:413:ARG:N	2.75	0.40
1:A:758:LEU:CD1	1:A:810:SER:OG	2.53	0.40
1:A:89:TRP:CH2	1:A:134:VAL:HG21	2.55	0.40
1:A:341:ASP:O	1:A:388:LYS:CE	2.70	0.40
1:A:893:MET:N	1:A:894:PRO:HD2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ASP:O	1:B:607:ARG:NH2[2_655]	2.17	0.03

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	893/980 (91%)	813 (91%)	76 (8%)	4 (0%)	39 75
1	B	878/980 (90%)	800 (91%)	71 (8%)	7 (1%)	24 63
All	All	1771/1960 (90%)	1613 (91%)	147 (8%)	11 (1%)	30 68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	598	PRO
1	A	289	PRO
1	A	592	VAL
1	B	289	PRO
1	B	730	VAL
1	B	263	PRO
1	B	597	ALA
1	B	908	VAL
1	A	46	ILE
1	A	352	PRO
1	B	475	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/880 (67%)	555 (94%)	37 (6%)	22	58
1	B	569/880 (65%)	537 (94%)	32 (6%)	26	62
All	All	1161/1760 (66%)	1092 (94%)	69 (6%)	24	60

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	47	PHE
1	A	56	SER
1	A	64	THR
1	A	89	TRP
1	A	94	GLU
1	A	103	TYR
1	A	215	TYR
1	A	229	ASN
1	A	252	THR
1	A	328	LEU
1	A	330	ASN
1	A	337	ARG

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Mol	Chain	Res	Type
1	A	343	TYR
1	A	348	THR
1	A	392	ASP
1	A	396	GLU
1	A	397	TRP
1	A	424	ASN
1	A	441	SER
1	A	456	GLN
1	A	502	CYS
1	A	511	LEU
1	A	528	SER
1	A	542	ARG
1	A	546	ASN
1	A	561	ARG
1	A	568	LYS
1	A	570	VAL
1	A	583	ASP
1	A	603	ASN
1	A	687	GLU
1	A	711	PHE
1	A	723	SER
1	A	764	LEU
1	A	766	HIS
1	A	835	TYR
1	B	47	PHE
1	B	56	SER
1	B	64	THR
1	B	89	TRP
1	B	200	SER
1	B	215	TYR
1	B	229	ASN
1	B	246	ARG
1	B	252	THR
1	B	283	GLN
1	B	328	LEU
1	B	330	ASN
1	B	334	TYR
1	B	337	ARG
1	B	343	TYR
1	B	373	SER
1	B	392	ASP
1	B	397	TRP

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Mol	Chain	Res	Type
1	B	408	GLU
1	B	424	ASN
1	B	441	SER
1	B	456	GLN
1	B	511	LEU
1	B	542	ARG
1	B	546	ASN
1	B	583	ASP
1	B	603	ASN
1	B	617	LEU
1	B	711	PHE
1	B	734	MET
1	B	764	LEU
1	B	766	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	77	ASN
1	A	82	GLN
1	A	106	ASN
1	A	109	GLN
1	A	132	GLN
1	A	145	ASN
1	A	204	ASN
1	A	223	ASN
1	A	229	ASN
1	A	258	ASN
1	A	271	ASN
1	A	300	ASN
1	A	302	GLN
1	A	327	GLN
1	A	330	ASN
1	A	424	ASN
1	A	456	GLN
1	A	504	HIS
1	A	506	HIS
1	A	546	ASN
1	A	572	ASN
1	A	603	ASN
1	A	676	ASN

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Mol	Chain	Res	Type
1	A	841	ASN
1	B	8	ASN
1	B	77	ASN
1	B	82	GLN
1	B	106	ASN
1	B	109	GLN
1	B	123	ASN
1	B	132	GLN
1	B	145	ASN
1	B	183	ASN
1	B	229	ASN
1	B	271	ASN
1	B	283	GLN
1	B	300	ASN
1	B	302	GLN
1	B	327	GLN
1	B	330	ASN
1	B	420	GLN
1	B	424	ASN
1	B	456	GLN
1	B	504	HIS
1	B	506	HIS
1	B	546	ASN
1	B	603	ASN
1	B	676	ASN
1	B	696	ASN
1	B	728	ASN
1	B	777	ASN
1	B	841	ASN

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	917/980 (93%)	0.10	39 (4%)	39	18	47, 117, 195, 201	0
1	B	902/980 (92%)	0.08	34 (3%)	44	21	56, 120, 195, 201	0
All	All	1819/1960 (92%)	0.09	73 (4%)	42	20	47, 118, 195, 201	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	948	SER	5.9
1	B	947	ALA	5.4
1	B	854	ALA	5.4
1	A	287	THR	5.3
1	A	948	SER	4.9
1	A	691	TRP	4.9
1	A	751	MET	4.8
1	B	806	ASP	4.6
1	A	973	LEU	4.3
1	B	946	MET	4.1
1	B	731	GLY	4.1
1	A	950	TYR	4.1
1	A	951	LEU	3.9
1	A	970	ILE	3.9
1	B	287	THR	3.7
1	A	949	GLU	3.7
1	B	773	MET	3.7
1	A	662	GLU	3.5
1	B	714	ASP	3.5
1	A	947	ALA	3.5
1	B	588	SER	3.5
1	B	475	PRO	3.5
1	A	752	ASN	3.5
1	A	953	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	642	LEU	3.2
1	B	937	PHE	3.2
1	B	628	GLY	3.1
1	A	930	SER	3.1
1	A	645	ALA	3.0
1	A	971	GLN	3.0
1	B	945	VAL	3.0
1	B	589	VAL	2.9
1	A	946	MET	2.9
1	B	855	THR	2.9
1	B	629	ASN	2.9
1	A	952	GLN	2.8
1	B	857	LYS	2.8
1	A	669	CYS	2.7
1	B	858	SER	2.7
1	A	47	PHE	2.7
1	B	915	GLY	2.6
1	B	587	ILE	2.6
1	A	736	PRO	2.5
1	A	834	VAL	2.5
1	B	776	THR	2.5
1	A	602	LEU	2.5
1	A	665	ILE	2.5
1	A	731	GLY	2.4
1	A	698	ALA	2.4
1	A	732	PRO	2.4
1	B	324	CYS	2.3
1	B	698	ALA	2.3
1	B	787	ILE	2.3
1	A	931	TYR	2.3
1	B	30	ILE	2.3
1	A	734	MET	2.3
1	A	566	ILE	2.3
1	A	972	ALA	2.3
1	A	705	ILE	2.3
1	B	477	ALA	2.3
1	A	168	VAL	2.2
1	B	944	ASP	2.2
1	B	476	ASP	2.2
1	B	846	PHE	2.2
1	B	502	CYS	2.1
1	B	635	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	802	VAL	2.1
1	A	592	VAL	2.1
1	A	666	SER	2.1
1	A	939	THR	2.1
1	A	587	ILE	2.0
1	B	669	CYS	2.0
1	A	646	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	A	2001	1/1	0.94	0.16	-1.70	53,53,53,53	0
2	CA	B	2001	1/1	0.95	0.14	-2.49	53,53,53,53	0
2	CA	A	2002	1/1	0.98	0.04	-6.68	52,52,52,52	0
2	CA	B	2002	1/1	0.98	0.04	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.