



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 3NMS / pdb\_00003nms  
Title : Staphylococcal Complement Inhibitor (SCIN) in complex with Human Complement C3c  
Authors : Geisbrecht, B.V.; Garcia, B.L.  
Deposited on : 2010-06-22  
Resolution : 4.10 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](mailto: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>.

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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

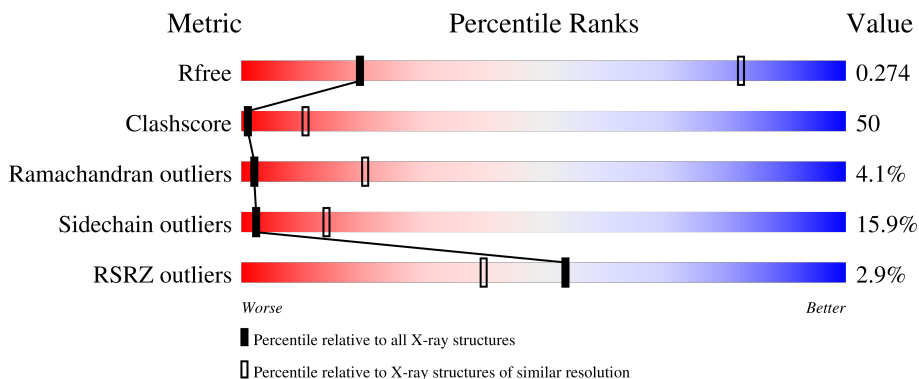
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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))
$R_{free}$	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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  $\geq 3$ , 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	645	 3% 42% 48% 8% ..
2	C	343	 3% 26% 45% 14% • 14%
3	M	88	 3% 34% 48% 14% 5%
4	B	206	 22% 50% 16% • 11%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9561 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	641	4989	3175	846	953	15	0	0	0

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	294	2388	1506	391	471	20	0	0	0

- Molecule 3 is a protein called Staphylococcal complement inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	84	682	432	111	137	2	0	0	0

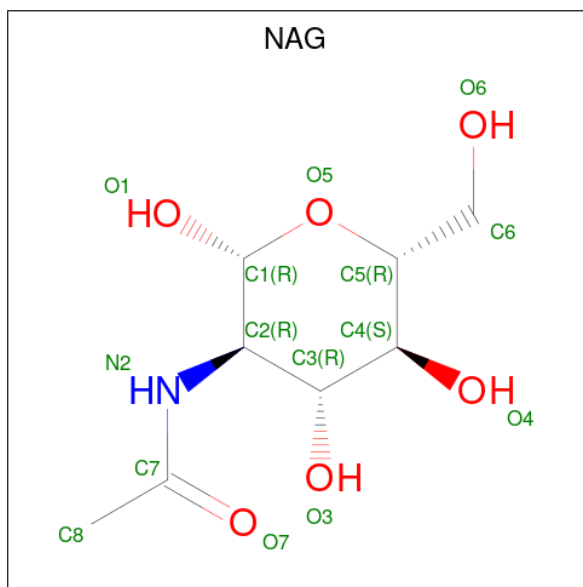
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP Q931M7
M	-1	THR	-	expression tag	UNP Q931M7
M	0	SER	-	expression tag	UNP Q931M7

- Molecule 4 is a protein called Complement C3.

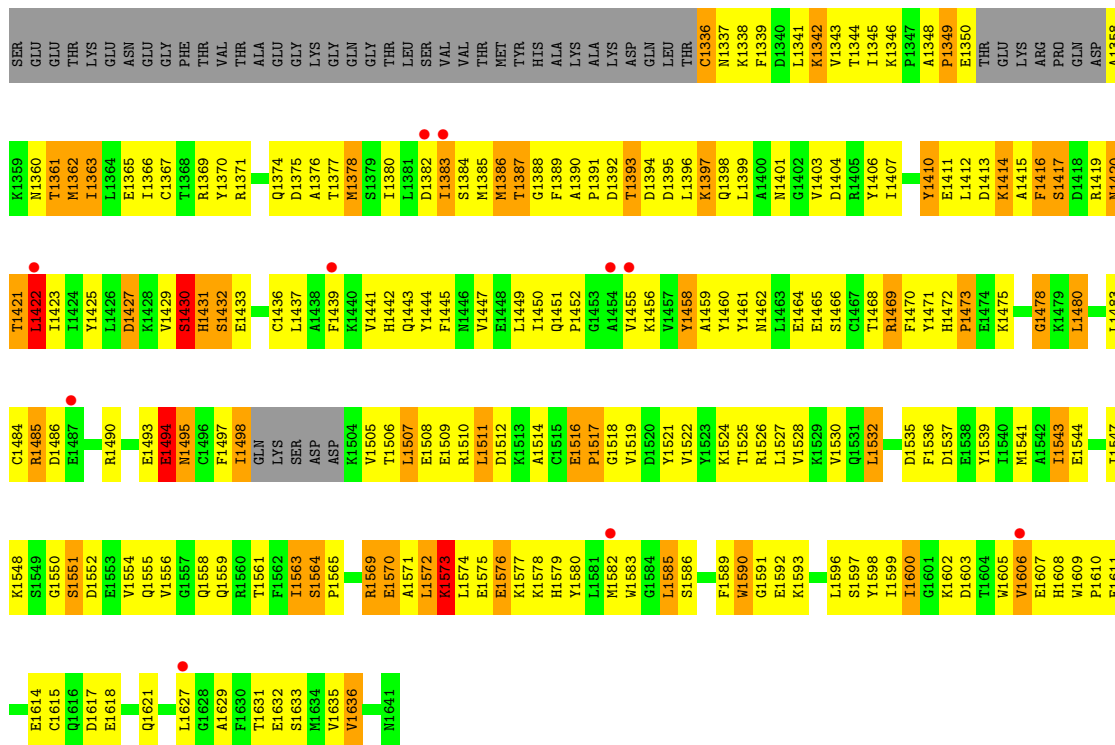
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	184	1488	956	250	277	5	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

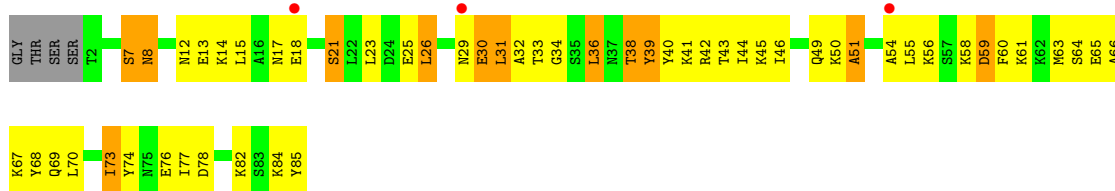


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

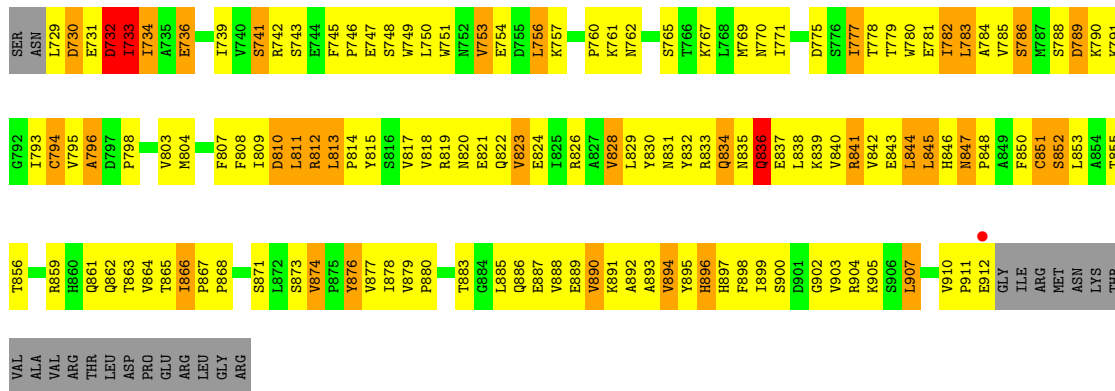




• Molecule 3: Staphylococcal complement inhibitor



• Molecule 4: Complement C3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.07Å 68.43Å 114.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 4.10 49.39 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.39-4.10) 98.1 (49.39-4.10)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 4.14Å)	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.271 , 0.289 0.253 , 0.274	Depositor DCC
$R_{free}$ test set	1364 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.4	Xtrriage
Anisotropy	0.376	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 146.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	9561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	161.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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

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	0.56	0/5089	0.96	11/6916 (0.2%)
2	C	0.62	0/2434	1.01	9/3280 (0.3%)
3	M	0.59	0/690	0.99	3/923 (0.3%)
4	B	0.90	1/1520 (0.1%)	1.18	10/2066 (0.5%)
All	All	0.64	1/9733 (0.0%)	1.01	33/13185 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	733	ILE	CA-CB	-5.77	1.51	1.55

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	76	GLU	N-CA-C	-9.52	101.66	113.28
1	A	162	ASN	N-CA-C	-8.44	100.89	113.72
4	B	866	ILE	CB-CA-C	-8.32	101.28	110.52
4	B	733	ILE	CB-CA-C	-7.86	104.35	111.74
2	C	1427	ASP	N-CA-C	-7.37	104.42	113.41
2	C	1362	MET	N-CA-C	7.36	120.36	109.24
1	A	535	ASP	CB-CA-C	-7.22	98.46	110.29
2	C	1606	VAL	N-CA-C	7.18	118.40	107.77
2	C	1484	CYS	N-CA-C	6.75	119.83	108.02
1	A	151	ILE	N-CA-C	6.73	114.21	107.55
4	B	847	ASN	CA-C-N	6.72	126.35	119.56
4	B	847	ASN	C-N-CA	6.72	126.35	119.56
1	A	239	TYR	N-CA-C	-6.58	100.57	110.24
4	B	730	ASP	N-CA-C	-6.42	97.14	110.80
1	A	535	ASP	N-CA-C	6.40	119.03	109.25
2	C	1478	GLY	N-CA-C	-6.03	106.42	114.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1431	HIS	N-CA-C	-5.90	105.92	113.23
1	A	257	GLU	N-CA-C	-5.81	106.05	114.12
3	M	73	ILE	O-C-N	5.76	127.69	121.87
1	A	333	ILE	N-CA-C	5.67	116.15	107.77
2	C	1564	SER	N-CA-C	5.60	114.74	108.25
4	B	798	PRO	N-CA-C	-5.57	102.83	111.13
2	C	1417	SER	N-CA-C	5.44	117.21	111.28
4	B	733	ILE	N-CA-C	5.44	114.34	107.70
4	B	810	ASP	CA-C-N	-5.40	115.82	122.84
4	B	810	ASP	C-N-CA	-5.40	115.82	122.84
3	M	46	ILE	CB-CA-C	-5.38	104.80	112.22
1	A	491	ASP	N-CA-C	-5.34	107.31	113.88
1	A	182	TRP	CB-CA-C	-5.27	107.81	114.40
1	A	356	ASN	CA-C-N	-5.20	113.34	119.84
1	A	356	ASN	C-N-CA	-5.20	113.34	119.84
2	C	1636	VAL	N-CA-C	5.06	115.83	110.72
4	B	815	TYR	CA-CB-CG	-5.02	104.87	113.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4989	0	5052	482	0
2	C	2388	0	2295	251	0
3	M	682	0	697	61	0
4	B	1488	0	1513	216	0
5	A	14	0	13	4	0
All	All	9561	0	9570	958	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 50.

All (958) 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:280:LEU:CD2	1:A:285:LEU:HD11	1.33	1.56
1:A:230:GLU:HA	1:A:279:VAL:CG1	1.37	1.50
4:B:811:LEU:CD1	4:B:813:LEU:HD22	1.56	1.36
1:A:280:LEU:HD21	1:A:285:LEU:CD1	1.55	1.34
1:A:161:GLN:O	1:A:162:ASN:CG	1.82	1.22
1:A:290:GLN:NE2	1:A:292:PRO:HG3	1.53	1.21
2:C:1525:THR:HG22	2:C:1543:ILE:HA	1.25	1.15
1:A:287:ASP:N	1:A:291:ASN:HB3	1.61	1.13
4:B:810:ASP:HB3	4:B:828:VAL:HG23	1.30	1.13
1:A:590:THR:HG22	1:A:592:SER:H	1.13	1.13
1:A:161:GLN:O	1:A:162:ASN:ND2	1.83	1.12
1:A:230:GLU:CA	1:A:279:VAL:CG1	2.26	1.12
4:B:811:LEU:HD12	4:B:811:LEU:C	1.75	1.12
2:C:1497:PHE:HE2	2:C:1571:ALA:HB1	1.05	1.12
1:A:290:GLN:HE21	1:A:292:PRO:HG3	1.00	1.10
1:A:230:GLU:HG2	1:A:279:VAL:HG11	1.12	1.10
1:A:289:VAL:O	1:A:290:GLN:HB3	1.48	1.09
1:A:161:GLN:C	1:A:162:ASN:CG	2.15	1.08
1:A:591:GLN:HB2	4:B:795:VAL:CB	1.82	1.08
1:A:286:LEU:H	1:A:286:LEU:HD23	1.05	1.07
4:B:810:ASP:CG	4:B:812:ARG:HD3	1.80	1.06
1:A:281:SER:OG	1:A:284:VAL:HG21	1.56	1.05
1:A:230:GLU:HA	1:A:279:VAL:HG13	1.37	1.05
4:B:811:LEU:HD11	4:B:813:LEU:HD22	1.09	1.05
3:M:26:LEU:HA	3:M:74:TYR:OH	1.57	1.05
1:A:230:GLU:CA	1:A:279:VAL:HG12	1.85	1.04
1:A:290:GLN:HG2	1:A:290:GLN:O	1.58	1.04
1:A:280:LEU:CG	1:A:285:LEU:HD11	1.88	1.03
1:A:591:GLN:N	4:B:795:VAL:HG11	1.73	1.02
1:A:287:ASP:HA	1:A:291:ASN:N	1.75	1.02
4:B:811:LEU:CD1	4:B:811:LEU:C	2.29	1.02
1:A:287:ASP:HA	1:A:291:ASN:H	1.21	1.02
4:B:831:ASN:ND2	4:B:868:PRO:HA	1.74	1.02
1:A:280:LEU:HD11	1:A:285:LEU:HD12	1.40	1.01
1:A:281:SER:O	1:A:284:VAL:HG23	1.60	1.01
4:B:795:VAL:HG12	4:B:795:VAL:O	1.60	1.00
1:A:206:VAL:HG11	4:B:813:LEU:O	1.61	1.00
1:A:280:LEU:CD2	1:A:285:LEU:CD1	2.27	1.00
1:A:286:LEU:HD23	1:A:286:LEU:N	1.60	0.99
2:C:1497:PHE:CE2	2:C:1571:ALA:HB1	1.97	0.99
1:A:230:GLU:HA	1:A:279:VAL:HG12	1.04	0.99
1:A:591:GLN:HB2	4:B:795:VAL:HB	1.03	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:734:ILE:HD13	4:B:893:ALA:HB1	1.44	0.99
4:B:811:LEU:HD11	4:B:813:LEU:CD2	1.93	0.98
4:B:810:ASP:OD1	4:B:812:ARG:HD3	1.64	0.98
1:A:230:GLU:CG	1:A:279:VAL:HG11	1.94	0.98
1:A:290:GLN:HE21	1:A:292:PRO:CG	1.77	0.97
1:A:541:LEU:HD22	4:B:786:SER:HB3	1.46	0.96
2:C:1343:VAL:HG21	2:C:1469:ARG:HB3	1.48	0.96
1:A:287:ASP:CA	1:A:291:ASN:HB3	1.95	0.96
1:A:290:GLN:C	1:A:292:PRO:HD3	1.92	0.94
1:A:286:LEU:N	1:A:286:LEU:CD2	2.30	0.94
1:A:590:THR:HG22	1:A:592:SER:N	1.83	0.94
1:A:281:SER:CB	1:A:284:VAL:CG2	2.45	0.94
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.48	0.94
1:A:280:LEU:CG	1:A:285:LEU:CD1	2.46	0.93
3:M:39:TYR:CE1	3:M:43:THR:OG1	2.21	0.92
1:A:287:ASP:CA	1:A:291:ASN:H	1.82	0.92
4:B:734:ILE:HD12	4:B:734:ILE:H	1.35	0.92
2:C:1516:GLU:HB3	2:C:1517:PRO:HD2	1.50	0.91
2:C:1575:GLU:HB2	2:C:1578:LYS:HD2	1.49	0.91
1:A:161:GLN:C	1:A:162:ASN:OD1	2.14	0.90
1:A:591:GLN:H	4:B:795:VAL:HG11	1.30	0.89
1:A:10:ASN:HB3	1:A:635:ARG:HH11	1.37	0.89
1:A:281:SER:C	1:A:284:VAL:HG23	1.98	0.89
2:C:1573:LYS:O	2:C:1574:LEU:HD23	1.73	0.88
2:C:1539:TYR:CE1	2:C:1574:LEU:HD12	2.08	0.88
4:B:811:LEU:CD1	4:B:813:LEU:CD2	2.48	0.88
1:A:591:GLN:CB	4:B:795:VAL:HB	1.99	0.87
1:A:346:MET:O	1:A:391:THR:HG22	1.74	0.86
1:A:142:MET:HG3	1:A:187:TYR:CE1	2.10	0.86
4:B:883:THR:HG21	4:B:911:PRO:HG3	1.58	0.85
2:C:1497:PHE:CD1	2:C:1498:ILE:HG13	2.11	0.85
1:A:287:ASP:N	1:A:291:ASN:CB	2.39	0.85
4:B:811:LEU:CG	4:B:813:LEU:HD22	2.05	0.85
4:B:822:GLN:HB2	4:B:879:VAL:HG22	1.55	0.85
4:B:733:ILE:HG12	4:B:734:ILE:N	1.90	0.85
1:A:280:LEU:HD11	1:A:285:LEU:CD1	2.06	0.85
1:A:281:SER:CB	1:A:284:VAL:HG23	2.06	0.85
1:A:281:SER:HB2	1:A:284:VAL:HG23	1.58	0.84
2:C:1386:MET:HE3	2:C:1389:PHE:CG	2.12	0.84
4:B:811:LEU:HG	4:B:813:LEU:CD2	2.08	0.84
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:822:GLN:O	4:B:822:GLN:HG2	1.78	0.84
1:A:8:THR:HG22	1:A:20:MET:HB2	1.60	0.84
1:A:126:ARG:HG3	4:B:751:TRP:CZ2	2.13	0.84
4:B:833:ARG:HD2	4:B:834:GLN:HE22	1.42	0.83
1:A:229:LEU:O	1:A:279:VAL:HG12	1.78	0.83
1:A:591:GLN:OE1	4:B:795:VAL:HG23	1.79	0.83
4:B:810:ASP:OD1	4:B:812:ARG:CD	2.26	0.83
4:B:811:LEU:CG	4:B:813:LEU:CD2	2.58	0.82
4:B:833:ARG:HD2	4:B:834:GLN:NE2	1.95	0.82
1:A:223:ILE:HD11	1:A:298:VAL:HG23	1.61	0.82
2:C:1391:PRO:HB2	2:C:1396:LEU:HD11	1.61	0.82
4:B:811:LEU:CD1	4:B:812:ARG:N	2.41	0.82
2:C:1444:TYR:CD1	2:C:1445:PHE:HB2	2.16	0.81
1:A:590:THR:HB	1:A:593:LYS:HG3	1.61	0.81
2:C:1451:GLN:HG3	2:C:1452:PRO:HD2	1.63	0.80
2:C:1518:GLY:O	2:C:1585:LEU:HA	1.82	0.80
1:A:400:ILE:HD13	1:A:419:MET:HE3	1.60	0.80
2:C:1497:PHE:CD1	2:C:1498:ILE:CG1	2.64	0.80
1:A:55:THR:HG22	1:A:57:ALA:H	1.45	0.80
1:A:161:GLN:CG	1:A:162:ASN:OD1	2.30	0.80
1:A:281:SER:OG	1:A:284:VAL:CG2	2.30	0.80
1:A:281:SER:O	1:A:284:VAL:CG2	2.29	0.80
1:A:161:GLN:CB	1:A:162:ASN:OD1	2.30	0.79
1:A:541:LEU:HB2	4:B:794:CYS:SG	2.23	0.79
3:M:29:ASN:ND2	3:M:44:ILE:HD12	1.97	0.79
1:A:286:LEU:C	1:A:291:ASN:HA	2.08	0.79
1:A:281:SER:HB2	1:A:284:VAL:CG2	2.13	0.79
3:M:70:LEU:HG	3:M:74:TYR:CD1	2.17	0.78
4:B:811:LEU:HD12	4:B:812:ARG:N	1.97	0.78
2:C:1536:PHE:HD1	2:C:1563:ILE:HG21	1.47	0.78
4:B:831:ASN:HD21	4:B:868:PRO:HA	1.45	0.78
4:B:810:ASP:OD2	4:B:812:ARG:HD3	1.82	0.78
2:C:1343:VAL:HG21	2:C:1469:ARG:CB	2.14	0.77
3:M:29:ASN:ND2	3:M:44:ILE:CD1	2.48	0.77
1:A:180:GLY:O	1:A:182:TRP:HD1	1.66	0.77
1:A:290:GLN:O	1:A:290:GLN:CG	2.33	0.77
2:C:1490:ARG:NH1	2:C:1599:ILE:HG21	2.00	0.77
4:B:841:ARG:HG2	4:B:841:ARG:HH11	1.50	0.77
4:B:741:SER:HB3	4:B:902:GLY:C	2.09	0.76
1:A:297:LEU:HD23	1:A:326:ILE:HD13	1.67	0.76
1:A:365:VAL:HG13	1:A:379:THR:OG1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD11	1:A:64:VAL:HG23	1.67	0.75
2:C:1497:PHE:C	2:C:1498:ILE:HG13	2.10	0.75
4:B:795:VAL:O	4:B:795:VAL:CG1	2.34	0.75
4:B:810:ASP:CB	4:B:828:VAL:HG23	2.13	0.75
1:A:530:TRP:HD1	1:A:531:VAL:N	1.85	0.75
3:M:73:ILE:O	3:M:77:ILE:HG12	1.87	0.75
4:B:788:SER:O	4:B:790:LYS:N	2.20	0.74
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.16	0.74
1:A:610:GLY:HA3	1:A:616:VAL:N	2.02	0.74
3:M:70:LEU:HG	3:M:74:TYR:CE1	2.22	0.74
1:A:12:LEU:HB2	1:A:101:VAL:HG22	1.70	0.74
1:A:117:TYR:CZ	1:A:123:VAL:HG13	2.22	0.74
1:A:180:GLY:O	1:A:182:TRP:CD1	2.41	0.74
1:A:20:MET:O	1:A:64:VAL:HB	1.87	0.74
1:A:223:ILE:O	1:A:282:ARG:NH1	2.21	0.74
2:C:1403:VAL:O	2:C:1404:ASP:HB2	1.88	0.74
1:A:290:GLN:O	1:A:292:PRO:HD3	1.86	0.73
2:C:1573:LYS:N	2:C:1573:LYS:HD2	2.02	0.73
1:A:280:LEU:CD1	1:A:285:LEU:CD1	2.65	0.73
1:A:369:VAL:HG12	1:A:370:GLN:N	2.03	0.73
4:B:822:GLN:HB2	4:B:879:VAL:CG2	2.18	0.73
2:C:1444:TYR:CE1	2:C:1445:PHE:HB2	2.24	0.73
4:B:813:LEU:HD12	4:B:814:PRO:CD	2.19	0.73
2:C:1370:TYR:CD2	2:C:1376:ALA:HB2	2.24	0.73
1:A:290:GLN:HG2	1:A:292:PRO:HD3	1.70	0.72
1:A:180:GLY:O	1:A:181:GLN:C	2.30	0.72
1:A:287:ASP:H	1:A:291:ASN:HB3	1.54	0.72
2:C:1575:GLU:O	2:C:1578:LYS:HB2	1.89	0.72
4:B:777:ILE:HG22	4:B:777:ILE:O	1.88	0.72
4:B:756:LEU:N	4:B:756:LEU:HD23	2.05	0.72
4:B:810:ASP:HB3	4:B:828:VAL:CG2	2.16	0.72
4:B:833:ARG:HH22	4:B:899:ILE:HD11	1.53	0.72
4:B:749:TRP:CE3	4:B:750:LEU:HB2	2.26	0.71
1:A:390:ASN:OD1	1:A:390:ASN:O	2.07	0.71
4:B:874:VAL:HG12	4:B:874:VAL:O	1.90	0.71
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.72	0.71
1:A:289:VAL:O	1:A:290:GLN:CB	2.33	0.71
3:M:36:LEU:HD23	3:M:36:LEU:N	2.06	0.71
1:A:6:ILE:HD11	1:A:22:LEU:HD23	1.72	0.71
1:A:6:ILE:HD11	1:A:20:MET:HE3	1.73	0.71
1:A:257:GLU:N	1:A:257:GLU:CD	2.49	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:17:ASN:CG	3:M:17:ASN:O	2.34	0.71
1:A:280:LEU:HD21	1:A:285:LEU:HD11	0.72	0.71
1:A:161:GLN:HB3	1:A:162:ASN:OD1	1.91	0.71
1:A:591:GLN:HA	4:B:795:VAL:HG21	1.72	0.70
1:A:495:LEU:HD12	1:A:496:PRO:HD2	1.73	0.70
1:A:230:GLU:HG2	1:A:279:VAL:CG1	2.07	0.70
1:A:268:ARG:HB2	2:C:1378:MET:HE3	1.72	0.70
2:C:1341:LEU:HD23	2:C:1469:ARG:H	1.56	0.70
2:C:1343:VAL:CG2	2:C:1469:ARG:HB3	2.21	0.70
2:C:1345:ILE:HD12	2:C:1363:ILE:O	1.92	0.70
1:A:239:TYR:HB2	4:B:804:MET:SD	2.32	0.69
1:A:330:PRO:O	1:A:357:PRO:HD3	1.92	0.69
1:A:237:PHE:CE2	1:A:243:VAL:HG22	2.27	0.69
1:A:281:SER:CB	1:A:284:VAL:HG21	2.16	0.69
4:B:731:GLU:O	4:B:733:ILE:N	2.25	0.69
1:A:38:HIS:CE1	1:A:45:LEU:HD12	2.27	0.69
1:A:161:GLN:C	1:A:163:GLN:H	1.98	0.69
1:A:591:GLN:OE1	4:B:795:VAL:CG2	2.39	0.69
1:A:369:VAL:HG12	1:A:370:GLN:H	1.58	0.69
3:M:38:THR:O	3:M:39:TYR:C	2.34	0.69
1:A:229:LEU:C	1:A:279:VAL:HG12	2.18	0.69
1:A:589:LEU:HD12	1:A:590:THR:H	1.57	0.69
2:C:1416:PHE:C	2:C:1416:PHE:CD2	2.70	0.69
2:C:1510:ARG:NH1	2:C:1627:LEU:HD23	2.08	0.69
4:B:811:LEU:HD13	4:B:812:ARG:N	2.06	0.69
2:C:1386:MET:HE3	2:C:1389:PHE:CD1	2.28	0.69
1:A:281:SER:O	1:A:282:ARG:C	2.36	0.69
2:C:1342:LYS:CB	2:C:1367:CYS:HB2	2.23	0.69
4:B:813:LEU:HD12	4:B:814:PRO:HD3	1.74	0.69
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.74	0.68
4:B:777:ILE:O	4:B:777:ILE:CG2	2.41	0.68
2:C:1391:PRO:CB	2:C:1396:LEU:HD11	2.24	0.68
4:B:831:ASN:HD22	4:B:868:PRO:HA	1.57	0.68
2:C:1342:LYS:HB2	2:C:1367:CYS:HB2	1.74	0.68
1:A:19:THR:HA	1:A:64:VAL:O	1.94	0.68
2:C:1590:TRP:HB3	2:C:1597:SER:HB2	1.75	0.68
1:A:216:PRO:HB2	1:A:218:GLU:O	1.95	0.67
1:A:280:LEU:HG	1:A:285:LEU:CD1	2.24	0.67
2:C:1391:PRO:HB2	2:C:1396:LEU:CD1	2.24	0.67
1:A:294:ALA:O	1:A:295:GLU:C	2.36	0.67
3:M:26:LEU:CA	3:M:74:TYR:OH	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HB3	1:A:291:ASN:HB2	1.77	0.67
4:B:734:ILE:CD1	4:B:893:ALA:HB1	2.22	0.67
3:M:70:LEU:O	3:M:74:TYR:HD1	1.77	0.66
1:A:286:LEU:C	1:A:291:ASN:CA	2.68	0.66
4:B:742:ARG:HB3	4:B:775:ASP:HB3	1.78	0.66
3:M:36:LEU:HB3	3:M:40:TYR:CD2	2.30	0.66
4:B:793:ILE:HG23	4:B:793:ILE:O	1.95	0.66
4:B:841:ARG:HG2	4:B:841:ARG:NH1	2.09	0.66
1:A:130:VAL:HG12	1:A:136:PRO:HA	1.78	0.66
2:C:1532:LEU:HD21	2:C:1569:ARG:HE	1.60	0.66
2:C:1570:GLU:HG3	2:C:1571:ALA:H	1.61	0.66
1:A:282:ARG:O	1:A:284:VAL:N	2.29	0.66
1:A:567:HIS:ND1	4:B:760:PRO:HG3	2.10	0.66
2:C:1451:GLN:CG	2:C:1452:PRO:HD2	2.26	0.66
2:C:1600:ILE:O	2:C:1600:ILE:HG22	1.94	0.66
4:B:841:ARG:HH11	4:B:841:ARG:CG	2.08	0.66
2:C:1585:LEU:HD21	2:C:1603:ASP:HB3	1.76	0.66
3:M:84:LYS:O	3:M:84:LYS:HG3	1.96	0.66
4:B:835:ASN:OD1	4:B:835:ASN:O	2.13	0.66
4:B:883:THR:CG2	4:B:911:PRO:HG3	2.26	0.65
2:C:1490:ARG:HH11	2:C:1599:ILE:HG21	1.61	0.65
1:A:293:ARG:NH1	1:A:295:GLU:OE2	2.29	0.65
2:C:1510:ARG:HH12	2:C:1627:LEU:CD2	2.09	0.65
4:B:843:GLU:OE2	4:B:859:ARG:HD3	1.96	0.65
1:A:281:SER:O	1:A:284:VAL:N	2.30	0.65
1:A:223:ILE:CD1	1:A:298:VAL:HG23	2.26	0.65
3:M:39:TYR:O	3:M:40:TYR:C	2.38	0.65
1:A:8:THR:HG22	1:A:20:MET:CB	2.26	0.65
2:C:1494:GLU:HB2	2:C:1602:LYS:HB3	1.79	0.65
2:C:1532:LEU:HD23	2:C:1537:ASP:HB3	1.79	0.64
2:C:1450:ILE:HG13	2:C:1450:ILE:O	1.96	0.64
2:C:1590:TRP:HA	2:C:1590:TRP:CE3	2.32	0.64
1:A:285:LEU:O	1:A:286:LEU:C	2.40	0.64
2:C:1518:GLY:HA3	2:C:1585:LEU:HD22	1.80	0.64
1:A:572:VAL:HG12	4:B:753:VAL:HG22	1.79	0.64
1:A:281:SER:O	1:A:284:VAL:CB	2.45	0.64
1:A:294:ALA:O	1:A:296:ASP:N	2.30	0.64
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.79	0.64
1:A:287:ASP:O	1:A:290:GLN:N	2.30	0.64
1:A:335:PHE:CD2	1:A:419:MET:HB3	2.33	0.64
2:C:1416:PHE:HA	2:C:1419:ARG:HH12	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1470:PHE:CZ	4:B:822:GLN:O	2.50	0.64
3:M:17:ASN:O	3:M:17:ASN:ND2	2.31	0.64
4:B:833:ARG:CD	4:B:834:GLN:NE2	2.60	0.64
1:A:6:ILE:HG22	1:A:625:THR:HB	1.80	0.64
1:A:295:GLU:O	1:A:296:ASP:C	2.42	0.64
1:A:407:GLN:O	1:A:408:GLU:HB2	1.96	0.63
4:B:811:LEU:HG	4:B:813:LEU:HD23	1.79	0.63
4:B:874:VAL:O	4:B:874:VAL:CG1	2.45	0.63
2:C:1461:TYR:CD1	2:C:1462:ASN:HB2	2.34	0.63
1:A:445:PRO:HA	1:A:499:ILE:O	1.98	0.63
1:A:93:GLN:OE1	1:A:93:GLN:HA	1.97	0.63
1:A:105:SER:HB2	1:A:188:TYR:CD1	2.33	0.63
1:A:295:GLU:O	1:A:298:VAL:N	2.30	0.63
1:A:610:GLY:HA3	1:A:616:VAL:H	1.63	0.63
1:A:307:THR:HG23	1:A:318:GLN:HG3	1.81	0.62
2:C:1451:GLN:HB2	4:B:853:LEU:HD12	1.79	0.62
1:A:10:ASN:CG	1:A:635:ARG:HD2	2.24	0.62
1:A:114:LYS:HE3	1:A:116:ILE:O	1.99	0.62
1:A:287:ASP:CA	1:A:291:ASN:CB	2.74	0.62
1:A:340:LYS:O	1:A:341:TYR:CD1	2.53	0.62
1:A:136:PRO:CG	4:B:789:ASP:HA	2.30	0.62
1:A:239:TYR:HB2	4:B:804:MET:HG3	1.79	0.62
2:C:1527:LEU:HD21	2:C:1530:VAL:CG2	2.29	0.62
4:B:811:LEU:C	4:B:811:LEU:HD13	2.23	0.62
4:B:833:ARG:HH11	4:B:833:ARG:HG2	1.64	0.62
1:A:154:LYS:HE2	1:A:156:ASP:OD1	2.00	0.62
2:C:1575:GLU:OE2	2:C:1578:LYS:HD2	2.00	0.62
1:A:281:SER:CA	1:A:284:VAL:HG23	2.29	0.62
2:C:1527:LEU:HD21	2:C:1530:VAL:HG22	1.81	0.62
4:B:745:PHE:CE2	4:B:905:LYS:HG2	2.34	0.62
1:A:161:GLN:C	1:A:163:GLN:N	2.54	0.61
1:A:251:PHE:CD1	1:A:280:LEU:HB2	2.35	0.61
1:A:346:MET:HE1	1:A:454:LEU:HG	1.82	0.61
2:C:1550:GLY:C	2:C:1552:ASP:H	2.07	0.61
1:A:126:ARG:HG3	4:B:751:TRP:CH2	2.35	0.61
1:A:433:TYR:HB2	1:A:456:ARG:HB3	1.81	0.61
4:B:844:LEU:HD12	4:B:845:LEU:N	2.14	0.61
4:B:907:LEU:HD23	4:B:907:LEU:H	1.64	0.61
2:C:1497:PHE:CD1	2:C:1498:ILE:HG12	2.36	0.61
1:A:282:ARG:C	1:A:284:VAL:N	2.54	0.61
2:C:1506:THR:OG1	2:C:1509:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:26:LEU:C	3:M:26:LEU:HD12	2.26	0.61
4:B:840:VAL:CG1	4:B:892:ALA:HB1	2.30	0.61
1:A:487:GLU:O	1:A:490:GLN:HB2	2.01	0.61
2:C:1572:LEU:HD13	2:C:1574:LEU:HG	1.82	0.61
2:C:1358:ALA:HB1	2:C:1361:THR:CG2	2.31	0.61
2:C:1527:LEU:HD13	2:C:1541:MET:HG2	1.83	0.61
1:A:438:VAL:O	1:A:440:ARG:HG3	2.00	0.60
4:B:847:ASN:CB	4:B:850:PHE:HD1	2.14	0.60
1:A:73:GLU:HB3	1:A:82:LYS:NZ	2.16	0.60
1:A:239:TYR:CE1	4:B:832:TYR:CE1	2.89	0.60
1:A:282:ARG:O	1:A:285:LEU:N	2.26	0.60
1:A:179:MET:HG2	1:A:203:LYS:HA	1.83	0.60
1:A:297:LEU:HD23	1:A:326:ILE:CD1	2.31	0.60
1:A:513:TYR:CE1	1:A:525:VAL:HB	2.37	0.60
1:A:530:TRP:CD1	1:A:531:VAL:N	2.69	0.60
1:A:160:SER:HA	1:A:167:LEU:HD21	1.82	0.60
4:B:833:ARG:CD	4:B:834:GLN:HE22	2.11	0.60
1:A:134:LEU:HD11	1:A:598:VAL:HG21	1.84	0.60
1:A:241:LYS:HG3	4:B:832:TYR:CE2	2.36	0.60
2:C:1575:GLU:HB2	2:C:1578:LYS:CD	2.26	0.60
1:A:334:HIS:HB2	1:A:353:PHE:HB3	1.83	0.60
1:A:455:LEU:HD11	1:A:457:MET:HG2	1.82	0.60
2:C:1360:ASN:HD22	2:C:1443:GLN:HB3	1.66	0.60
1:A:606:THR:HG22	1:A:608:GLY:N	2.17	0.59
2:C:1590:TRP:HA	2:C:1590:TRP:HE3	1.67	0.59
4:B:808:PHE:HE1	4:B:830:TYR:CD2	2.20	0.59
1:A:591:GLN:CA	4:B:795:VAL:HG21	2.32	0.59
1:A:10:ASN:HB3	1:A:635:ARG:NH1	2.15	0.59
1:A:22:LEU:HB2	1:A:62:GLY:HA3	1.82	0.59
1:A:135:LEU:HD22	4:B:789:ASP:O	2.02	0.59
2:C:1343:VAL:CG2	2:C:1469:ARG:CB	2.79	0.59
2:C:1528:VAL:HG21	2:C:1559:GLN:OE1	2.00	0.59
1:A:99:VAL:HG12	1:A:100:LEU:N	2.18	0.59
2:C:1530:VAL:HG23	2:C:1576:GLU:HG2	1.84	0.59
4:B:822:GLN:O	4:B:822:GLN:CG	2.48	0.59
1:A:446:GLY:N	1:A:499:ILE:O	2.32	0.59
4:B:808:PHE:CE1	4:B:830:TYR:HB2	2.38	0.59
4:B:841:ARG:HG2	4:B:841:ARG:O	2.03	0.59
1:A:536:SER:O	1:A:537:CYS:C	2.46	0.59
2:C:1589:PHE:CE1	2:C:1598:TYR:CE2	2.91	0.59
1:A:177:VAL:HG21	1:A:182:TRP:HH2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:MET:HG2	1:A:64:VAL:HG21	1.84	0.59
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.85	0.59
2:C:1569:ARG:NH1	2:C:1569:ARG:HG3	2.17	0.58
3:M:38:THR:O	3:M:39:TYR:O	2.20	0.58
2:C:1507:LEU:HD11	2:C:1629:ALA:HB1	1.85	0.58
4:B:808:PHE:CD1	4:B:808:PHE:C	2.81	0.58
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.32	0.58
1:A:589:LEU:HD12	1:A:590:THR:N	2.18	0.58
2:C:1505:VAL:HG12	2:C:1510:ARG:HE	1.68	0.58
4:B:902:GLY:C	4:B:903:VAL:CG2	2.76	0.58
2:C:1336:CYS:O	2:C:1337:ASN:CG	2.47	0.58
4:B:844:LEU:HB2	4:B:876:TYR:CE2	2.39	0.58
1:A:533:VAL:HG12	1:A:534:LYS:N	2.17	0.58
4:B:732:ASP:O	4:B:896:HIS:N	2.33	0.58
1:A:47:LEU:HD11	1:A:66:PHE:HB2	1.84	0.58
1:A:117:TYR:CG	1:A:123:VAL:HG22	2.37	0.58
1:A:230:GLU:CB	1:A:279:VAL:CG1	2.81	0.58
1:A:61:MET:HE2	1:A:483:ARG:HG2	1.85	0.58
1:A:118:THR:HG23	1:A:205:TYR:CZ	2.38	0.58
1:A:345:GLY:H	1:A:391:THR:HG23	1.68	0.58
2:C:1470:PHE:HB2	2:C:1478:GLY:HA3	1.85	0.57
4:B:835:ASN:O	4:B:836:GLN:CB	2.51	0.57
1:A:246:THR:OG1	2:C:1425:TYR:CZ	2.57	0.57
1:A:290:GLN:C	1:A:292:PRO:CD	2.73	0.57
1:A:513:TYR:CZ	1:A:525:VAL:HB	2.39	0.57
2:C:1572:LEU:C	2:C:1573:LYS:HD2	2.28	0.57
3:M:55:LEU:O	3:M:58:LYS:HD3	2.04	0.57
1:A:477:ARG:NH2	1:A:479:LEU:HD13	2.20	0.57
2:C:1519:VAL:HG12	2:C:1548:LYS:NZ	2.20	0.57
3:M:39:TYR:O	3:M:42:ARG:N	2.37	0.57
2:C:1617:ASP:O	2:C:1621:GLN:HG3	2.04	0.57
2:C:1569:ARG:HG3	2:C:1569:ARG:HH11	1.70	0.57
1:A:99:VAL:HG12	1:A:100:LEU:H	1.70	0.57
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.87	0.57
1:A:282:ARG:C	1:A:284:VAL:H	2.12	0.57
1:A:541:LEU:CD2	4:B:786:SER:HB3	2.28	0.57
2:C:1536:PHE:CD1	2:C:1563:ILE:HG21	2.36	0.57
3:M:70:LEU:O	3:M:74:TYR:CD1	2.57	0.57
1:A:541:LEU:HD22	4:B:794:CYS:HB3	1.87	0.56
1:A:594:ILE:O	1:A:598:VAL:HG23	2.05	0.56
3:M:29:ASN:ND2	3:M:44:ILE:HD11	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1444:TYR:CD1	2:C:1444:TYR:C	2.82	0.56
3:M:84:LYS:O	3:M:85:TYR:HB2	2.05	0.56
1:A:6:ILE:CD1	1:A:22:LEU:HD23	2.33	0.56
1:A:345:GLY:N	1:A:391:THR:HG23	2.20	0.56
4:B:741:SER:HB3	4:B:903:VAL:N	2.19	0.56
1:A:292:PRO:O	1:A:293:ARG:O	2.24	0.56
1:A:257:GLU:CD	1:A:257:GLU:H	2.13	0.56
1:A:287:ASP:HA	1:A:291:ASN:CB	2.36	0.56
1:A:406:LYS:H	1:A:414:GLN:HE22	1.54	0.56
2:C:1410:TYR:C	2:C:1410:TYR:CD2	2.83	0.56
3:M:70:LEU:CG	3:M:74:TYR:CE1	2.89	0.56
1:A:281:SER:CA	1:A:284:VAL:CG2	2.84	0.56
2:C:1572:LEU:O	2:C:1573:LYS:HB3	2.06	0.56
4:B:761:LYS:O	4:B:762:ASN:HB2	2.06	0.56
1:A:210:PHE:CE2	1:A:310:LEU:HD21	2.41	0.56
1:A:239:TYR:HE1	4:B:832:TYR:CZ	2.24	0.56
1:A:443:LEU:O	1:A:533:VAL:HG13	2.06	0.56
2:C:1510:ARG:NH1	2:C:1627:LEU:CD2	2.68	0.56
1:A:430:SER:O	1:A:431:ASN:HB2	2.06	0.55
1:A:239:TYR:HB2	4:B:804:MET:CG	2.36	0.55
1:A:290:GLN:O	1:A:292:PRO:CD	2.55	0.55
2:C:1386:MET:CE	2:C:1389:PHE:CD1	2.88	0.55
1:A:230:GLU:N	1:A:279:VAL:HG12	2.22	0.55
2:C:1366:ILE:HD11	2:C:1455:VAL:HG21	1.88	0.55
2:C:1530:VAL:HG12	2:C:1530:VAL:O	2.07	0.55
3:M:64:SER:O	3:M:67:LYS:HB3	2.05	0.55
4:B:788:SER:C	4:B:790:LYS:N	2.63	0.55
1:A:142:MET:HG3	1:A:187:TYR:HE1	1.64	0.55
1:A:239:TYR:CB	4:B:804:MET:HG3	2.36	0.55
1:A:536:SER:O	1:A:537:CYS:O	2.24	0.55
1:A:610:GLY:N	1:A:616:VAL:HG23	2.22	0.55
1:A:148:PRO:HG3	1:A:182:TRP:CD1	2.42	0.55
1:A:440:ARG:NH2	1:A:529:VAL:HG23	2.22	0.55
1:A:586:LYS:O	1:A:587:ASN:HB2	2.05	0.55
2:C:1389:PHE:CZ	2:C:1443:GLN:HB2	2.41	0.55
2:C:1407:ILE:HB	2:C:1412:LEU:HD11	1.89	0.55
2:C:1421:THR:OG1	2:C:1422:LEU:N	2.39	0.55
1:A:177:VAL:HG21	1:A:182:TRP:CH2	2.42	0.55
4:B:785:VAL:HG13	4:B:794:CYS:O	2.07	0.55
1:A:161:GLN:O	1:A:162:ASN:CB	2.46	0.55
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:835:ASN:O	4:B:836:GLN:CG	2.55	0.55
1:A:287:ASP:O	1:A:288:GLY:C	2.51	0.54
1:A:34:THR:HG22	1:A:51:LYS:HE2	1.88	0.54
1:A:577:ASP:HB2	4:B:780:TRP:CZ3	2.42	0.54
2:C:1386:MET:O	2:C:1387:THR:C	2.50	0.54
1:A:297:LEU:O	1:A:298:VAL:C	2.51	0.54
4:B:844:LEU:HB2	4:B:876:TYR:CZ	2.43	0.54
4:B:778:THR:HG23	4:B:779:THR:N	2.21	0.54
1:A:126:ARG:CG	4:B:751:TRP:CZ2	2.88	0.54
1:A:136:PRO:CD	4:B:789:ASP:HA	2.37	0.54
2:C:1575:GLU:O	2:C:1576:GLU:C	2.51	0.54
1:A:147:ASN:HB2	1:A:148:PRO:HD3	1.90	0.54
1:A:363:TYR:CZ	1:A:364:ARG:HG3	2.43	0.54
2:C:1421:THR:O	2:C:1422:LEU:CB	2.56	0.54
1:A:54:LEU:HB3	1:A:60:HIS:HA	1.90	0.54
4:B:749:TRP:CZ3	4:B:750:LEU:HB2	2.43	0.54
1:A:471:LEU:O	1:A:509:LEU:HD12	2.06	0.53
2:C:1413:ASP:O	2:C:1414:LYS:C	2.50	0.53
4:B:793:ILE:O	4:B:793:ILE:CG2	2.56	0.53
1:A:524:VAL:HB	1:A:613:TYR:CD1	2.43	0.53
1:A:577:ASP:HB2	4:B:780:TRP:HZ3	1.73	0.53
2:C:1392:ASP:HB2	2:C:1442:HIS:NE2	2.23	0.53
2:C:1416:PHE:HA	2:C:1419:ARG:NH1	2.23	0.53
1:A:146:GLU:CD	1:A:185:ARG:HD2	2.33	0.53
1:A:287:ASP:CA	1:A:291:ASN:N	2.53	0.53
2:C:1586:SER:HA	2:C:1589:PHE:CE2	2.42	0.53
1:A:124:LEU:N	1:A:124:LEU:HD23	2.24	0.53
1:A:297:LEU:HA	1:A:300:LYS:HD2	1.91	0.53
1:A:567:HIS:CG	4:B:760:PRO:HG3	2.44	0.53
1:A:239:TYR:HE1	4:B:832:TYR:CE1	2.26	0.53
4:B:833:ARG:HH11	4:B:833:ARG:CG	2.22	0.53
2:C:1507:LEU:HD22	2:C:1511:LEU:HD12	1.91	0.53
4:B:902:GLY:C	4:B:903:VAL:HG23	2.32	0.53
1:A:34:THR:CG2	1:A:51:LYS:HE2	2.38	0.53
2:C:1358:ALA:HB1	2:C:1361:THR:HG22	1.91	0.53
2:C:1403:VAL:HG22	2:C:1404:ASP:N	2.23	0.53
4:B:847:ASN:HB3	4:B:850:PHE:HD1	1.74	0.53
2:C:1461:TYR:HD1	2:C:1462:ASN:HB2	1.74	0.53
1:A:117:TYR:CD1	1:A:123:VAL:HG22	2.44	0.52
2:C:1384:SER:HA	2:C:1421:THR:HA	1.91	0.52
1:A:39:ASP:OD1	1:A:44:LYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:O	1:A:155:GLN:HA	2.10	0.52
1:A:290:GLN:HE21	1:A:292:PRO:CD	2.21	0.52
1:A:468:TYR:HE1	1:A:513:TYR:HD2	1.57	0.52
4:B:887:GLU:CG	4:B:887:GLU:O	2.57	0.52
1:A:357:PRO:O	1:A:358:ASP:C	2.53	0.52
1:A:365:VAL:CG1	1:A:379:THR:OG1	2.56	0.52
1:A:581:PHE:CE1	1:A:588:LYS:HD2	2.45	0.52
2:C:1514:ALA:HA	2:C:1519:VAL:HG21	1.92	0.52
2:C:1554:VAL:O	2:C:1554:VAL:HG13	2.09	0.52
1:A:468:TYR:HE1	1:A:513:TYR:CD2	2.28	0.52
1:A:510:VAL:HG12	1:A:528:SER:CB	2.30	0.52
2:C:1366:ILE:HD11	2:C:1455:VAL:CG2	2.39	0.52
2:C:1582:MET:SD	2:C:1606:VAL:HG22	2.50	0.52
2:C:1570:GLU:HG3	2:C:1571:ALA:N	2.23	0.52
1:A:363:TYR:CE1	1:A:364:ARG:HG3	2.44	0.52
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.45	0.52
2:C:1516:GLU:HB3	2:C:1517:PRO:CD	2.32	0.52
4:B:895:TYR:HB3	4:B:896:HIS:CE1	2.44	0.52
1:A:136:PRO:HD2	4:B:789:ASP:HA	1.91	0.52
2:C:1461:TYR:CD1	2:C:1462:ASN:N	2.78	0.52
1:A:404:THR:C	1:A:414:GLN:OE1	2.53	0.52
1:A:403:ARG:HG2	1:A:404:THR:O	2.10	0.52
2:C:1375:ASP:OD2	2:C:1430:SER:HA	2.10	0.52
3:M:59:ASP:C	3:M:59:ASP:OD1	2.52	0.51
4:B:788:SER:O	4:B:791:LYS:N	2.43	0.51
1:A:193:GLN:HG2	1:A:194:GLN:N	2.24	0.51
1:A:287:ASP:N	1:A:291:ASN:CA	2.72	0.51
1:A:472:ILE:HG13	1:A:480:LYS:HB3	1.92	0.51
3:M:36:LEU:HB3	3:M:40:TYR:HD2	1.73	0.51
3:M:66:ALA:O	3:M:67:LYS:C	2.53	0.51
4:B:811:LEU:HD12	4:B:813:LEU:HD22	1.77	0.51
4:B:907:LEU:HD23	4:B:907:LEU:N	2.24	0.51
1:A:37:VAL:HB	1:A:46:VAL:HG23	1.93	0.51
1:A:343:LYS:HD2	1:A:343:LYS:N	2.25	0.51
1:A:19:THR:HG23	1:A:64:VAL:O	2.10	0.51
1:A:590:THR:HG21	1:A:592:SER:HB2	1.92	0.51
2:C:1345:ILE:HG23	2:C:1345:ILE:O	2.09	0.51
3:M:70:LEU:O	3:M:74:TYR:HB2	2.11	0.51
1:A:367:VAL:HG23	1:A:387:LEU:HD11	1.92	0.51
1:A:591:GLN:HB2	4:B:795:VAL:CG1	2.38	0.51
2:C:1483:LEU:HD23	2:C:1599:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1575:GLU:CB	2:C:1578:LYS:HD2	2.32	0.51
4:B:842:VAL:HG23	4:B:892:ALA:HB2	1.91	0.51
1:A:148:PRO:HG2	1:A:179:MET:O	2.11	0.51
1:A:468:TYR:CE1	1:A:513:TYR:HD2	2.28	0.51
1:A:595:TRP:CE3	1:A:595:TRP:HA	2.45	0.51
2:C:1385:MET:HG3	2:C:1390:ALA:HA	1.93	0.51
2:C:1444:TYR:CD1	2:C:1445:PHE:CB	2.93	0.51
2:C:1586:SER:O	2:C:1589:PHE:HD2	1.93	0.51
2:C:1415:ALA:O	2:C:1416:PHE:C	2.54	0.51
2:C:1416:PHE:C	2:C:1416:PHE:HD2	2.16	0.51
2:C:1550:GLY:C	2:C:1552:ASP:N	2.67	0.51
1:A:38:HIS:HE1	1:A:45:LEU:HD12	1.73	0.51
1:A:138:GLY:HA2	1:A:160:SER:OG	2.10	0.51
1:A:369:VAL:CG1	1:A:370:GLN:H	2.24	0.51
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.92	0.51
3:M:29:ASN:HD22	3:M:44:ILE:HD11	1.74	0.51
4:B:788:SER:C	4:B:790:LYS:H	2.18	0.51
1:A:4:TYR:HB3	1:A:90:PHE:CE2	2.46	0.50
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.11	0.50
2:C:1510:ARG:HH12	2:C:1627:LEU:HD23	1.68	0.50
4:B:739:ILE:HG22	4:B:739:ILE:O	2.11	0.50
1:A:285:LEU:O	1:A:286:LEU:O	2.29	0.50
2:C:1507:LEU:HD11	2:C:1629:ALA:CB	2.42	0.50
2:C:1585:LEU:N	2:C:1585:LEU:HD23	2.26	0.50
3:M:49:GLN:O	3:M:50:LYS:C	2.53	0.50
1:A:3:MET:HE2	1:A:626:SER:CB	2.41	0.50
2:C:1365:GLU:HG3	2:C:1437:LEU:O	2.11	0.50
2:C:1451:GLN:CG	2:C:1452:PRO:CD	2.90	0.50
2:C:1573:LYS:O	2:C:1573:LYS:CD	2.59	0.50
1:A:162:ASN:OD1	1:A:162:ASN:N	2.43	0.50
1:A:184:ILE:HG13	1:A:200:PHE:HE2	1.77	0.50
1:A:291:ASN:O	1:A:291:ASN:OD1	2.29	0.50
1:A:495:LEU:HD12	1:A:496:PRO:CD	2.40	0.50
1:A:624:PHE:O	1:A:631:GLN:HA	2.11	0.50
2:C:1360:ASN:ND2	2:C:1443:GLN:O	2.44	0.50
1:A:63:ASN:HD21	5:A:646:NAG:C1	2.24	0.50
1:A:180:GLY:O	1:A:181:GLN:O	2.30	0.50
1:A:462:GLU:HG3	1:A:486:ARG:HH22	1.76	0.50
3:M:7:SER:O	3:M:8:ASN:C	2.54	0.50
1:A:25:HIS:O	1:A:26:ASP:HB2	2.12	0.50
1:A:289:VAL:O	1:A:289:VAL:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLN:NE2	4:B:804:MET:HE3	2.26	0.50
2:C:1382:ASP:HB3	2:C:1456:LYS:HB3	1.94	0.50
1:A:351:MET:SD	1:A:440:ARG:HD3	2.52	0.50
2:C:1444:TYR:HD1	2:C:1445:PHE:HB2	1.68	0.50
1:A:160:SER:OG	1:A:160:SER:O	2.30	0.50
1:A:634:GLN:HG2	1:A:635:ARG:N	2.26	0.50
2:C:1338:LYS:HG3	2:C:1370:TYR:HE1	1.77	0.50
2:C:1480:LEU:HD12	4:B:851:CYS:O	2.11	0.50
2:C:1506:THR:O	2:C:1510:ARG:HG3	2.12	0.50
3:M:18:GLU:O	3:M:21:SER:HB2	2.11	0.50
1:A:224:TYR:N	1:A:224:TYR:CD2	2.79	0.49
1:A:552:GLN:HE22	4:B:804:MET:HE3	1.77	0.49
1:A:588:LYS:NZ	4:B:781:GLU:OE2	2.46	0.49
2:C:1393:THR:CG2	2:C:1419:ARG:HH22	2.25	0.49
2:C:1605:TRP:HE1	2:C:1607:GLU:CD	2.20	0.49
2:C:1632:GLU:HA	2:C:1635:VAL:HG22	1.93	0.49
4:B:852:SER:HA	4:B:878:ILE:HG22	1.93	0.49
1:A:440:ARG:HH22	1:A:529:VAL:HG23	1.77	0.49
1:A:286:LEU:HB3	1:A:291:ASN:CB	2.42	0.49
1:A:472:ILE:HA	1:A:508:ARG:O	2.11	0.49
4:B:731:GLU:CB	4:B:733:ILE:HG22	2.43	0.49
4:B:836:GLN:HE22	4:B:897:HIS:CE1	2.31	0.49
3:M:64:SER:O	3:M:65:GLU:C	2.55	0.49
4:B:890:VAL:O	4:B:891:LYS:CG	2.60	0.49
2:C:1593:LYS:HG2	2:C:1596:LEU:HD11	1.95	0.49
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.95	0.49
1:A:402:VAL:HG12	1:A:403:ARG:N	2.27	0.49
1:A:406:LYS:N	1:A:414:GLN:HE22	2.10	0.49
3:M:26:LEU:HD12	3:M:26:LEU:O	2.13	0.49
1:A:239:TYR:HE1	4:B:832:TYR:OH	1.95	0.49
1:A:271:ILE:HD13	1:A:276:GLY:HA3	1.94	0.49
1:A:403:ARG:NH1	1:A:416:THR:HG21	2.28	0.49
1:A:504:ILE:CG2	1:A:505:PRO:HA	2.43	0.49
2:C:1569:ARG:HH11	2:C:1569:ARG:CG	2.24	0.49
1:A:280:LEU:HD21	1:A:285:LEU:CG	2.36	0.49
1:A:281:SER:H	1:A:284:VAL:HG21	1.76	0.49
1:A:439:LEU:HD12	1:A:439:LEU:O	2.12	0.49
3:M:29:ASN:O	3:M:30:GLU:C	2.55	0.49
1:A:509:LEU:HB3	1:A:529:VAL:HG13	1.94	0.49
3:M:30:GLU:OE2	3:M:45:LYS:HE3	2.13	0.49
2:C:1413:ASP:O	2:C:1414:LYS:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:847:ASN:HB3	4:B:850:PHE:HB2	1.95	0.49
1:A:434:LEU:HD12	1:A:435:HIS:N	2.28	0.48
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.95	0.48
2:C:1591:GLY:O	2:C:1596:LEU:HD23	2.12	0.48
1:A:161:GLN:HG3	1:A:162:ASN:OD1	2.13	0.48
1:A:278:VAL:C	1:A:279:VAL:HG22	2.38	0.48
2:C:1497:PHE:HD1	2:C:1498:ILE:CG1	2.23	0.48
2:C:1550:GLY:O	2:C:1552:ASP:N	2.46	0.48
3:M:39:TYR:O	3:M:41:LYS:N	2.46	0.48
1:A:530:TRP:CD1	1:A:530:TRP:C	2.91	0.48
2:C:1485:ARG:HB2	2:C:1590:TRP:HE1	1.78	0.48
1:A:183:LYS:HD2	1:A:185:ARG:HD2	1.94	0.48
1:A:445:PRO:HA	1:A:499:ILE:HG22	1.95	0.48
1:A:606:THR:HG22	1:A:608:GLY:H	1.78	0.48
2:C:1374:GLN:O	2:C:1431:HIS:HB3	2.14	0.48
1:A:63:ASN:OD1	5:A:646:NAG:N2	2.46	0.48
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.49	0.48
1:A:287:ASP:HA	1:A:291:ASN:CA	2.44	0.48
1:A:477:ARG:HH22	1:A:479:LEU:HD13	1.78	0.48
2:C:1348:ALA:O	2:C:1349:PRO:O	2.31	0.48
2:C:1423:ILE:HG21	2:C:1425:TYR:CZ	2.48	0.48
2:C:1470:PHE:CB	2:C:1478:GLY:HA3	2.43	0.48
4:B:745:PHE:CD2	4:B:905:LYS:HG2	2.49	0.48
1:A:20:MET:H	1:A:64:VAL:HB	1.79	0.48
1:A:183:LYS:HD3	1:A:185:ARG:CD	2.44	0.48
4:B:795:VAL:O	4:B:796:ALA:C	2.54	0.48
4:B:783:LEU:HD12	4:B:784:ALA:H	1.79	0.48
1:A:161:GLN:HB3	1:A:162:ASN:CG	2.39	0.48
1:A:615:GLY:O	1:A:616:VAL:C	2.56	0.48
1:A:437:SER:O	1:A:452:ASN:HB2	2.13	0.48
1:A:510:VAL:HG21	1:A:622:LEU:HD12	1.95	0.48
2:C:1429:VAL:O	2:C:1430:SER:C	2.56	0.48
1:A:83:PHE:HD1	1:A:99:VAL:O	1.97	0.48
1:A:280:LEU:HG	1:A:285:LEU:HD13	1.94	0.48
1:A:403:ARG:CB	1:A:416:THR:HG22	2.44	0.48
2:C:1508:GLU:C	2:C:1510:ARG:N	2.69	0.48
1:A:364:ARG:O	1:A:378:LEU:HD22	2.14	0.47
1:A:603:ILE:HD12	1:A:621:GLY:HA3	1.94	0.47
1:A:7:ILE:HA	1:A:623:THR:O	2.14	0.47
1:A:59:ASN:HB3	1:A:483:ARG:NH1	2.30	0.47
1:A:171:TRP:CH2	1:A:182:TRP:CZ3	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:MET:HE1	1:A:386:LYS:HB2	1.96	0.47
4:B:807:PHE:C	4:B:807:PHE:CD2	2.92	0.47
1:A:282:ARG:O	1:A:283:LYS:C	2.58	0.47
2:C:1526:ARG:HB2	2:C:1579:HIS:CD2	2.49	0.47
2:C:1563:ILE:O	2:C:1600:ILE:HB	2.15	0.47
4:B:844:LEU:HD22	4:B:876:TYR:CD2	2.49	0.47
1:A:61:MET:HE2	1:A:483:ARG:CG	2.44	0.47
2:C:1370:TYR:O	2:C:1431:HIS:HA	2.14	0.47
2:C:1444:TYR:C	2:C:1444:TYR:HD1	2.20	0.47
2:C:1544:GLU:OE1	2:C:1579:HIS:CD2	2.68	0.47
1:A:613:TYR:CE2	1:A:614:ALA:HB2	2.48	0.47
2:C:1429:VAL:O	2:C:1429:VAL:HG23	2.15	0.47
4:B:749:TRP:O	4:B:750:LEU:HB3	2.13	0.47
1:A:73:GLU:HB3	1:A:82:LYS:HZ1	1.80	0.47
1:A:97:LYS:HG3	1:A:98:VAL:N	2.30	0.47
1:A:203:LYS:HG2	1:A:204:GLU:N	2.30	0.47
1:A:214:VAL:HG11	1:A:304:VAL:CG2	2.45	0.47
1:A:369:VAL:CG1	1:A:370:GLN:N	2.72	0.47
1:A:475:LYS:HG2	1:A:598:VAL:HG11	1.96	0.47
2:C:1369:ARG:HD2	2:C:1432:SER:O	2.13	0.47
4:B:888:VAL:HG12	4:B:889:GLU:N	2.28	0.47
1:A:290:GLN:O	1:A:291:ASN:C	2.57	0.47
1:A:368:ALA:O	1:A:402:VAL:HG13	2.15	0.47
1:A:462:GLU:HG3	1:A:486:ARG:NH2	2.29	0.47
1:A:475:LYS:HG2	1:A:598:VAL:CG1	2.45	0.47
3:M:64:SER:O	3:M:67:LYS:N	2.47	0.47
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.45	0.47
1:A:230:GLU:CA	1:A:279:VAL:HG13	2.22	0.47
2:C:1362:MET:HE3	2:C:1389:PHE:CE1	2.49	0.47
2:C:1586:SER:HA	2:C:1589:PHE:HE2	1.80	0.47
1:A:59:ASN:HB3	1:A:483:ARG:HH12	1.80	0.47
1:A:230:GLU:CB	1:A:279:VAL:HG11	2.40	0.47
2:C:1521:TYR:O	2:C:1583:TRP:HB2	2.14	0.47
2:C:1536:PHE:HD1	2:C:1563:ILE:CG2	2.20	0.47
2:C:1589:PHE:CE1	2:C:1598:TYR:CZ	3.03	0.47
1:A:105:SER:O	1:A:132:HIS:CD2	2.68	0.46
1:A:111:GLN:O	1:A:125:TYR:HA	2.16	0.46
1:A:248:PHE:CZ	2:C:1380:ILE:HD11	2.49	0.46
1:A:251:PHE:CE1	1:A:304:VAL:CG1	2.98	0.46
1:A:403:ARG:HB2	1:A:416:THR:HG22	1.95	0.46
1:A:591:GLN:OE1	4:B:795:VAL:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:23:LEU:HD11	3:M:51:ALA:HB1	1.97	0.46
4:B:736:GLU:HA	4:B:739:ILE:HD12	1.97	0.46
4:B:808:PHE:CD1	4:B:808:PHE:O	2.68	0.46
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.50	0.46
2:C:1336:CYS:O	2:C:1337:ASN:ND2	2.48	0.46
2:C:1341:LEU:HD23	2:C:1469:ARG:N	2.28	0.46
3:M:70:LEU:CG	3:M:74:TYR:HE1	2.27	0.46
4:B:813:LEU:CD1	4:B:814:PRO:HD3	2.45	0.46
1:A:47:LEU:C	1:A:47:LEU:HD23	2.41	0.46
1:A:298:VAL:O	1:A:298:VAL:HG12	2.16	0.46
1:A:510:VAL:CG1	1:A:528:SER:HB3	2.33	0.46
2:C:1472:HIS:ND1	2:C:1473:PRO:HD2	2.31	0.46
2:C:1510:ARG:HH12	2:C:1627:LEU:HD21	1.79	0.46
4:B:885:LEU:HD12	4:B:907:LEU:O	2.15	0.46
2:C:1445:PHE:CD1	2:C:1445:PHE:C	2.93	0.46
2:C:1475:LYS:HE2	2:C:1493:GLU:OE2	2.16	0.46
2:C:1582:MET:CG	2:C:1606:VAL:HG22	2.45	0.46
3:M:8:ASN:ND2	3:M:12:ASN:OD1	2.46	0.46
4:B:789:ASP:OD1	4:B:790:LYS:HG3	2.16	0.46
1:A:309:ILE:HG12	1:A:316:MET:HG3	1.97	0.46
2:C:1572:LEU:CD1	2:C:1574:LEU:HG	2.45	0.46
2:C:1388:GLY:O	2:C:1443:GLN:HA	2.16	0.46
1:A:375:VAL:CG2	1:A:387:LEU:HD22	2.46	0.46
1:A:549:GLU:O	1:A:550:ASP:HB2	2.14	0.46
2:C:1393:THR:HG22	2:C:1419:ARG:HH22	1.79	0.46
2:C:1582:MET:HG2	2:C:1605:TRP:O	2.16	0.46
4:B:886:GLN:OE1	4:B:886:GLN:HA	2.15	0.46
1:A:85:THR:HG23	1:A:98:VAL:HG22	1.98	0.46
2:C:1342:LYS:HB2	2:C:1367:CYS:CB	2.44	0.46
2:C:1421:THR:O	2:C:1422:LEU:HB2	2.15	0.46
2:C:1539:TYR:CE1	2:C:1574:LEU:CD1	2.90	0.46
1:A:185:ARG:HA	1:A:196:PHE:O	2.16	0.46
2:C:1451:GLN:HG3	2:C:1452:PRO:CD	2.42	0.46
2:C:1522:VAL:O	2:C:1547:ILE:HB	2.16	0.46
1:A:301:SER:HB2	1:A:323:GLY:HA2	1.98	0.46
2:C:1366:ILE:O	2:C:1436:CYS:HA	2.16	0.46
1:A:36:THR:HA	1:A:47:LEU:O	2.17	0.45
1:A:40:PHE:CE2	1:A:41:PRO:HG3	2.51	0.45
2:C:1386:MET:SD	2:C:1471:TYR:HE1	2.39	0.45
2:C:1519:VAL:HG12	2:C:1548:LYS:HZ2	1.81	0.45
4:B:907:LEU:N	4:B:907:LEU:CD2	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:CG1	1:A:102:SER:N	2.80	0.45
1:A:379:THR:HG22	1:A:384:VAL:N	2.31	0.45
2:C:1341:LEU:O	2:C:1469:ARG:HG2	2.16	0.45
1:A:6:ILE:HA	1:A:6:ILE:HD12	1.56	0.45
1:A:287:ASP:CB	1:A:291:ASN:HB3	2.44	0.45
2:C:1459:ALA:O	2:C:1460:TYR:C	2.58	0.45
4:B:897:HIS:O	4:B:898:PHE:CD1	2.69	0.45
1:A:271:ILE:O	1:A:271:ILE:HG22	2.16	0.45
1:A:461:HIS:O	1:A:464:LYS:HB2	2.16	0.45
4:B:733:ILE:HB	4:B:895:TYR:HD2	1.82	0.45
1:A:339:PRO:O	1:A:340:LYS:HD3	2.16	0.45
1:A:406:LYS:HG3	1:A:407:GLN:O	2.17	0.45
1:A:591:GLN:OE1	4:B:795:VAL:HB	2.17	0.45
2:C:1399:LEU:HD23	2:C:1399:LEU:HA	1.80	0.45
2:C:1530:VAL:HG13	2:C:1539:TYR:HE1	1.80	0.45
3:M:29:ASN:O	3:M:32:ALA:N	2.49	0.45
2:C:1524:LYS:HA	2:C:1580:TYR:O	2.16	0.45
2:C:1383:ILE:CD1	2:C:1439:PHE:HZ	2.30	0.45
4:B:808:PHE:C	4:B:808:PHE:HD1	2.25	0.45
4:B:894:VAL:HG23	4:B:899:ILE:O	2.16	0.45
1:A:20:MET:HG2	1:A:64:VAL:CB	2.47	0.45
1:A:644:ALA:O	1:A:645:ALA:HB3	2.16	0.45
2:C:1361:THR:HB	2:C:1442:HIS:HD1	1.82	0.45
2:C:1505:VAL:HG11	2:C:1607:GLU:OE2	2.16	0.45
4:B:823:VAL:HG23	4:B:824:GLU:N	2.32	0.45
4:B:866:ILE:HG22	4:B:867:PRO:O	2.16	0.45
1:A:287:ASP:C	1:A:290:GLN:H	2.23	0.45
1:A:591:GLN:CB	4:B:795:VAL:CB	2.74	0.45
1:A:210:PHE:HB3	1:A:237:PHE:HA	1.99	0.45
1:A:251:PHE:CD2	1:A:251:PHE:N	2.85	0.45
1:A:380:GLN:O	1:A:382:ASP:N	2.50	0.45
2:C:1505:VAL:CG1	2:C:1510:ARG:HE	2.28	0.45
4:B:910:VAL:HA	4:B:911:PRO:HD3	1.82	0.45
1:A:30:ASP:OD1	1:A:30:ASP:N	2.50	0.44
1:A:114:LYS:HZ2	4:B:747:GLU:CD	2.25	0.44
3:M:26:LEU:O	3:M:29:ASN:N	2.50	0.44
1:A:97:LYS:NZ	1:A:632:THR:O	2.48	0.44
1:A:215:GLU:HA	1:A:216:PRO:HD3	1.68	0.44
1:A:346:MET:O	1:A:391:THR:CG2	2.57	0.44
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.81	0.44
4:B:734:ILE:HD13	4:B:893:ALA:CB	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:813:LEU:HA	4:B:814:PRO:HD3	1.88	0.44
4:B:853:LEU:HA	4:B:853:LEU:HD23	1.57	0.44
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.52	0.44
1:A:281:SER:O	1:A:284:VAL:HB	2.16	0.44
2:C:1497:PHE:CE1	2:C:1498:ILE:CG1	3.01	0.44
2:C:1543:ILE:HD11	2:C:1554:VAL:HG21	1.99	0.44
3:M:70:LEU:HG	3:M:74:TYR:HD1	1.77	0.44
4:B:835:ASN:O	4:B:835:ASN:CG	2.59	0.44
1:A:179:MET:CG	1:A:202:VAL:O	2.65	0.44
1:A:380:GLN:C	1:A:382:ASP:H	2.25	0.44
1:A:516:ILE:C	1:A:516:ILE:HD12	2.42	0.44
2:C:1539:TYR:CZ	2:C:1574:LEU:HD12	2.49	0.44
2:C:1573:LYS:O	2:C:1574:LEU:CD2	2.56	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.48	0.44
2:C:1617:ASP:OD1	2:C:1618:GLU:N	2.48	0.44
2:C:1631:THR:O	2:C:1635:VAL:HG22	2.18	0.44
4:B:741:SER:CB	4:B:902:GLY:C	2.85	0.44
4:B:822:GLN:CB	4:B:879:VAL:HG22	2.39	0.44
1:A:604:GLY:HA2	1:A:619:ASP:O	2.18	0.44
2:C:1472:HIS:CG	2:C:1473:PRO:HD2	2.52	0.44
2:C:1575:GLU:OE2	2:C:1575:GLU:N	2.50	0.44
1:A:38:HIS:HE1	1:A:45:LEU:CD1	2.31	0.44
1:A:97:LYS:HD3	1:A:625:THR:OG1	2.18	0.44
1:A:465:ILE:HD11	1:A:515:LEU:HD13	2.00	0.44
2:C:1404:ASP:O	2:C:1427:ASP:HB2	2.18	0.44
2:C:1411:GLU:OE2	2:C:1414:LYS:HD2	2.17	0.44
2:C:1494:GLU:HG3	2:C:1602:LYS:HB3	2.00	0.44
4:B:830:TYR:CD1	4:B:871:SER:HB3	2.53	0.44
1:A:86:VAL:O	1:A:96:GLU:HB2	2.18	0.44
1:A:641:PRO:O	1:A:642:GLN:C	2.59	0.44
2:C:1336:CYS:HB3	2:C:1337:ASN:H	1.57	0.44
2:C:1464:GLU:O	2:C:1466:SER:N	2.45	0.44
2:C:1493:GLU:C	2:C:1494:GLU:O	2.59	0.44
1:A:251:PHE:CE1	1:A:280:LEU:HB2	2.52	0.44
2:C:1383:ILE:HG23	2:C:1455:VAL:HG22	1.99	0.44
2:C:1410:TYR:CD2	2:C:1410:TYR:O	2.71	0.44
2:C:1514:ALA:HB2	2:C:1583:TRP:CE2	2.53	0.44
2:C:1610:PRO:HB2	2:C:1615:CYS:SG	2.57	0.44
3:M:33:THR:O	3:M:34:GLY:C	2.61	0.44
1:A:40:PHE:HA	1:A:41:PRO:HA	1.69	0.43
1:A:161:GLN:HG2	1:A:162:ASN:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:SER:OG	1:A:413:GLU:HG3	2.18	0.43
2:C:1415:ALA:O	2:C:1417:SER:N	2.51	0.43
2:C:1511:LEU:HD11	2:C:1633:SER:OG	2.17	0.43
2:C:1578:LYS:NZ	2:C:1608:HIS:NE2	2.50	0.43
2:C:1589:PHE:CZ	2:C:1598:TYR:CE2	3.05	0.43
2:C:1589:PHE:CZ	2:C:1598:TYR:HE2	2.36	0.43
3:M:14:LYS:O	3:M:15:LEU:C	2.61	0.43
4:B:731:GLU:C	4:B:733:ILE:N	2.75	0.43
1:A:351:MET:HE2	1:A:351:MET:HA	1.99	0.43
2:C:1337:ASN:O	2:C:1371:ARG:HD2	2.19	0.43
4:B:784:ALA:HB3	4:B:796:ALA:HB3	2.00	0.43
4:B:840:VAL:HG11	4:B:892:ALA:HB1	1.99	0.43
1:A:453:PHE:CE2	1:A:495:LEU:HB2	2.53	0.43
3:M:15:LEU:HD22	3:M:60:PHE:CE1	2.53	0.43
3:M:51:ALA:O	3:M:54:ALA:N	2.52	0.43
4:B:788:SER:O	4:B:789:ASP:C	2.60	0.43
4:B:808:PHE:CE1	4:B:830:TYR:CD2	3.03	0.43
1:A:227:LYS:HE2	1:A:227:LYS:HB2	1.64	0.43
1:A:458:ASP:OD2	1:A:460:ALA:HB3	2.18	0.43
2:C:1632:GLU:O	2:C:1636:VAL:HG12	2.17	0.43
4:B:746:PRO:HB3	4:B:748:SER:O	2.19	0.43
1:A:287:ASP:N	1:A:287:ASP:OD1	2.50	0.43
4:B:734:ILE:HD12	4:B:734:ILE:N	2.17	0.43
1:A:148:PRO:HG3	1:A:182:TRP:NE1	2.33	0.43
1:A:541:LEU:HD12	1:A:541:LEU:HA	1.77	0.43
1:A:584:ASN:C	1:A:584:ASN:OD1	2.61	0.43
1:A:283:LYS:O	1:A:287:ASP:OD1	2.36	0.43
2:C:1342:LYS:HB3	2:C:1367:CYS:HB2	1.98	0.43
2:C:1397:LYS:O	2:C:1401:ASN:ND2	2.40	0.43
1:A:220:PHE:HB3	1:A:357:PRO:HG2	2.01	0.43
1:A:255:ASP:O	1:A:258:GLN:HB3	2.18	0.43
1:A:454:LEU:HA	1:A:491:ASP:O	2.18	0.43
1:A:458:ASP:O	1:A:460:ALA:N	2.52	0.43
1:A:590:THR:HB	1:A:593:LYS:CG	2.39	0.43
2:C:1362:MET:HE3	2:C:1389:PHE:CZ	2.54	0.43
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.71	0.43
2:C:1380:ILE:HB	2:C:1458:TYR:CE1	2.54	0.43
3:M:29:ASN:C	3:M:31:LEU:N	2.76	0.43
1:A:20:MET:HG2	1:A:64:VAL:CG2	2.47	0.43
5:A:646:NAG:H62	5:A:646:NAG:O3	2.19	0.43
2:C:1577:LYS:HA	2:C:1577:LYS:HD3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:15:LEU:O	3:M:18:GLU:HB2	2.19	0.43
4:B:894:VAL:HG21	4:B:899:ILE:HB	2.01	0.43
1:A:281:SER:N	1:A:284:VAL:HG21	2.34	0.42
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.31	0.42
2:C:1460:TYR:CG	2:C:1461:TYR:N	2.86	0.42
4:B:899:ILE:HG22	4:B:900:SER:N	2.35	0.42
1:A:182:TRP:CD1	1:A:182:TRP:N	2.86	0.42
2:C:1526:ARG:NH1	2:C:1526:ARG:HB3	2.34	0.42
3:M:43:THR:HG21	3:M:73:ILE:HD13	2.01	0.42
3:M:82:LYS:C	3:M:84:LYS:H	2.27	0.42
4:B:731:GLU:HB3	4:B:733:ILE:HG22	1.98	0.42
4:B:835:ASN:O	4:B:836:GLN:HB3	2.19	0.42
1:A:87:GLN:HG3	1:A:96:GLU:HB3	2.01	0.42
1:A:168:PRO:O	1:A:169:LEU:HG	2.20	0.42
4:B:894:VAL:CG2	4:B:899:ILE:O	2.67	0.42
1:A:61:MET:HE1	1:A:482:GLY:HA2	2.01	0.42
3:M:68:TYR:O	3:M:69:GLN:C	2.61	0.42
4:B:819:ARG:NE	4:B:883:THR:HG23	2.35	0.42
1:A:402:VAL:HG12	1:A:403:ARG:H	1.84	0.42
1:A:442:GLU:OE1	1:A:534:LYS:HD3	2.18	0.42
2:C:1341:LEU:HB3	2:C:1469:ARG:HG2	2.02	0.42
2:C:1386:MET:H	2:C:1386:MET:HG3	1.34	0.42
2:C:1576:GLU:C	2:C:1578:LYS:H	2.28	0.42
4:B:750:LEU:HG	4:B:750:LEU:O	2.20	0.42
4:B:907:LEU:H	4:B:907:LEU:CD2	2.28	0.42
1:A:177:VAL:HG22	1:A:178:ASN:N	2.34	0.42
1:A:455:LEU:HB2	1:A:468:TYR:OH	2.19	0.42
1:A:468:TYR:CE1	1:A:513:TYR:CD2	3.05	0.42
2:C:1472:HIS:CE1	2:C:1473:PRO:HD2	2.55	0.42
4:B:838:LEU:HD23	4:B:838:LEU:HA	1.77	0.42
1:A:203:LYS:HG2	1:A:204:GLU:H	1.85	0.42
1:A:533:VAL:CG1	1:A:534:LYS:N	2.81	0.42
1:A:603:ILE:HB	1:A:635:ARG:HH12	1.84	0.42
3:M:29:ASN:O	3:M:31:LEU:N	2.53	0.42
4:B:783:LEU:HD12	4:B:784:ALA:N	2.34	0.42
4:B:819:ARG:O	4:B:820:ASN:HB2	2.20	0.42
1:A:3:MET:HE2	1:A:626:SER:HB2	2.01	0.42
1:A:296:ASP:O	1:A:297:LEU:C	2.62	0.42
2:C:1472:HIS:HA	2:C:1473:PRO:HD3	1.81	0.42
2:C:1483:LEU:HD23	2:C:1599:ILE:HG23	2.01	0.42
2:C:1524:LYS:HD2	2:C:1609:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1575:GLU:CD	2:C:1578:LYS:HD2	2.45	0.42
4:B:829:LEU:N	4:B:829:LEU:HD12	2.35	0.42
1:A:504:ILE:HG23	1:A:505:PRO:HA	2.02	0.42
1:A:613:TYR:CD2	1:A:614:ALA:N	2.88	0.42
2:C:1337:ASN:OD1	2:C:1338:LYS:N	2.52	0.42
2:C:1341:LEU:HD12	2:C:1341:LEU:HA	1.84	0.42
2:C:1403:VAL:CG2	2:C:1404:ASP:N	2.82	0.42
1:A:4:TYR:HB3	1:A:90:PHE:CZ	2.55	0.41
1:A:101:VAL:HG12	1:A:102:SER:N	2.35	0.41
1:A:195:VAL:CG1	1:A:196:PHE:N	2.82	0.41
1:A:239:TYR:CE1	4:B:832:TYR:HE1	2.35	0.41
2:C:1564:SER:OG	2:C:1565:PRO:HD2	2.19	0.41
3:M:23:LEU:HD23	3:M:23:LEU:HA	1.81	0.41
4:B:821:GLU:O	4:B:880:PRO:HD3	2.20	0.41
4:B:890:VAL:O	4:B:891:LYS:HG3	2.20	0.41
1:A:20:MET:HG2	1:A:64:VAL:HG11	2.01	0.41
1:A:207:LEU:O	4:B:812:ARG:NH2	2.53	0.41
1:A:350:LEU:O	1:A:351:MET:HE2	2.19	0.41
2:C:1419:ARG:O	2:C:1421:THR:N	2.52	0.41
3:M:13:GLU:O	3:M:13:GLU:HG2	2.20	0.41
4:B:771:ILE:O	4:B:771:ILE:HG13	2.18	0.41
1:A:179:MET:CB	1:A:202:VAL:O	2.69	0.41
1:A:219:LYS:HD2	1:A:358:ASP:OD2	2.19	0.41
1:A:389:ILE:O	1:A:389:ILE:HG13	2.20	0.41
2:C:1494:GLU:CB	2:C:1602:LYS:HB3	2.47	0.41
2:C:1632:GLU:HA	2:C:1635:VAL:CG2	2.49	0.41
3:M:58:LYS:C	3:M:63:MET:HE2	2.45	0.41
4:B:786:SER:O	4:B:794:CYS:N	2.33	0.41
1:A:106:GLY:HA2	1:A:132:HIS:CD2	2.55	0.41
1:A:173:ILE:HA	1:A:174:PRO:HD3	1.92	0.41
2:C:1497:PHE:HD1	2:C:1498:ILE:HG12	1.84	0.41
2:C:1554:VAL:CG2	2:C:1558:GLN:HB2	2.50	0.41
4:B:736:GLU:C	4:B:736:GLU:OE1	2.63	0.41
1:A:14:LEU:HD11	1:A:103:LEU:CD2	2.51	0.41
1:A:171:TRP:HH2	1:A:182:TRP:CZ3	2.39	0.41
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.76	0.41
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.85	0.41
4:B:813:LEU:HA	4:B:813:LEU:HD13	1.28	0.41
4:B:839:LYS:HE2	4:B:895:TYR:HD1	1.85	0.41
4:B:841:ARG:HD2	4:B:861:GLN:OE1	2.20	0.41
1:A:33:VAL:HG22	1:A:90:PHE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:CD1	1:A:100:LEU:HA	2.56	0.41
1:A:289:VAL:HG23	1:A:290:GLN:NE2	2.36	0.41
2:C:1404:ASP:O	2:C:1427:ASP:N	2.51	0.41
2:C:1495:ASN:OD1	2:C:1495:ASN:N	2.54	0.41
2:C:1543:ILE:CD1	2:C:1554:VAL:HG11	2.50	0.41
1:A:63:ASN:ND2	5:A:646:NAG:C1	2.84	0.41
1:A:343:LYS:N	1:A:343:LYS:CD	2.83	0.41
1:A:533:VAL:HG12	1:A:534:LYS:H	1.86	0.41
2:C:1508:GLU:C	2:C:1510:ARG:H	2.28	0.41
2:C:1530:VAL:HG13	2:C:1539:TYR:CE1	2.54	0.41
3:M:15:LEU:HA	3:M:15:LEU:HD12	1.82	0.41
3:M:58:LYS:HD2	3:M:58:LYS:HA	1.75	0.41
4:B:811:LEU:HD13	4:B:812:ARG:H	1.85	0.41
4:B:847:ASN:HB3	4:B:850:PHE:CD1	2.55	0.41
1:A:265:SER:O	1:A:267:LYS:HG2	2.21	0.41
3:M:84:LYS:O	3:M:85:TYR:CB	2.69	0.41
4:B:841:ARG:HA	4:B:862:GLN:O	2.20	0.41
4:B:889:GLU:HB2	4:B:904:ARG:HG3	2.03	0.41
1:A:114:LYS:HE2	1:A:117:TYR:CD1	2.56	0.41
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.03	0.41
1:A:474:ASN:O	1:A:475:LYS:C	2.64	0.41
1:A:508:ARG:CZ	1:A:604:GLY:HA3	2.51	0.41
1:A:509:LEU:HB3	1:A:529:VAL:CG1	2.50	0.41
2:C:1375:ASP:CG	2:C:1430:SER:HA	2.46	0.41
4:B:754:GLU:HB3	4:B:767:LYS:HE3	2.02	0.41
4:B:812:ARG:HA	4:B:812:ARG:HD2	1.58	0.41
4:B:847:ASN:HA	4:B:848:PRO:HD2	1.77	0.41
4:B:855:THR:O	4:B:856:THR:C	2.64	0.41
4:B:897:HIS:O	4:B:898:PHE:HD1	2.04	0.41
1:A:252:GLY:HA3	1:A:303:TYR:CZ	2.56	0.41
1:A:278:VAL:O	1:A:279:VAL:HG13	2.21	0.41
1:A:453:PHE:HE2	1:A:495:LEU:HB2	1.85	0.41
2:C:1339:PHE:HE2	2:C:1429:VAL:HG21	1.85	0.41
2:C:1395:ASP:O	2:C:1398:GLN:HB3	2.21	0.41
2:C:1497:PHE:HE2	2:C:1571:ALA:CB	1.99	0.41
2:C:1497:PHE:O	2:C:1498:ILE:HG13	2.20	0.41
4:B:839:LYS:HG2	4:B:863:THR:HG23	2.03	0.41
1:A:615:GLY:C	1:A:617:PHE:N	2.79	0.40
1:A:632:THR:O	1:A:633:ALA:C	2.63	0.40
4:B:846:HIS:CE1	4:B:855:THR:HA	2.56	0.40
1:A:272:GLU:O	1:A:273:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ILE:N	1:A:400:ILE:HD12	2.35	0.40
2:C:1611:GLU:HB3	2:C:1614:GLU:HB2	2.03	0.40
1:A:108:LEU:HB2	1:A:196:PHE:CG	2.57	0.40
1:A:590:THR:HG22	1:A:591:GLN:N	2.35	0.40
2:C:1384:SER:HB3	4:B:826:ARG:HH12	1.87	0.40
2:C:1544:GLU:OE1	2:C:1579:HIS:HD2	2.03	0.40
1:A:239:TYR:CZ	4:B:808:PHE:HZ	2.39	0.40
1:A:345:GLY:HA2	1:A:393:PRO:HD3	2.04	0.40
1:A:502:ASP:N	1:A:502:ASP:OD1	2.53	0.40
4:B:852:SER:O	4:B:853:LEU:HD23	2.21	0.40
1:A:61:MET:CE	1:A:483:ARG:HG2	2.50	0.40
2:C:1555:GLN:O	2:C:1556:VAL:C	2.63	0.40
2:C:1590:TRP:N	2:C:1597:SER:O	2.54	0.40
4:B:750:LEU:HD23	4:B:782:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/645 (99%)	545 (86%)	73 (12%)	19 (3%)	3	25
2	C	288/343 (84%)	232 (81%)	39 (14%)	17 (6%)	1	16
3	M	82/88 (93%)	56 (68%)	22 (27%)	4 (5%)	1	18
4	B	182/206 (88%)	145 (80%)	28 (15%)	9 (5%)	1	18
All	All	1189/1282 (93%)	978 (82%)	162 (14%)	49 (4%)	2	20

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	290	GLN
1	A	293	ARG
1	A	294	ALA
1	A	295	GLU
1	A	537	CYS
2	C	1494	GLU
2	C	1573	LYS
4	B	730	ASP
4	B	789	ASP
4	B	836	GLN
1	A	282	ARG
2	C	1377	THR
2	C	1414	LYS
2	C	1430	SER
3	M	51	ALA
4	B	732	ASP
4	B	852	SER
1	A	181	GLN
1	A	283	LYS
1	A	296	ASP
2	C	1349	PRO
2	C	1422	LEU
2	C	1432	SER
2	C	1458	TYR
2	C	1551	SER
2	C	1576	GLU
3	M	30	GLU
3	M	61	LYS
4	B	743	SER
4	B	837	GLU
1	A	179	MET
2	C	1420	ASN
2	C	1486	ASP
3	M	39	TYR
4	B	753	VAL
4	B	796	ALA
1	A	72	ARG
1	A	291	ASN
1	A	370	GLN
1	A	459	ARG
2	C	1406	TYR
2	C	1517	PRO

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Mol	Chain	Res	Type
1	A	298	VAL
1	A	381	GLY
2	C	1516	GLU
1	A	616	VAL
1	A	359	GLY
2	C	1473	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	563/567 (99%)	494 (88%)	69 (12%)	4 20
2	C	267/309 (86%)	218 (82%)	49 (18%)	1 11
3	M	76/79 (96%)	65 (86%)	11 (14%)	3 16
4	B	172/191 (90%)	130 (76%)	42 (24%)	1 5
All	All	1078/1146 (94%)	907 (84%)	171 (16%)	2 14

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	6	ILE
1	A	21	VAL
1	A	30	ASP
1	A	51	LYS
1	A	52	THR
1	A	61	MET
1	A	64	VAL
1	A	84	VAL
1	A	85	THR
1	A	110	ILE
1	A	124	LEU
1	A	127	ILE
1	A	137	VAL
1	A	149	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	155	GLN
1	A	156	ASP
1	A	157	SER
1	A	162	ASN
1	A	163	GLN
1	A	169	LEU
1	A	176	LEU
1	A	178	ASN
1	A	191	SER
1	A	198	THR
1	A	207	LEU
1	A	213	ILE
1	A	215	GLU
1	A	217	THR
1	A	223	ILE
1	A	241	LYS
1	A	251	PHE
1	A	257	GLU
1	A	278	VAL
1	A	279	VAL
1	A	281	SER
1	A	282	ARG
1	A	283	LYS
1	A	284	VAL
1	A	286	LEU
1	A	289	VAL
1	A	290	GLN
1	A	295	GLU
1	A	297	LEU
1	A	298	VAL
1	A	304	VAL
1	A	314	SER
1	A	365	VAL
1	A	375	VAL
1	A	404	THR
1	A	410	SER
1	A	422	LEU
1	A	438	VAL
1	A	451	VAL
1	A	454	LEU
1	A	472	ILE
1	A	477	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	501	THR
1	A	515	LEU
1	A	516	ILE
1	A	524	VAL
1	A	538	VAL
1	A	542	VAL
1	A	548	SER
1	A	554	VAL
1	A	559	MET
1	A	603	ILE
1	A	616	VAL
1	A	634	GLN
2	C	1336	CYS
2	C	1342	LYS
2	C	1344	THR
2	C	1346	LYS
2	C	1350	GLU
2	C	1361	THR
2	C	1363	ILE
2	C	1378	MET
2	C	1383	ILE
2	C	1386	MET
2	C	1387	THR
2	C	1393	THR
2	C	1394	ASP
2	C	1397	LYS
2	C	1410	TYR
2	C	1416	PHE
2	C	1420	ASN
2	C	1421	THR
2	C	1422	LEU
2	C	1430	SER
2	C	1433	GLU
2	C	1441	VAL
2	C	1447	VAL
2	C	1449	LEU
2	C	1465	GLU
2	C	1468	THR
2	C	1469	ARG
2	C	1480	LEU
2	C	1485	ARG
2	C	1494	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	1495	ASN
2	C	1498	ILE
2	C	1507	LEU
2	C	1511	LEU
2	C	1512	ASP
2	C	1532	LEU
2	C	1535	ASP
2	C	1543	ILE
2	C	1551	SER
2	C	1561	THR
2	C	1563	ILE
2	C	1569	ARG
2	C	1570	GLU
2	C	1572	LEU
2	C	1573	LYS
2	C	1585	LEU
2	C	1590	TRP
2	C	1592	GLU
2	C	1600	ILE
3	M	7	SER
3	M	8	ASN
3	M	21	SER
3	M	25	GLU
3	M	26	LEU
3	M	31	LEU
3	M	36	LEU
3	M	38	THR
3	M	56	LYS
3	M	59	ASP
3	M	78	ASP
4	B	729	LEU
4	B	732	ASP
4	B	733	ILE
4	B	734	ILE
4	B	736	GLU
4	B	741	SER
4	B	756	LEU
4	B	757	LYS
4	B	765	SER
4	B	769	MET
4	B	770	ASN
4	B	777	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	B	782	ILE
4	B	783	LEU
4	B	786	SER
4	B	794	CYS
4	B	803	VAL
4	B	809	ILE
4	B	811	LEU
4	B	812	ARG
4	B	813	LEU
4	B	817	VAL
4	B	818	VAL
4	B	823	VAL
4	B	828	VAL
4	B	834	GLN
4	B	836	GLN
4	B	841	ARG
4	B	844	LEU
4	B	845	LEU
4	B	851	CYS
4	B	864	VAL
4	B	865	THR
4	B	873	SER
4	B	874	VAL
4	B	876	TYR
4	B	877	VAL
4	B	890	VAL
4	B	894	VAL
4	B	896	HIS
4	B	907	LEU
4	B	912	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	132	HIS
1	A	144	ASN
1	A	155	GLN
1	A	290	GLN
1	A	390	ASN
2	C	1579	HIS
3	M	17	ASN
3	M	69	GLN

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Mol	Chain	Res	Type
4	B	897	HIS

### 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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	646	-	14,14,15	0.47	0	17,19,21	1.46	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	646	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	646	NAG	C1-O5-C5	4.96	118.83	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	646	NAG	O5-C5-C6-O6
5	A	646	NAG	C8-C7-N2-C2
5	A	646	NAG	O7-C7-N2-C2
5	A	646	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	646	NAG	4	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	641/645 (99%)	0.44	21 (3%) 49 37	26, 151, 213, 245	0
2	C	294/343 (85%)	0.48	10 (3%) 48 36	118, 187, 274, 305	0
3	M	84/88 (95%)	0.40	3 (3%) 46 35	121, 146, 199, 261	0
4	B	184/206 (89%)	0.21	1 (0%) 87 74	99, 130, 161, 183	0
All	All	1203/1282 (93%)	0.41	35 (2%) 53 40	26, 151, 238, 305	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1582	MET	5.3
2	C	1439	PHE	5.2
1	A	347	PRO	4.7
2	C	1382	ASP	4.7
2	C	1454	ALA	4.4
2	C	1487	GLU	3.9
1	A	398	LEU	3.8
1	A	324	ILE	3.7
1	A	471	LEU	3.3
1	A	436	LEU	3.3
3	M	29	ASN	3.3
1	A	421	ALA	3.1
1	A	369	VAL	3.1
2	C	1606	VAL	2.9
3	M	54	ALA	2.8
1	A	527	ASP	2.6
1	A	589	LEU	2.6
2	C	1422	LEU	2.5
2	C	1383	ILE	2.4
2	C	1627	LEU	2.3
1	A	66	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	518	ALA	2.3
1	A	388	SER	2.2
1	A	35	VAL	2.2
1	A	314	SER	2.2
1	A	507	PHE	2.2
4	B	912	GLU	2.2
3	M	18	GLU	2.2
1	A	494	VAL	2.1
1	A	573	LEU	2.1
1	A	492	LEU	2.1
1	A	294	ALA	2.1
2	C	1455	VAL	2.1
1	A	475	LYS	2.0
1	A	63	ASN	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	646	14/15	0.78	0.16	159,175,186,189	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.