



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 01:46 AM EDT

PDB ID : 3OHX  
Title : Molecular Basis for Complement Recognition and Inhibition Determined by Crystallographic Studies of the Staphylococcal Complement Inhibitor (SCIN) Bound to C3c and C3b  
Authors : Geisbrecht, B.V.; Garcia, B.L.  
Deposited on : unknown  
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

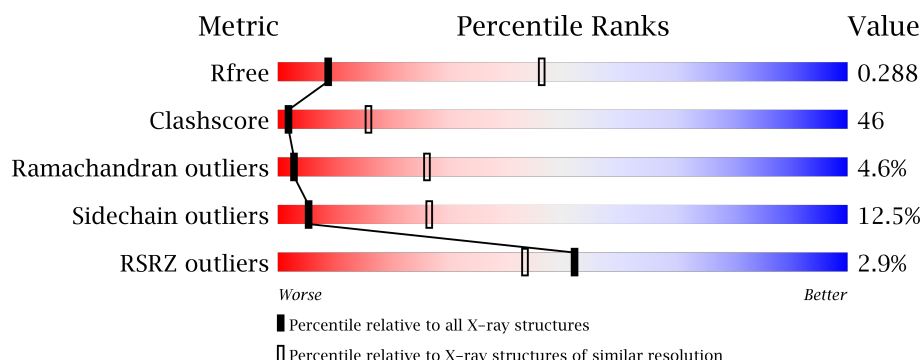
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div>48%</div> <div>47%</div> <div>• •</div> </div>
1	D	645	<div> <div>2%</div> <div>48%</div> <div>47%</div> <div>• •</div> </div>
2	B	206	<div> <div>37%</div> <div>41%</div> <div>10%</div> <div>11%</div> </div>
2	E	206	<div> <div>36%</div> <div>43%</div> <div>10%</div> <div>11%</div> </div>
3	C	343	<div> <div>7%</div> <div>27%</div> <div>41%</div> <div>14%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	343	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%21%38%23%.14%</div></div>
4	M	88	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%47%39%10%5%</div></div>
4	P	88	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%48%36%11%5%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19119 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
1	A	641	Total	C	N	O	S	0	0	0
			4989	3175	846	953	15			
1	D	641	Total	C	N	O	S	0	0	0
			4989	3175	846	953	15			

- Molecule 2 is a protein called Complement C3.

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

- Molecule 3 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	293	Total	C	N	O	S	0	0	0
			2377	1495	390	472	20			
3	F	295	Total	C	N	O	S	0	0	0
			2396	1510	392	474	20			

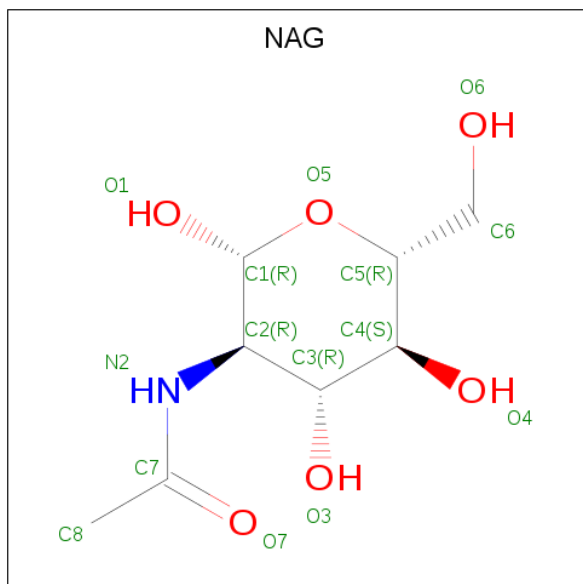
- Molecule 4 is a protein called Staphylococcal complement inhibitor.

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

There are 6 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
P	-2	GLY	-	EXPRESSION TAG	UNP Q931M7
P	-1	THR	-	EXPRESSION TAG	UNP Q931M7
P	0	SER	-	EXPRESSION TAG	UNP Q931M7

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

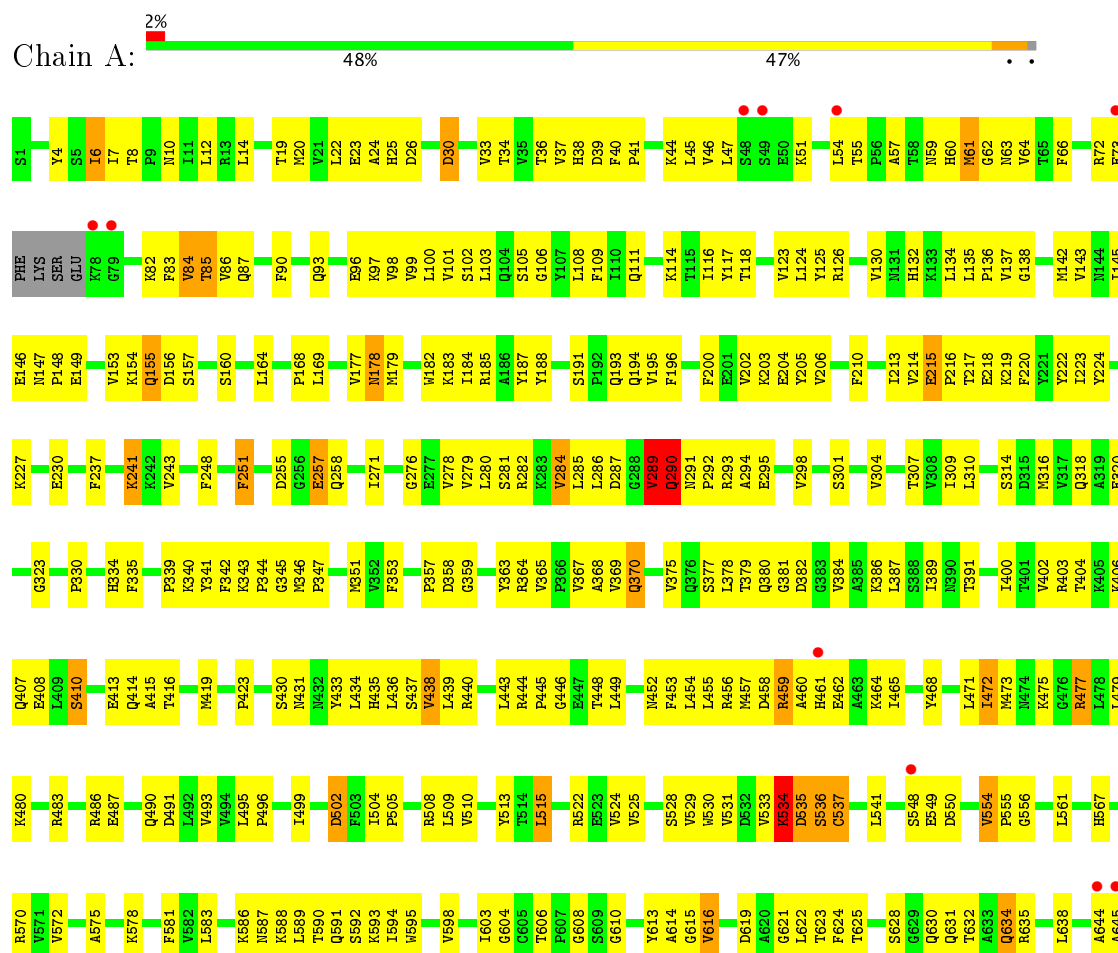


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

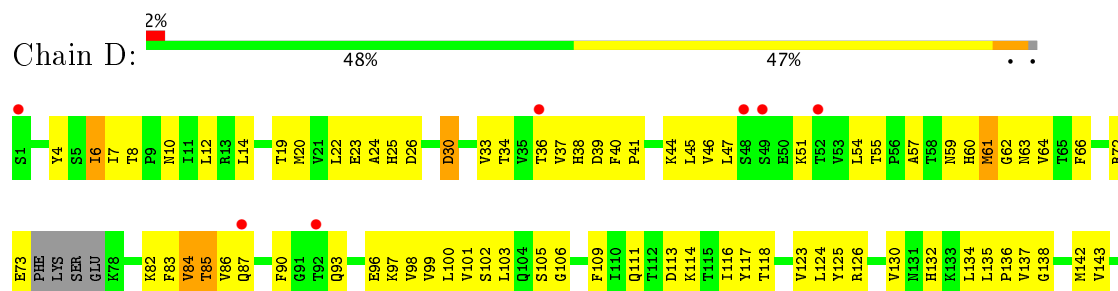
### 3 Residue-property plots

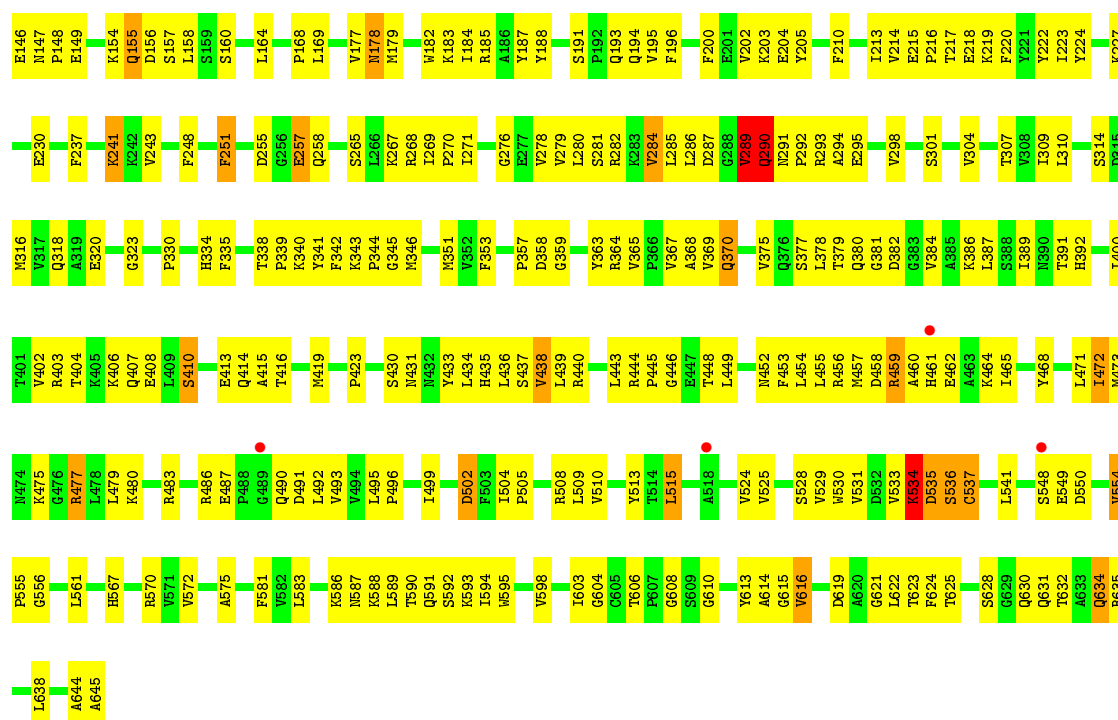
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Complement C3



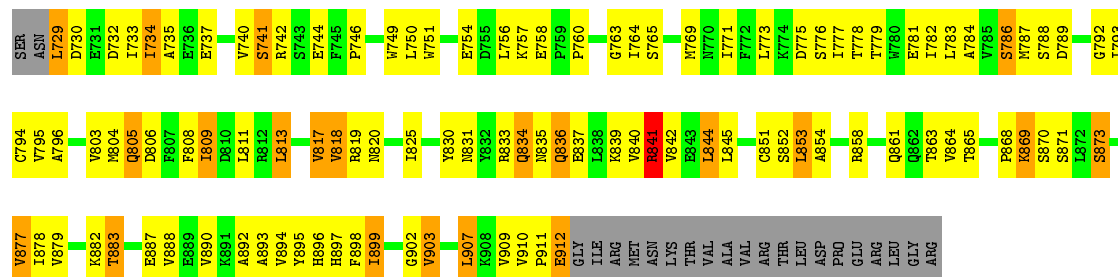
#### • Molecule 1: Complement C3





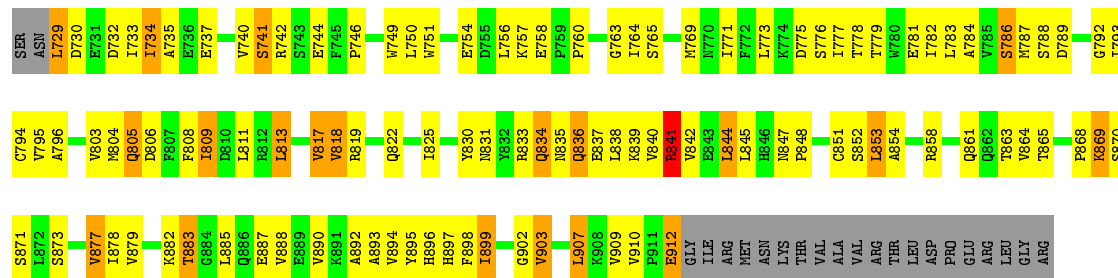
### • Molecule 2: Complement C3

Chain B: 37% 41% 10% 11%



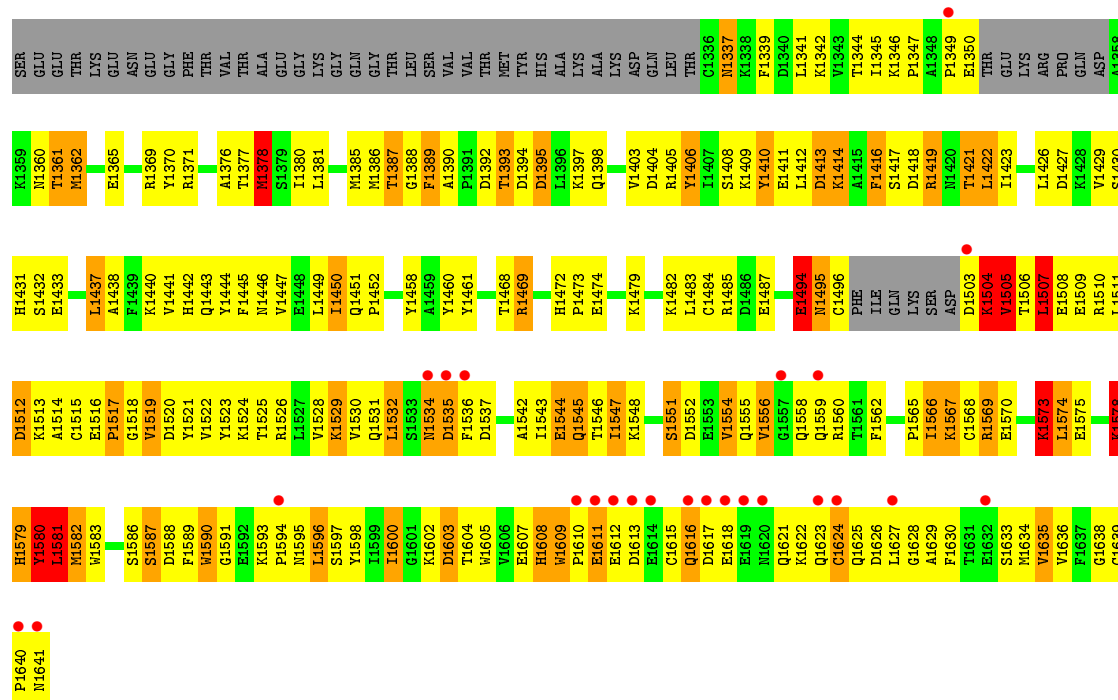
### • Molecule 2: Complement C3

Chain E: 36% 43% 10% 11%

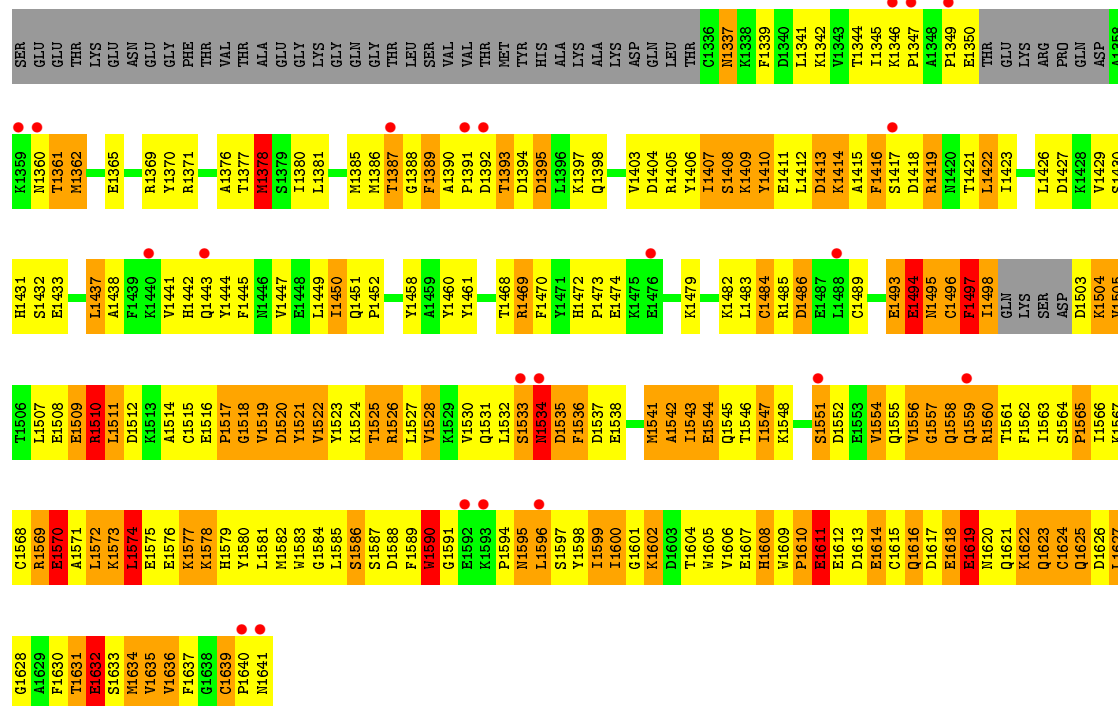
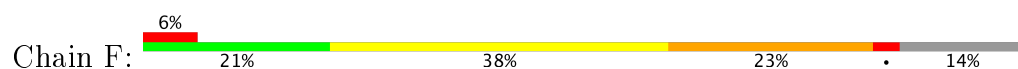


### • Molecule 3: Complement C3

Chain C: 7% 27% 41% 14% 15%



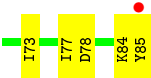
• Molecule 3: Complement C3



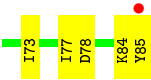
• Molecule 4: Staphylococcal complement inhibitor







● Molecule 4: Staphylococcal complement inhibitor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.16Å 231.50Å 68.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.27 – 3.50 46.96 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (46.27-3.50) 93.2 (46.96-3.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.5 _2	Depositor
R, $R_{free}$	0.274 , 0.294 0.267 , 0.288	Depositor DCC
$R_{free}$ test set	2014 reflections (4.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	19119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3878e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.45	0/5089	0.63	0/6916
1	D	0.45	0/5089	0.63	0/6916
2	B	0.51	0/1520	0.70	1/2066 (0.0%)
2	E	0.51	0/1520	0.70	1/2066 (0.0%)
3	C	0.49	0/2422	0.73	2/3264 (0.1%)
3	F	0.56	0/2442	0.74	1/3291 (0.0%)
4	M	0.39	0/690	0.59	0/923
4	P	0.39	0/690	0.59	0/923
All	All	0.48	0/19462	0.67	5/26365 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1609	TRP	N-CA-C	-5.93	94.98	111.00
3	C	1581	LEU	CA-CB-CG	-5.75	102.08	115.30
2	E	841	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	B	841	ARG	NE-CZ-NH1	5.07	122.84	120.30
3	F	1536	PHE	N-CA-C	-5.05	97.36	111.00

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	5051	367	0
1	D	4989	0	5051	372	0
2	B	1488	0	1512	125	0
2	E	1488	0	1512	119	0
3	C	2377	0	2279	319	0
3	F	2396	0	2299	474	0
4	M	682	0	697	56	0
4	P	682	0	697	50	0
5	A	14	0	13	4	0
5	D	14	0	13	3	0
All	All	19119	0	19124	1763	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 46.

All (1763) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1497:PHE:CZ	3:F:1498:ILE:HG13	1.39	1.57
3:C:1639:CYS:SG	3:C:1640:PRO:HD2	1.45	1.56
3:F:1497:PHE:CE2	3:F:1498:ILE:HG13	1.52	1.44
3:F:1571:ALA:C	3:F:1572:LEU:HD22	1.41	1.39
3:F:1569:ARG:CG	3:F:1570:GLU:OE1	1.73	1.33
3:C:1581:LEU:HD12	3:C:1582:MET:N	1.45	1.27
3:C:1578:LYS:HB3	3:C:1580:TYR:CE2	1.71	1.25
3:F:1595:ASN:O	3:F:1596:LEU:HG	1.36	1.22
3:C:1578:LYS:HD3	3:C:1608:HIS:CE1	1.73	1.22
3:F:1504:LYS:O	3:F:1505:VAL:HG22	1.07	1.22
3:F:1504:LYS:O	3:F:1505:VAL:CG2	1.87	1.20
3:C:1526:ARG:NH1	3:C:1542:ALA:HB1	1.58	1.18
3:F:1533:SER:OG	3:F:1538:GLU:HG3	1.42	1.18
2:E:853:LEU:CD1	3:F:1451:GLN:HB2	1.75	1.17
3:F:1507:LEU:HB3	3:F:1510:ARG:NH2	1.59	1.16
3:F:1497:PHE:CE2	3:F:1498:ILE:CG1	2.30	1.14
3:C:1639:CYS:SG	3:C:1640:PRO:CD	2.36	1.14
3:F:1572:LEU:CB	3:F:1574:LEU:HD21	1.77	1.14
3:F:1574:LEU:N	3:F:1574:LEU:HD23	1.59	1.13
3:C:1581:LEU:C	3:C:1581:LEU:HD12	1.66	1.11
3:C:1515:CYS:SG	3:C:1640:PRO:HD2	1.90	1.11
3:F:1558:GLN:O	3:F:1559:GLN:HG3	1.49	1.11
3:C:1349:PRO:O	3:C:1350:GLU:HB2	1.47	1.11
3:F:1497:PHE:CZ	3:F:1498:ILE:CG1	2.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:912:GLU:H	2:B:912:GLU:CD	1.52	1.10
3:F:1507:LEU:CB	3:F:1510:ARG:HH21	1.62	1.10
1:D:289:VAL:C	1:D:290:GLN:HG2	1.71	1.08
3:C:1526:ARG:HG2	3:C:1542:ALA:HB3	1.13	1.08
1:D:634:GLN:HE21	1:D:635:ARG:N	1.51	1.08
3:F:1558:GLN:C	3:F:1559:GLN:HG3	1.70	1.08
3:F:1533:SER:HB2	3:F:1537:ASP:HA	1.19	1.08
1:D:590:THR:HG22	1:D:592:SER:H	1.13	1.08
3:F:1554:VAL:HG23	3:F:1558:GLN:OE1	1.52	1.08
3:F:1349:PRO:O	3:F:1350:GLU:HB2	1.47	1.08
1:A:634:GLN:HE21	1:A:635:ARG:N	1.50	1.07
3:F:1572:LEU:O	3:F:1573:LYS:CD	2.02	1.06
3:C:1578:LYS:HD3	3:C:1608:HIS:HE1	0.89	1.06
3:F:1574:LEU:H	3:F:1574:LEU:HD23	1.05	1.06
1:A:289:VAL:C	1:A:290:GLN:HG2	1.71	1.06
3:F:1569:ARG:HG2	3:F:1570:GLU:OE1	0.89	1.06
1:A:590:THR:HG22	1:A:592:SER:H	1.13	1.06
3:C:1507:LEU:HD21	3:C:1629:ALA:HB3	1.33	1.05
1:D:634:GLN:NE2	1:D:635:ARG:N	2.05	1.05
3:C:1608:HIS:NE2	3:C:1610:PRO:HA	1.72	1.04
3:F:1507:LEU:CD1	3:F:1626:ASP:HB3	1.88	1.04
1:A:634:GLN:NE2	1:A:635:ARG:N	2.05	1.03
3:F:1572:LEU:O	3:F:1573:LYS:HG3	1.58	1.03
3:F:1572:LEU:O	3:F:1573:LYS:CG	2.06	1.02
2:E:841:ARG:HG2	2:E:841:ARG:HH11	1.22	1.02
2:E:853:LEU:HD11	3:F:1451:GLN:CB	1.89	1.02
3:F:1406:TYR:O	3:F:1407:ILE:HG12	1.57	1.02
2:E:912:GLU:H	2:E:912:GLU:CD	1.52	1.02
3:F:1572:LEU:HB2	3:F:1574:LEU:HD21	1.38	1.02
3:F:1483:LEU:HG	3:F:1590:TRP:CH2	1.95	1.02
3:C:1360:ASN:ND2	3:C:1443:GLN:HB3	1.75	1.01
3:F:1572:LEU:C	3:F:1573:LYS:HG3	1.80	1.01
3:F:1574:LEU:CD2	3:F:1574:LEU:H	1.61	1.01
3:F:1360:ASN:ND2	3:F:1443:GLN:HB3	1.75	1.00
3:F:1571:ALA:C	3:F:1572:LEU:CD2	2.29	1.00
2:B:841:ARG:HG2	2:B:841:ARG:HH11	1.23	1.00
3:F:1495:ASN:ND2	3:F:1495:ASN:H	1.59	1.00
3:F:1497:PHE:CD2	3:F:1497:PHE:C	2.34	0.99
3:F:1378:MET:HE3	1:D:268:ARG:HB2	1.42	0.99
3:F:1535:ASP:O	3:F:1566:ILE:HG23	1.62	0.99
3:F:1526:ARG:CZ	3:F:1579:HIS:NE2	2.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1520:ASP:O	3:F:1521:TYR:HB3	1.60	0.98
3:F:1497:PHE:CE1	3:F:1498:ILE:HG13	1.98	0.98
3:C:1543:ILE:HD12	3:C:1554:VAL:HG21	1.47	0.97
3:C:1580:TYR:CD2	3:C:1580:TYR:N	2.30	0.96
3:C:1360:ASN:HD22	3:C:1443:GLN:HB3	1.30	0.96
3:C:1578:LYS:HB3	3:C:1580:TYR:HE2	1.12	0.95
3:C:1582:MET:HB2	3:C:1605:TRP:O	1.66	0.95
3:F:1507:LEU:HB3	3:F:1510:ARG:HH21	0.80	0.95
3:F:1536:PHE:CD2	3:F:1566:ILE:CG1	2.49	0.95
2:B:853:LEU:HD11	3:C:1451:GLN:HB2	1.45	0.95
1:D:510:VAL:HG12	1:D:528:SER:HB3	1.48	0.94
3:C:1578:LYS:HE3	3:C:1578:LYS:HA	1.48	0.94
3:C:1609:TRP:CZ3	3:C:1627:LEU:HD22	2.02	0.94
1:D:38:HIS:O	1:D:85:THR:HG23	1.67	0.94
3:F:1509:GLU:HG2	3:F:1510:ARG:H	1.29	0.94
2:E:853:LEU:HD11	3:F:1451:GLN:HB2	0.97	0.94
3:C:1578:LYS:CD	3:C:1608:HIS:HE1	1.80	0.94
3:C:1495:ASN:HD22	3:C:1495:ASN:H	0.97	0.94
3:F:1485:ARG:HH21	3:F:1591:GLY:HA3	1.33	0.94
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.48	0.93
3:C:1516:GLU:HB3	3:C:1517:PRO:CD	1.97	0.93
3:C:1495:ASN:ND2	3:C:1495:ASN:H	1.65	0.93
1:D:590:THR:HG22	1:D:592:SER:N	1.83	0.93
3:F:1572:LEU:CD2	3:F:1572:LEU:N	2.30	0.93
1:A:38:HIS:O	1:A:85:THR:HG23	1.67	0.93
3:F:1532:LEU:HA	3:F:1569:ARG:HH12	1.34	0.93
3:F:1595:ASN:C	3:F:1596:LEU:HG	1.88	0.92
1:A:590:THR:HG22	1:A:592:SER:N	1.83	0.92
3:C:1543:ILE:O	3:C:1556:VAL:HG13	1.68	0.92
3:C:1581:LEU:CD1	3:C:1581:LEU:C	2.30	0.92
3:C:1522:VAL:O	3:C:1523:TYR:CD1	2.23	0.92
3:C:1526:ARG:HG2	3:C:1542:ALA:CB	2.00	0.92
3:F:1485:ARG:O	3:F:1486:ASP:HB2	1.68	0.92
3:F:1378:MET:CE	1:D:268:ARG:HB2	2.00	0.91
3:C:1609:TRP:CE3	3:C:1627:LEU:HD22	2.05	0.91
3:F:1590:TRP:CE3	3:F:1590:TRP:HA	2.03	0.91
1:A:634:GLN:NE2	1:A:635:ARG:H	1.66	0.90
3:F:1507:LEU:HD11	3:F:1626:ASP:HB3	1.51	0.90
1:A:223:ILE:HD11	1:A:298:VAL:HG23	1.53	0.90
3:C:1504:LYS:N	3:C:1504:LYS:HD3	1.86	0.90
3:F:1496:CYS:O	3:F:1497:PHE:HB3	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:HB3	1:A:635:ARG:HH11	1.37	0.90
3:F:1360:ASN:HD22	3:F:1443:GLN:HB3	1.30	0.90
1:D:634:GLN:HE21	1:D:635:ARG:H	0.91	0.90
3:F:1497:PHE:CD2	3:F:1498:ILE:CG1	2.54	0.90
1:D:223:ILE:HD11	1:D:298:VAL:HG23	1.53	0.89
3:F:1450:ILE:O	3:F:1450:ILE:HG13	1.72	0.89
3:F:1519:VAL:H	3:F:1585:LEU:HD21	1.37	0.89
4:M:10:TYR:HE2	3:F:1417:SER:HG	1.16	0.89
3:F:1589:PHE:O	3:F:1590:TRP:HB2	1.71	0.89
1:A:634:GLN:HE21	1:A:635:ARG:H	0.91	0.89
1:D:634:GLN:NE2	1:D:635:ARG:H	1.66	0.89
3:F:1543:ILE:CD1	3:F:1559:GLN:HA	2.02	0.89
3:C:1526:ARG:NH1	3:C:1542:ALA:CB	2.36	0.89
3:C:1578:LYS:CB	3:C:1580:TYR:CE2	2.54	0.89
3:C:1580:TYR:HD2	3:C:1580:TYR:H	1.01	0.89
1:D:10:ASN:HB3	1:D:635:ARG:HH11	1.37	0.89
3:F:1572:LEU:HD22	3:F:1572:LEU:N	1.84	0.89
3:C:1506:THR:OG1	3:C:1509:GLU:HG2	1.71	0.89
3:C:1555:GLN:O	3:C:1558:GLN:HB2	1.73	0.89
3:F:1569:ARG:O	3:F:1570:GLU:HG2	1.74	0.88
3:C:1513:LYS:O	3:C:1516:GLU:HG3	1.72	0.88
3:F:1495:ASN:N	3:F:1495:ASN:HD22	1.60	0.88
1:A:346:MET:O	1:A:391:THR:HG22	1.74	0.88
3:F:1497:PHE:C	3:F:1497:PHE:HD2	1.74	0.88
3:C:1450:ILE:HG13	3:C:1450:ILE:O	1.72	0.88
1:A:138:GLY:HA2	1:A:160:SER:OG	1.74	0.88
3:F:1536:PHE:CE2	3:F:1566:ILE:HD11	2.09	0.88
3:C:1532:LEU:HB3	3:C:1569:ARG:NH1	1.90	0.87
3:F:1535:ASP:CG	3:F:1536:PHE:H	1.77	0.87
3:F:1542:ALA:C	3:F:1543:ILE:HD12	1.94	0.87
3:F:1522:VAL:HG13	3:F:1583:TRP:HB3	1.55	0.87
3:F:1497:PHE:CD2	3:F:1498:ILE:N	2.42	0.87
1:D:138:GLY:HA2	1:D:160:SER:OG	1.74	0.87
3:C:1544:GLU:O	3:C:1545:GLN:HG3	1.73	0.87
4:M:10:TYR:HE2	3:F:1417:SER:OG	1.56	0.87
3:F:1521:TYR:HE2	3:F:1584:GLY:HA3	1.37	0.87
1:D:453:PHE:HB2	1:D:493:VAL:HG23	1.57	0.86
1:A:142:MET:HG3	1:A:187:TYR:CE1	2.10	0.86
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.57	0.86
1:D:142:MET:HG3	1:D:187:TYR:CE1	2.10	0.86
1:D:346:MET:O	1:D:391:THR:HG22	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1495:ASN:HD22	3:F:1495:ASN:H	0.90	0.86
3:F:1524:LYS:HD2	3:F:1525:THR:H	1.38	0.86
3:F:1574:LEU:CD2	3:F:1574:LEU:N	2.29	0.86
3:C:1495:ASN:HD22	3:C:1495:ASN:N	1.71	0.86
3:F:1507:LEU:HD12	3:F:1626:ASP:HB3	1.56	0.86
3:F:1590:TRP:HE3	3:F:1590:TRP:HA	1.38	0.86
3:C:1515:CYS:SG	3:C:1640:PRO:CD	2.63	0.86
3:C:1506:THR:H	3:C:1509:GLU:CG	1.89	0.85
3:F:1494:GLU:OE2	3:F:1494:GLU:HA	1.76	0.85
3:C:1581:LEU:O	3:C:1581:LEU:HG	1.75	0.85
3:C:1520:ASP:HB2	3:C:1586:SER:HB3	1.59	0.85
3:C:1578:LYS:O	3:C:1579:HIS:HB2	1.76	0.85
3:F:1533:SER:HB2	3:F:1536:PHE:O	1.76	0.85
2:B:734:ILE:HD12	2:B:734:ILE:H	1.42	0.85
2:B:912:GLU:N	2:B:912:GLU:CD	2.30	0.85
1:A:289:VAL:C	1:A:290:GLN:CG	2.44	0.84
3:F:1536:PHE:CD2	3:F:1566:ILE:HG12	2.11	0.84
3:F:1504:LYS:C	3:F:1505:VAL:HG22	1.96	0.84
3:F:1524:LYS:HD2	3:F:1525:THR:N	1.92	0.83
2:E:734:ILE:HD12	2:E:734:ILE:H	1.42	0.83
1:D:289:VAL:C	1:D:290:GLN:CG	2.44	0.83
2:B:853:LEU:CD1	3:C:1451:GLN:HB2	2.08	0.83
3:F:1571:ALA:O	3:F:1572:LEU:HD22	1.77	0.83
3:F:1572:LEU:C	3:F:1574:LEU:HD23	1.99	0.83
1:D:590:THR:HB	1:D:593:LYS:HG3	1.61	0.82
3:F:1533:SER:CB	3:F:1536:PHE:O	2.27	0.82
3:F:1497:PHE:CG	3:F:1498:ILE:HG12	2.15	0.82
1:A:590:THR:HB	1:A:593:LYS:HG3	1.62	0.82
3:C:1507:LEU:CD2	3:C:1629:ALA:HB3	2.09	0.82
3:F:1572:LEU:HB3	3:F:1574:LEU:HD21	1.62	0.82
3:F:1503:ASP:O	3:F:1505:VAL:HG13	1.79	0.81
3:F:1406:TYR:CG	3:F:1407:ILE:N	2.48	0.81
1:A:55:THR:HG22	1:A:57:ALA:H	1.46	0.81
3:F:1572:LEU:O	3:F:1574:LEU:HD23	1.79	0.81
4:M:6:THR:HA	3:F:1445:PHE:HE1	1.45	0.81
3:F:1526:ARG:HH21	3:F:1544:GLU:CD	1.84	0.81
1:A:8:THR:HG22	1:A:20:MET:HB2	1.60	0.81
3:C:1578:LYS:HG2	3:C:1580:TYR:CZ	2.16	0.81
1:D:8:THR:HG22	1:D:20:MET:HB2	1.60	0.81
3:F:1497:PHE:CE1	3:F:1498:ILE:CG1	2.62	0.81
1:D:55:THR:HG22	1:D:57:ALA:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1445:PHE:HE1	4:P:6:THR:HA	1.42	0.81
3:F:1408:SER:OG	3:F:1410:TYR:HB3	1.81	0.81
3:F:1484:CYS:HB3	3:F:1489:CYS:HB2	1.61	0.80
3:F:1485:ARG:NH2	3:F:1591:GLY:HA3	1.96	0.80
1:D:289:VAL:O	1:D:290:GLN:CG	2.30	0.80
3:F:1572:LEU:O	3:F:1573:LYS:HD2	1.79	0.80
3:F:1569:ARG:O	3:F:1570:GLU:CB	2.30	0.80
1:D:83:PHE:HD1	1:D:99:VAL:O	1.64	0.80
3:F:1622:LYS:HG3	3:F:1623:GLN:N	1.97	0.80
3:C:1507:LEU:HG	3:C:1626:ASP:HB3	1.61	0.79
1:A:289:VAL:O	1:A:290:GLN:CG	2.30	0.79
3:F:1507:LEU:H	3:F:1507:LEU:HD23	1.47	0.79
3:F:1569:ARG:CB	3:F:1570:GLU:OE1	2.30	0.79
3:F:1614:GLU:O	3:F:1614:GLU:HG3	1.82	0.79
1:A:83:PHE:HD1	1:A:99:VAL:O	1.64	0.79
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.65	0.79
3:F:1521:TYR:CE2	3:F:1584:GLY:CA	2.66	0.79
3:C:1522:VAL:O	3:C:1523:TYR:HD1	1.63	0.79
3:F:1406:TYR:O	3:F:1407:ILE:CG1	2.30	0.79
3:F:1521:TYR:CE2	3:F:1584:GLY:HA3	2.18	0.78
3:F:1533:SER:CB	3:F:1537:ASP:HA	2.10	0.78
3:F:1569:ARG:HG2	3:F:1570:GLU:CD	1.98	0.78
3:F:1569:ARG:O	3:F:1570:GLU:CG	2.30	0.78
3:C:1337:ASN:O	3:C:1371:ARG:HD2	1.84	0.78
3:C:1446:ASN:HB2	4:P:4:LEU:HB2	1.63	0.78
2:B:841:ARG:NH1	2:B:841:ARG:HG2	1.95	0.78
3:F:1337:ASN:O	3:F:1371:ARG:HD2	1.84	0.78
3:F:1536:PHE:HD2	3:F:1566:ILE:HG12	1.49	0.78
2:E:912:GLU:N	2:E:912:GLU:CD	2.30	0.77
3:F:1494:GLU:OE2	3:F:1494:GLU:CA	2.30	0.77
2:B:833:ARG:HH22	2:B:899:ILE:HD11	1.47	0.77
3:F:1543:ILE:HD13	3:F:1559:GLN:HA	1.65	0.77
2:B:819:ARG:HH21	2:B:911:PRO:HB3	1.49	0.77
3:F:1532:LEU:HA	3:F:1569:ARG:NH1	1.99	0.77
3:F:1601:GLY:H	3:F:1604:THR:CG2	1.97	0.77
1:A:22:LEU:HD11	1:A:64:VAL:HG23	1.67	0.77
3:C:1516:GLU:HB3	3:C:1517:PRO:HD2	1.65	0.77
3:F:1524:LYS:HE3	3:F:1579:HIS:HB3	1.67	0.77
1:D:98:VAL:O	1:D:634:GLN:CG	2.33	0.77
3:F:1558:GLN:O	3:F:1559:GLN:CG	2.29	0.76
3:F:1406:TYR:C	3:F:1407:ILE:CG1	2.53	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:786:SER:HB3	1:D:541:LEU:HD22	1.67	0.76
2:E:833:ARG:HH22	2:E:899:ILE:HD11	1.47	0.76
1:A:365:VAL:HG13	1:A:379:THR:OG1	1.85	0.76
1:A:98:VAL:O	1:A:634:GLN:CG	2.33	0.76
3:C:1548:LYS:HG2	3:C:1548:LYS:O	1.84	0.76
1:D:22:LEU:HD11	1:D:64:VAL:HG23	1.67	0.76
3:F:1534:ASN:HD22	3:F:1534:ASN:C	1.85	0.76
3:C:1506:THR:H	3:C:1509:GLU:HG2	1.49	0.76
3:F:1572:LEU:C	3:F:1574:LEU:CD2	2.54	0.76
2:B:733:ILE:HG12	2:B:734:ILE:N	2.01	0.75
3:F:1509:GLU:O	3:F:1510:ARG:C	2.24	0.75
2:E:733:ILE:HG12	2:E:734:ILE:N	2.01	0.75
3:F:1521:TYR:CE2	3:F:1584:GLY:N	2.55	0.75
3:F:1483:LEU:CD1	3:F:1590:TRP:CZ2	2.69	0.75
1:D:20:MET:O	1:D:64:VAL:HB	1.87	0.75
1:A:20:MET:O	1:A:64:VAL:HB	1.87	0.75
1:D:47:LEU:CD1	1:D:66:PHE:HB2	2.16	0.75
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.16	0.75
3:F:1497:PHE:CD2	3:F:1498:ILE:HG13	2.17	0.75
1:D:117:TYR:CZ	1:D:123:VAL:HG13	2.22	0.74
3:F:1521:TYR:HE2	3:F:1584:GLY:CA	2.00	0.74
3:F:1534:ASN:C	3:F:1534:ASN:ND2	2.40	0.74
1:D:365:VAL:HG13	1:D:379:THR:OG1	1.85	0.74
1:D:610:GLY:HA3	1:D:616:VAL:N	2.03	0.74
4:M:10:TYR:CE2	3:F:1417:SER:OG	2.34	0.74
1:A:530:TRP:HD1	1:A:531:VAL:N	1.85	0.74
3:F:1509:GLU:CG	3:F:1510:ARG:H	1.98	0.74
2:B:733:ILE:HD11	2:B:893:ALA:HB3	1.70	0.74
3:C:1416:PHE:HE2	3:C:1444:TYR:HD2	1.36	0.74
1:A:117:TYR:CZ	1:A:123:VAL:HG13	2.22	0.74
3:C:1634:MET:O	3:C:1638:GLY:N	2.21	0.74
1:A:369:VAL:HG12	1:A:370:GLN:N	2.03	0.73
1:D:530:TRP:HD1	1:D:531:VAL:N	1.85	0.73
1:A:610:GLY:HA3	1:A:616:VAL:N	2.02	0.73
3:F:1541:MET:HE1	3:F:1582:MET:SD	2.28	0.73
1:A:248:PHE:HD1	3:C:1378:MET:HE3	1.53	0.73
4:M:14:LYS:NZ	3:F:1415:ALA:CB	2.50	0.73
1:D:369:VAL:HG12	1:D:370:GLN:N	2.03	0.73
1:A:12:LEU:HB2	1:A:101:VAL:HG22	1.70	0.73
1:D:12:LEU:HB2	1:D:101:VAL:HG22	1.70	0.73
3:F:1497:PHE:CD2	3:F:1498:ILE:HG12	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:733:ILE:HD11	2:E:893:ALA:HB3	1.70	0.73
3:F:1535:ASP:OD2	3:F:1536:PHE:N	2.14	0.73
3:F:1510:ARG:O	3:F:1511:LEU:CB	2.37	0.72
3:F:1519:VAL:H	3:F:1585:LEU:CD2	2.01	0.72
3:F:1573:LYS:HD3	3:F:1573:LYS:C	2.10	0.72
3:C:1504:LYS:H	3:C:1504:LYS:HD3	1.55	0.72
3:C:1504:LYS:HE2	3:C:1506:THR:HG23	1.70	0.72
3:C:1544:GLU:O	3:C:1545:GLN:CG	2.38	0.72
3:C:1388:GLY:O	3:C:1443:GLN:HA	1.89	0.72
2:E:733:ILE:HG12	2:E:734:ILE:H	1.55	0.72
3:F:1536:PHE:HE2	3:F:1566:ILE:HD11	1.53	0.72
4:M:4:LEU:HD13	3:F:1444:TYR:C	2.09	0.72
3:C:1445:PHE:CE1	4:P:7:SER:N	2.58	0.72
3:C:1578:LYS:CD	3:C:1608:HIS:CE1	2.62	0.72
3:F:1416:PHE:HE2	3:F:1444:TYR:HD2	1.36	0.72
1:A:6:ILE:HD11	1:A:22:LEU:HD23	1.72	0.72
1:D:6:ILE:HD11	1:D:20:MET:HE3	1.72	0.72
3:F:1388:GLY:O	3:F:1443:GLN:HA	1.89	0.71
1:A:289:VAL:O	1:A:290:GLN:CD	2.29	0.71
3:C:1608:HIS:NE2	3:C:1610:PRO:CA	2.53	0.71
1:D:6:ILE:HD11	1:D:22:LEU:HD23	1.72	0.71
3:C:1485:ARG:HH22	3:C:1591:GLY:HA3	1.55	0.71
3:C:1610:PRO:O	3:C:1611:GLU:O	2.09	0.71
3:C:1445:PHE:HE1	4:P:6:THR:CA	2.03	0.71
1:D:289:VAL:O	1:D:290:GLN:CD	2.29	0.71
3:F:1347:PRO:HA	3:F:1362:MET:HB3	1.71	0.71
3:F:1509:GLU:HG2	3:F:1510:ARG:N	2.05	0.71
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.72	0.71
1:A:98:VAL:O	1:A:634:GLN:CD	2.29	0.71
3:C:1629:ALA:O	3:C:1633:SER:HB2	1.91	0.71
1:D:24:ALA:HB3	1:D:60:HIS:HB3	1.72	0.71
3:C:1578:LYS:HB3	3:C:1580:TYR:CZ	2.25	0.71
3:F:1536:PHE:CD2	3:F:1566:ILE:HD11	2.24	0.71
3:C:1347:PRO:HA	3:C:1362:MET:HB3	1.71	0.71
3:F:1542:ALA:O	3:F:1543:ILE:HG13	1.91	0.71
2:B:733:ILE:HG12	2:B:734:ILE:H	1.55	0.70
2:B:840:VAL:HG11	2:B:892:ALA:HB1	1.72	0.70
3:C:1605:TRP:HE1	3:C:1607:GLU:HB2	1.56	0.70
1:D:98:VAL:O	1:D:634:GLN:CD	2.29	0.70
3:F:1522:VAL:HG23	3:F:1548:LYS:HB3	1.71	0.70
1:A:281:SER:OG	1:A:284:VAL:HG23	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:THR:O	1:A:85:THR:OG1	2.03	0.70
1:D:281:SER:OG	1:D:284:VAL:HG23	1.91	0.70
4:M:36:LEU:N	4:M:36:LEU:HD23	2.05	0.70
3:C:1526:ARG:CZ	3:C:1542:ALA:CB	2.70	0.70
1:D:237:PHE:CE2	1:D:243:VAL:HG22	2.27	0.70
1:D:223:ILE:CD1	1:D:298:VAL:HG23	2.21	0.70
1:D:85:THR:O	1:D:85:THR:OG1	2.03	0.70
1:A:237:PHE:CE2	1:A:243:VAL:HG22	2.27	0.70
3:C:1389:PHE:HD1	3:C:1441:VAL:HG23	1.57	0.70
3:C:1495:ASN:ND2	3:C:1495:ASN:N	2.33	0.70
3:F:1568:CYS:O	3:F:1569:ARG:C	2.30	0.70
4:P:36:LEU:N	4:P:36:LEU:HD23	2.07	0.70
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.74	0.69
1:A:589:LEU:HD12	1:A:590:THR:H	1.57	0.69
1:D:504:ILE:HG12	1:D:533:VAL:HG11	1.73	0.69
3:F:1574:LEU:HB3	3:F:1580:TYR:CZ	2.26	0.69
4:P:36:LEU:HB3	4:P:40:TYR:CD2	2.27	0.69
1:A:6:ILE:HD11	1:A:20:MET:HE3	1.73	0.69
3:F:1569:ARG:C	3:F:1570:GLU:OE1	2.30	0.69
1:A:504:ILE:HG12	1:A:533:VAL:HG11	1.73	0.69
1:D:47:LEU:HD13	1:D:66:PHE:HB2	1.74	0.69
1:D:589:LEU:HD12	1:D:590:THR:H	1.58	0.69
3:F:1571:ALA:CA	3:F:1572:LEU:HD22	2.22	0.69
2:E:840:VAL:HG11	2:E:892:ALA:HB1	1.72	0.69
4:M:14:LYS:NZ	3:F:1415:ALA:HB1	2.08	0.69
3:C:1535:ASP:HB2	3:C:1536:PHE:HD2	1.57	0.69
3:C:1526:ARG:CG	3:C:1542:ALA:HB3	2.06	0.69
1:D:369:VAL:HG12	1:D:370:GLN:H	1.58	0.69
1:D:38:HIS:CE1	1:D:45:LEU:HD12	2.28	0.69
3:F:1389:PHE:HD1	3:F:1441:VAL:HG23	1.57	0.69
3:F:1530:VAL:O	3:F:1530:VAL:HG23	1.91	0.69
3:F:1588:ASP:HB3	3:F:1599:ILE:HG13	1.74	0.69
1:D:495:LEU:HD12	1:D:496:PRO:HD2	1.74	0.69
1:A:588:LYS:NZ	2:B:781:GLU:OE2	2.26	0.68
3:F:1536:PHE:HD2	3:F:1566:ILE:CG1	2.02	0.68
1:A:330:PRO:O	1:A:357:PRO:HD3	1.93	0.68
1:A:223:ILE:CD1	1:A:298:VAL:HG23	2.21	0.68
1:A:38:HIS:CE1	1:A:45:LEU:HD12	2.28	0.68
1:A:369:VAL:HG12	1:A:370:GLN:H	1.58	0.68
1:A:495:LEU:HD12	1:A:496:PRO:HD2	1.74	0.68
3:F:1532:LEU:HD12	3:F:1532:LEU:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1544:GLU:OE1	3:C:1579:HIS:CE1	2.46	0.68
1:D:286:LEU:O	1:D:289:VAL:HG23	1.94	0.68
1:D:330:PRO:O	1:D:357:PRO:HD3	1.93	0.68
2:E:781:GLU:OE2	1:D:588:LYS:NZ	2.27	0.68
2:B:825:ILE:CD1	2:B:888:VAL:HG11	2.24	0.68
1:A:286:LEU:O	1:A:289:VAL:HG23	1.94	0.68
3:C:1485:ARG:NH2	3:C:1591:GLY:HA3	2.09	0.68
3:F:1521:TYR:CG	3:F:1521:TYR:O	2.47	0.68
3:F:1557:GLY:O	3:F:1558:GLN:O	2.12	0.68
3:F:1605:TRP:C	3:F:1605:TRP:CD1	2.67	0.68
3:F:1507:LEU:HD21	3:F:1622:LYS:HE3	1.76	0.68
2:E:841:ARG:HG2	2:E:841:ARG:NH1	1.95	0.67
3:F:1537:ASP:HB2	3:F:1569:ARG:HD2	1.75	0.67
3:F:1569:ARG:C	3:F:1570:GLU:CG	2.62	0.67
3:F:1569:ARG:O	3:F:1570:GLU:HB2	1.93	0.67
1:D:19:THR:HA	1:D:64:VAL:O	1.94	0.67
3:F:1496:CYS:HA	3:F:1601:GLY:O	1.94	0.67
3:C:1506:THR:H	3:C:1509:GLU:HG3	1.59	0.67
2:E:825:ILE:CD1	2:E:888:VAL:HG11	2.24	0.67
3:C:1573:LYS:HD2	3:C:1573:LYS:O	1.95	0.67
3:C:1551:SER:CB	3:C:1593:LYS:HZ1	2.06	0.67
1:D:444:ARG:NH2	1:D:534:LYS:HD3	2.09	0.67
1:A:216:PRO:HB2	1:A:218:GLU:O	1.95	0.67
3:C:1526:ARG:CZ	3:C:1542:ALA:HB1	2.23	0.67
3:F:1601:GLY:N	3:F:1604:THR:HG21	2.09	0.67
3:C:1506:THR:C	3:C:1508:GLU:H	1.96	0.67
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.77	0.67
3:C:1590:TRP:CE3	3:C:1590:TRP:HA	2.30	0.67
3:F:1526:ARG:NH2	3:F:1579:HIS:NE2	2.43	0.67
1:A:444:ARG:NH2	1:A:534:LYS:HD3	2.09	0.67
2:B:837:GLU:HG2	4:P:64:SER:OG	1.95	0.67
3:C:1504:LYS:CE	3:C:1506:THR:HG23	2.25	0.67
2:E:742:ARG:HB3	2:E:775:ASP:HB3	1.77	0.67
3:F:1558:GLN:C	3:F:1559:GLN:CG	2.55	0.66
3:F:1543:ILE:HD11	3:F:1559:GLN:HA	1.77	0.66
1:A:19:THR:HA	1:A:64:VAL:O	1.94	0.66
3:F:1601:GLY:N	3:F:1604:THR:CG2	2.58	0.66
3:C:1578:LYS:O	3:C:1579:HIS:CB	2.44	0.66
3:C:1510:ARG:HB3	3:C:1630:PHE:CE1	2.30	0.66
3:C:1508:GLU:O	3:C:1512:ASP:CG	2.34	0.66
3:F:1497:PHE:O	3:F:1498:ILE:C	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:VAL:HG12	1:D:136:PRO:HA	1.78	0.66
1:D:257:GLU:N	1:D:257:GLU:CD	2.49	0.66
1:A:8:THR:HG22	1:A:20:MET:CB	2.26	0.66
3:C:1546:THR:O	3:C:1548:LYS:N	2.28	0.66
2:E:793:ILE:HG13	2:E:794:CYS:H	1.61	0.66
2:B:793:ILE:HG13	2:B:794:CYS:H	1.61	0.66
1:D:407:GLN:O	1:D:408:GLU:HB2	1.96	0.66
3:F:1507:LEU:N	3:F:1507:LEU:HD23	2.10	0.66
3:C:1535:ASP:HB2	3:C:1536:PHE:CD2	2.31	0.65
3:C:1562:PHE:CE2	3:C:1582:MET:CE	2.79	0.65
3:F:1483:LEU:HD11	3:F:1590:TRP:CZ2	2.31	0.65
3:F:1536:PHE:CD2	3:F:1566:ILE:CD1	2.78	0.65
3:F:1536:PHE:CE2	3:F:1566:ILE:CD1	2.79	0.65
3:C:1385:MET:HG3	3:C:1390:ALA:HA	1.79	0.65
3:C:1507:LEU:HD21	3:C:1629:ALA:CB	2.19	0.65
4:M:6:THR:HA	3:F:1445:PHE:CE1	2.29	0.65
3:F:1573:LYS:HZ2	3:F:1573:LYS:HB2	1.60	0.65
3:C:1581:LEU:CD1	3:C:1582:MET:N	2.41	0.65
1:D:624:PHE:O	1:D:631:GLN:HA	1.97	0.65
2:E:841:ARG:HH11	2:E:841:ARG:CG	2.06	0.65
4:M:36:LEU:HB3	4:M:40:TYR:CD2	2.30	0.65
2:B:795:VAL:HG12	2:B:795:VAL:O	1.96	0.65
3:F:1460:TYR:CD1	1:D:248:PHE:HB2	2.31	0.65
3:F:1611:GLU:O	3:F:1615:CYS:HB2	1.96	0.65
4:P:84:LYS:HG3	4:P:84:LYS:O	1.96	0.65
1:D:8:THR:HG22	1:D:20:MET:CB	2.26	0.65
3:F:1532:LEU:CA	3:F:1569:ARG:HH12	2.08	0.65
1:A:130:VAL:HG12	1:A:136:PRO:HA	1.78	0.65
1:A:257:GLU:CD	1:A:257:GLU:N	2.49	0.65
1:D:554:VAL:HG13	1:D:555:PRO:HD2	1.78	0.65
1:D:216:PRO:HB2	1:D:218:GLU:O	1.95	0.65
3:F:1497:PHE:CE2	3:F:1498:ILE:CB	2.80	0.65
4:M:84:LYS:O	4:M:84:LYS:HG3	1.96	0.65
2:B:839:LYS:NZ	4:P:12:ASN:OD1	2.30	0.65
1:A:624:PHE:O	1:A:631:GLN:HA	1.97	0.65
3:F:1607:GLU:O	3:F:1608:HIS:HB2	1.96	0.65
3:F:1624:CYS:O	3:F:1626:ASP:N	2.30	0.65
1:A:38:HIS:O	1:A:85:THR:CG2	2.44	0.65
1:D:93:GLN:OE1	1:D:93:GLN:HA	1.97	0.65
3:F:1520:ASP:OD1	3:F:1551:SER:HB2	1.97	0.65
1:D:37:VAL:HG12	1:D:84:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1556:VAL:O	3:F:1558:GLN:N	2.30	0.64
3:C:1582:MET:CB	3:C:1605:TRP:O	2.45	0.64
3:F:1485:ARG:CZ	3:F:1590:TRP:O	2.45	0.64
3:F:1570:GLU:N	3:F:1570:GLU:OE1	2.30	0.64
2:E:837:GLU:HG2	4:M:64:SER:OG	1.97	0.64
2:E:795:VAL:HG12	2:E:795:VAL:O	1.96	0.64
1:A:37:VAL:HG12	1:A:84:VAL:HG22	1.78	0.64
1:A:6:ILE:HG22	1:A:625:THR:HB	1.80	0.64
1:A:535:ASP:O	1:A:536:SER:HB3	1.97	0.64
3:F:1600:ILE:O	3:F:1600:ILE:HG22	1.95	0.64
3:C:1612:GLU:O	3:C:1616:GLN:NE2	2.30	0.64
1:D:335:PHE:CD2	1:D:419:MET:HB3	2.33	0.64
3:F:1536:PHE:CD2	3:F:1566:ILE:HG13	2.32	0.64
1:D:105:SER:HB2	1:D:188:TYR:CD1	2.33	0.64
1:D:610:GLY:HA3	1:D:616:VAL:H	1.63	0.64
3:F:1369:ARG:HD2	3:F:1432:SER:O	1.98	0.64
3:F:1595:ASN:O	3:F:1596:LEU:CG	2.30	0.64
3:F:1610:PRO:HG2	3:F:1624:CYS:SG	2.37	0.64
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.78	0.64
1:D:6:ILE:HG22	1:D:625:THR:HB	1.80	0.64
3:F:1385:MET:HG3	3:F:1390:ALA:HA	1.79	0.64
3:F:1572:LEU:O	3:F:1574:LEU:CD2	2.43	0.64
3:C:1590:TRP:HE3	3:C:1590:TRP:HA	1.63	0.64
1:D:445:PRO:HA	1:D:499:ILE:O	1.98	0.64
1:D:535:ASP:O	1:D:536:SER:HB3	1.97	0.63
3:C:1581:LEU:HD12	3:C:1582:MET:CA	2.27	0.63
2:B:819:ARG:HG2	2:B:820:ASN:ND2	2.13	0.63
3:C:1551:SER:O	3:C:1593:LYS:NZ	2.31	0.63
3:C:1600:ILE:HG22	3:C:1600:ILE:O	1.99	0.63
3:F:1495:ASN:N	3:F:1495:ASN:ND2	2.30	0.63
3:F:1526:ARG:NH2	3:F:1579:HIS:CE1	2.67	0.63
1:A:335:PHE:CD2	1:A:419:MET:HB3	2.33	0.63
1:A:610:GLY:HA3	1:A:616:VAL:H	1.63	0.63
3:C:1580:TYR:HD2	3:C:1580:TYR:N	1.80	0.63
1:A:407:GLN:O	1:A:408:GLU:HB2	1.96	0.63
1:A:433:TYR:HB2	1:A:456:ARG:HB3	1.81	0.63
3:C:1369:ARG:HD2	3:C:1432:SER:O	1.98	0.63
3:C:1546:THR:HG23	3:C:1556:VAL:HG23	1.80	0.63
3:C:1445:PHE:CE1	4:P:6:THR:C	2.72	0.63
1:D:307:THR:HG23	1:D:318:GLN:HG3	1.81	0.63
2:E:760:PRO:HG3	1:D:567:HIS:ND1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1572:LEU:HB2	3:F:1574:LEU:CD2	2.24	0.63
1:A:105:SER:HB2	1:A:188:TYR:CD1	2.33	0.63
3:C:1507:LEU:HG	3:C:1626:ASP:CB	2.29	0.63
1:D:433:TYR:HB2	1:D:456:ARG:HB3	1.80	0.63
3:F:1568:CYS:C	3:F:1569:ARG:O	2.37	0.63
1:A:445:PRO:HA	1:A:499:ILE:O	1.98	0.62
3:C:1551:SER:HB3	3:C:1593:LYS:HZ1	1.63	0.62
3:C:1581:LEU:O	3:C:1581:LEU:CG	2.41	0.62
1:D:154:LYS:HE2	1:D:156:ASP:OD1	1.99	0.62
1:D:340:LYS:O	1:D:341:TYR:CD1	2.52	0.62
1:D:84:VAL:HG13	1:D:85:THR:N	2.14	0.62
3:F:1535:ASP:CG	3:F:1536:PHE:N	2.45	0.62
1:A:114:LYS:HE3	1:A:116:ILE:O	1.99	0.62
1:A:286:LEU:HB3	1:A:291:ASN:ND2	2.14	0.62
1:D:286:LEU:HB3	1:D:291:ASN:ND2	2.15	0.62
2:E:839:LYS:NZ	4:M:12:ASN:OD1	2.32	0.62
2:E:840:VAL:CG1	2:E:892:ALA:HB1	2.28	0.62
3:F:1408:SER:O	3:F:1410:TYR:N	2.32	0.62
3:F:1507:LEU:HG	3:F:1626:ASP:OD2	1.98	0.62
3:C:1578:LYS:CB	3:C:1580:TYR:CZ	2.82	0.62
3:F:1378:MET:HG2	1:D:268:ARG:HH11	1.62	0.62
1:D:38:HIS:O	1:D:85:THR:CG2	2.44	0.62
1:A:248:PHE:CD1	3:C:1378:MET:HE3	2.35	0.62
1:A:93:GLN:HA	1:A:93:GLN:OE1	1.97	0.62
1:D:295:GLU:O	1:D:298:VAL:HB	2.00	0.62
2:E:877:VAL:HG13	3:F:1451:GLN:NE2	2.14	0.62
3:F:1497:PHE:CG	3:F:1498:ILE:CG1	2.80	0.62
1:D:438:VAL:O	1:D:440:ARG:HG3	2.00	0.62
1:A:340:LYS:O	1:A:341:TYR:CD1	2.52	0.62
2:B:840:VAL:CG1	2:B:892:ALA:HB1	2.28	0.62
1:A:84:VAL:HG13	1:A:85:THR:N	2.14	0.62
3:F:1639:CYS:O	3:F:1641:ASN:N	2.29	0.62
1:D:455:LEU:HD11	1:D:457:MET:HG2	1.82	0.62
3:C:1516:GLU:HB3	3:C:1517:PRO:HD3	1.82	0.62
3:C:1520:ASP:CB	3:C:1586:SER:HB3	2.30	0.62
1:D:142:MET:HG3	1:D:187:TYR:HE1	1.64	0.62
3:F:1497:PHE:CD1	3:F:1498:ILE:CG1	2.83	0.62
3:F:1507:LEU:CB	3:F:1510:ARG:NH2	2.38	0.62
3:F:1543:ILE:O	3:F:1545:GLN:N	2.31	0.62
3:C:1578:LYS:HE3	3:C:1578:LYS:CA	2.14	0.61
3:F:1406:TYR:C	3:F:1407:ILE:HG13	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1507:LEU:CD1	3:F:1626:ASP:CB	2.71	0.61
3:F:1554:VAL:O	3:F:1554:VAL:HG22	2.00	0.61
1:A:22:LEU:HB2	1:A:62:GLY:HA3	1.83	0.61
3:C:1510:ARG:HB3	3:C:1630:PHE:CD1	2.34	0.61
3:F:1507:LEU:HD12	3:F:1626:ASP:CB	2.30	0.61
2:B:912:GLU:N	2:B:912:GLU:OE1	2.30	0.61
3:F:1485:ARG:NH2	3:F:1590:TRP:O	2.33	0.61
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.15	0.61
4:M:10:TYR:HE2	3:F:1417:SER:CB	2.14	0.61
3:F:1572:LEU:HD23	3:F:1572:LEU:N	2.15	0.61
3:F:1601:GLY:H	3:F:1604:THR:HG21	1.65	0.61
1:A:295:GLU:O	1:A:298:VAL:HB	2.00	0.61
1:A:307:THR:HG23	1:A:318:GLN:HG3	1.81	0.61
1:D:114:LYS:HE3	1:D:116:ILE:O	1.99	0.61
3:F:1460:TYR:CD1	1:D:248:PHE:CB	2.84	0.61
3:F:1405:ARG:NE	3:F:1437:LEU:HD23	2.15	0.61
3:F:1526:ARG:NH2	3:F:1544:GLU:OE2	2.32	0.61
1:D:487:GLU:O	1:D:490:GLN:HB2	2.01	0.61
1:D:22:LEU:HB2	1:D:62:GLY:HA3	1.83	0.61
3:F:1409:LYS:O	3:F:1411:GLU:N	2.33	0.61
3:F:1533:SER:HB3	3:F:1536:PHE:O	2.00	0.61
3:F:1574:LEU:HA	3:F:1580:TYR:OH	2.00	0.61
3:F:1509:GLU:CG	3:F:1510:ARG:N	2.60	0.61
1:A:154:LYS:HE2	1:A:156:ASP:OD1	1.99	0.61
1:D:334:HIS:HB2	1:D:353:PHE:HB3	1.83	0.61
3:C:1445:PHE:HE1	4:P:6:THR:C	2.03	0.61
1:A:438:VAL:O	1:A:440:ARG:HG3	2.00	0.60
1:A:448:THR:HG21	1:D:377:SER:HB2	1.83	0.60
1:A:179:MET:HG3	1:A:203:LYS:HA	1.82	0.60
1:A:487:GLU:O	1:A:490:GLN:HB2	2.01	0.60
1:A:513:TYR:CE1	1:A:525:VAL:HB	2.36	0.60
2:E:912:GLU:OE1	2:E:912:GLU:N	2.30	0.60
3:F:1600:ILE:HA	3:F:1604:THR:HG21	1.82	0.60
3:C:1578:LYS:CG	3:C:1580:TYR:CE2	2.85	0.60
1:D:73:GLU:HB3	1:D:82:LYS:NZ	2.16	0.60
4:M:14:LYS:HZ3	3:F:1415:ALA:CB	2.14	0.60
1:A:134:LEU:HD11	1:A:598:VAL:HG21	1.84	0.60
1:A:455:LEU:HD11	1:A:457:MET:HG2	1.82	0.60
3:C:1339:PHE:HE2	3:C:1429:VAL:HG21	1.67	0.60
3:F:1577:LYS:O	3:F:1579:HIS:HD2	1.84	0.60
3:F:1526:ARG:HB2	3:F:1579:HIS:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1526:ARG:NE	3:F:1579:HIS:NE2	2.48	0.60
1:A:334:HIS:HB2	1:A:353:PHE:HB3	1.83	0.60
3:C:1405:ARG:NE	3:C:1437:LEU:HD23	2.15	0.60
3:F:1408:SER:HG	3:F:1410:TYR:HB3	1.65	0.60
3:C:1416:PHE:C	3:C:1416:PHE:CD2	2.75	0.60
1:A:20:MET:HG2	1:A:64:VAL:HG21	1.84	0.60
1:A:73:GLU:HB3	1:A:82:LYS:NZ	2.16	0.60
2:B:833:ARG:NH2	2:B:899:ILE:HD11	2.17	0.60
1:D:134:LEU:HD11	1:D:598:VAL:HG21	1.84	0.60
3:C:1422:LEU:HD12	3:C:1423:ILE:N	2.17	0.60
1:D:37:VAL:HG12	1:D:84:VAL:CG2	2.32	0.60
1:D:513:TYR:CE1	1:D:525:VAL:HB	2.37	0.60
1:D:179:MET:HG3	1:D:203:LYS:HA	1.82	0.60
3:C:1445:PHE:CE1	4:P:6:THR:HA	2.31	0.60
2:B:842:VAL:HG23	2:B:892:ALA:HB2	1.82	0.60
2:E:842:VAL:HG23	2:E:892:ALA:HB2	1.82	0.60
3:F:1483:LEU:CD2	3:F:1599:ILE:HG21	2.31	0.60
3:F:1571:ALA:N	3:F:1572:LEU:CD2	2.65	0.60
3:C:1640:PRO:C	3:C:1641:ASN:HD22	2.04	0.59
2:E:786:SER:HA	1:D:570:ARG:O	2.01	0.59
3:F:1416:PHE:C	3:F:1416:PHE:CD2	2.75	0.59
3:F:1533:SER:OG	3:F:1538:GLU:CG	2.34	0.59
2:B:841:ARG:HG2	2:B:841:ARG:O	2.01	0.59
1:A:534:LYS:CG	1:A:534:LYS:O	2.50	0.59
1:D:606:THR:HG22	1:D:608:GLY:N	2.17	0.59
2:E:831:ASN:ND2	2:E:868:PRO:HA	2.18	0.59
3:F:1497:PHE:CD1	3:F:1498:ILE:HG12	2.36	0.59
3:F:1595:ASN:C	3:F:1596:LEU:CG	2.67	0.59
1:A:377:SER:HB2	1:D:448:THR:HG21	1.84	0.59
3:C:1522:VAL:HG22	3:C:1583:TRP:HB3	1.83	0.59
2:B:804:MET:HG2	2:B:805:GLN:H	1.68	0.59
1:D:47:LEU:HD11	1:D:66:PHE:HB2	1.85	0.59
2:E:841:ARG:HG2	2:E:841:ARG:O	2.02	0.59
4:P:36:LEU:HB3	4:P:40:TYR:HD2	1.65	0.59
1:A:606:THR:HG22	1:A:608:GLY:N	2.17	0.59
3:C:1544:GLU:O	3:C:1545:GLN:CB	2.50	0.59
1:D:99:VAL:HG12	1:D:100:LEU:N	2.18	0.59
3:F:1526:ARG:NE	3:F:1544:GLU:OE2	2.36	0.59
1:A:117:TYR:CG	1:A:123:VAL:HG22	2.37	0.59
3:C:1360:ASN:HD22	3:C:1443:GLN:CB	2.11	0.59
3:C:1593:LYS:HG2	3:C:1596:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:TYR:CG	1:D:123:VAL:HG22	2.37	0.59
1:A:99:VAL:HG12	1:A:100:LEU:N	2.18	0.59
1:A:37:VAL:HG12	1:A:84:VAL:CG2	2.32	0.59
2:B:831:ASN:ND2	2:B:868:PRO:HA	2.18	0.59
1:D:345:GLY:H	1:D:391:THR:HG23	1.68	0.59
1:D:534:LYS:O	1:D:534:LYS:CG	2.50	0.59
3:F:1495:ASN:O	3:F:1496:CYS:HB3	2.01	0.59
4:M:10:TYR:CE2	3:F:1417:SER:CB	2.85	0.59
1:A:589:LEU:HD12	1:A:590:THR:N	2.18	0.59
3:C:1365:GLU:HG3	3:C:1438:ALA:HB2	1.85	0.59
3:C:1485:ARG:NH2	3:C:1591:GLY:CA	2.66	0.59
1:D:443:LEU:HD11	1:D:449:LEU:HD22	1.85	0.59
2:E:825:ILE:HD13	2:E:888:VAL:HG11	1.84	0.59
3:C:1634:MET:O	3:C:1635:VAL:C	2.42	0.59
3:F:1341:LEU:O	3:F:1469:ARG:HG2	2.03	0.59
1:A:136:PRO:HD2	2:B:789:ASP:HA	1.83	0.58
3:C:1341:LEU:O	3:C:1469:ARG:HG2	2.03	0.58
3:F:1422:LEU:HD12	3:F:1423:ILE:N	2.17	0.58
1:A:47:LEU:HD11	1:A:66:PHE:HB2	1.85	0.58
3:C:1532:LEU:HB3	3:C:1569:ARG:HH12	1.68	0.58
1:D:20:MET:HG2	1:D:64:VAL:HG21	1.84	0.58
2:E:804:MET:HG2	2:E:805:GLN:H	1.68	0.58
3:F:1339:PHE:HE2	3:F:1429:VAL:HG21	1.67	0.58
3:F:1365:GLU:HG3	3:F:1438:ALA:HB2	1.85	0.58
3:F:1615:CYS:O	3:F:1617:ASP:N	2.36	0.58
3:C:1608:HIS:HD2	3:C:1610:PRO:HG3	1.68	0.58
1:D:444:ARG:CZ	1:D:534:LYS:HD3	2.33	0.58
1:D:589:LEU:HD12	1:D:590:THR:N	2.18	0.58
3:F:1406:TYR:CD1	3:F:1407:ILE:N	2.72	0.58
3:F:1560:ARG:HD3	3:F:1598:TYR:HE1	1.68	0.58
1:A:444:ARG:CZ	1:A:534:LYS:HD3	2.33	0.58
1:A:510:VAL:HG12	1:A:528:SER:CB	2.30	0.58
1:A:6:ILE:CD1	1:A:22:LEU:HD23	2.33	0.58
3:C:1416:PHE:HE2	3:C:1444:TYR:CD2	2.21	0.58
3:C:1608:HIS:HD2	3:C:1610:PRO:CD	2.17	0.58
2:E:833:ARG:NH2	2:E:899:ILE:HD11	2.17	0.58
1:A:513:TYR:CZ	1:A:525:VAL:HB	2.39	0.58
2:B:873:SER:HB3	3:C:1421:THR:HG21	1.86	0.58
2:B:825:ILE:HD13	2:B:888:VAL:HG11	1.84	0.58
1:D:10:ASN:CG	1:D:635:ARG:HD2	2.24	0.58
3:F:1554:VAL:HB	3:F:1560:ARG:NH2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1341:LEU:HD23	3:C:1469:ARG:HB2	1.86	0.58
3:C:1525:THR:HA	3:C:1542:ALA:O	2.03	0.58
3:F:1345:ILE:O	3:F:1345:ILE:HG23	2.04	0.58
3:F:1510:ARG:O	3:F:1511:LEU:HB2	2.02	0.58
3:F:1554:VAL:CG2	3:F:1558:GLN:OE1	2.40	0.58
3:C:1526:ARG:O	3:C:1528:VAL:HG23	2.02	0.58
3:C:1578:LYS:CG	3:C:1580:TYR:CZ	2.86	0.58
1:D:118:THR:HG23	1:D:205:TYR:CZ	2.38	0.58
1:D:530:TRP:CD1	1:D:531:VAL:N	2.69	0.58
1:A:10:ASN:CG	1:A:635:ARG:HD2	2.24	0.58
1:D:453:PHE:HB2	1:D:493:VAL:CG2	2.32	0.58
1:A:118:THR:HG23	1:A:205:TYR:CZ	2.38	0.58
1:A:446:GLY:N	1:A:499:ILE:O	2.32	0.58
4:M:55:LEU:O	4:M:58:LYS:HD3	2.04	0.58
3:C:1360:ASN:ND2	3:C:1443:GLN:CB	2.60	0.57
3:F:1600:ILE:CA	3:F:1604:THR:HG21	2.34	0.57
3:F:1621:GLN:O	3:F:1625:GLN:HG3	2.03	0.57
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.85	0.57
1:A:477:ARG:NH2	1:A:479:LEU:HD13	2.20	0.57
3:F:1497:PHE:CG	3:F:1498:ILE:N	2.69	0.57
3:F:1515:CYS:SG	3:F:1634:MET:HE1	2.44	0.57
1:A:530:TRP:CD1	1:A:531:VAL:N	2.69	0.57
3:C:1559:GLN:O	3:C:1560:ARG:HG2	2.05	0.57
3:C:1608:HIS:HD2	3:C:1610:PRO:CG	2.18	0.57
1:A:345:GLY:H	1:A:391:THR:HG23	1.68	0.57
1:A:594:ILE:O	1:A:598:VAL:HG23	2.04	0.57
3:C:1578:LYS:HG2	3:C:1580:TYR:CE2	2.40	0.57
3:F:1378:MET:HG2	1:D:268:ARG:NH1	2.19	0.57
2:B:773:LEU:HD13	2:B:803:VAL:CG2	2.35	0.57
1:D:513:TYR:CZ	1:D:525:VAL:HB	2.39	0.57
1:D:6:ILE:CD1	1:D:22:LEU:HD23	2.33	0.57
3:F:1360:ASN:ND2	3:F:1443:GLN:CB	2.60	0.57
3:F:1628:GLY:O	3:F:1632:GLU:HG2	2.05	0.57
2:B:841:ARG:HH11	2:B:841:ARG:CG	2.06	0.57
3:C:1545:GLN:HA	3:C:1556:VAL:HG21	1.85	0.57
3:F:1393:THR:CG2	3:F:1419:ARG:HH22	2.17	0.57
3:F:1525:THR:OG1	3:F:1541:MET:HG2	2.05	0.57
1:A:534:LYS:HG3	1:A:534:LYS:O	2.05	0.57
1:A:567:HIS:CG	2:B:760:PRO:HG3	2.40	0.57
1:A:586:LYS:O	1:A:587:ASN:HB2	2.05	0.57
3:C:1506:THR:C	3:C:1508:GLU:N	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1589:PHE:HB3	3:C:1596:LEU:HD22	1.85	0.57
3:F:1408:SER:O	3:F:1409:LYS:C	2.42	0.57
4:M:26:LEU:HD12	4:M:26:LEU:C	2.25	0.57
3:C:1590:TRP:HB3	3:C:1597:SER:HB2	1.85	0.57
3:F:1568:CYS:O	3:F:1572:LEU:HD21	2.04	0.57
1:D:594:ILE:O	1:D:598:VAL:HG23	2.04	0.57
3:F:1341:LEU:HD23	3:F:1469:ARG:HB2	1.86	0.57
1:A:83:PHE:CD1	1:A:99:VAL:O	2.54	0.56
3:C:1393:THR:CG2	3:C:1419:ARG:HH22	2.17	0.56
1:D:477:ARG:NH2	1:D:479:LEU:HD13	2.20	0.56
1:D:83:PHE:CD1	1:D:99:VAL:O	2.54	0.56
3:F:1507:LEU:HD11	3:F:1626:ASP:CB	2.30	0.56
3:F:1533:SER:O	3:F:1536:PHE:O	2.23	0.56
1:A:364:ARG:HG2	1:A:378:LEU:HD23	1.87	0.56
2:E:789:ASP:HA	1:D:136:PRO:HD2	1.87	0.56
3:F:1630:PHE:O	3:F:1633:SER:HB3	2.05	0.56
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.87	0.56
1:A:570:ARG:O	2:B:786:SER:HA	2.05	0.56
3:C:1345:ILE:HG23	3:C:1345:ILE:O	2.04	0.56
3:F:1528:VAL:HG22	3:F:1542:ALA:H	1.69	0.56
4:M:84:LYS:O	4:M:85:TYR:HB2	2.05	0.56
1:A:10:ASN:HB3	1:A:635:ARG:NH1	2.15	0.56
1:A:34:THR:HG22	1:A:51:LYS:HE2	1.88	0.56
1:D:99:VAL:HG12	1:D:100:LEU:H	1.70	0.56
1:D:34:THR:HG22	1:D:51:LYS:HE2	1.88	0.56
1:D:510:VAL:HG12	1:D:528:SER:CB	2.30	0.56
3:F:1543:ILE:C	3:F:1545:GLN:H	2.09	0.56
2:B:734:ILE:HD13	2:B:893:ALA:HB1	1.88	0.56
3:F:1544:GLU:OE2	3:F:1579:HIS:CE1	2.58	0.56
4:M:64:SER:O	4:M:67:LYS:HB3	2.05	0.56
4:P:55:LEU:O	4:P:58:LYS:HD3	2.04	0.56
1:D:471:LEU:O	1:D:509:LEU:HD12	2.06	0.56
2:E:741:SER:HB3	2:E:902:GLY:C	2.26	0.56
4:M:4:LEU:HB3	3:F:1444:TYR:O	2.05	0.56
3:F:1483:LEU:HG	3:F:1590:TRP:CZ2	2.40	0.56
1:A:179:MET:HG3	1:A:202:VAL:O	2.06	0.56
1:A:210:PHE:CE2	1:A:310:LEU:HD21	2.41	0.56
3:C:1546:THR:HG23	3:C:1556:VAL:CG2	2.36	0.56
2:E:734:ILE:HD13	2:E:893:ALA:HB1	1.88	0.56
4:P:64:SER:O	4:P:67:LYS:HB3	2.05	0.56
3:C:1404:ASP:HA	3:C:1427:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1411:GLU:O	3:C:1414:LYS:HG3	2.06	0.56
3:C:1581:LEU:CD2	3:C:1627:LEU:HD21	2.36	0.56
3:C:1608:HIS:CD2	3:C:1610:PRO:CA	2.88	0.56
3:F:1546:THR:HG23	3:F:1546:THR:O	2.06	0.56
3:F:1574:LEU:HB3	3:F:1580:TYR:OH	2.05	0.56
1:A:430:SER:O	1:A:431:ASN:HB2	2.06	0.56
1:A:471:LEU:O	1:A:509:LEU:HD12	2.06	0.56
4:P:84:LYS:O	4:P:85:TYR:HB2	2.05	0.56
2:B:851:CYS:HB3	2:B:879:VAL:HB	1.87	0.56
3:C:1349:PRO:O	3:C:1350:GLU:CB	2.34	0.56
3:C:1524:LYS:O	3:C:1525:THR:HG23	2.06	0.56
3:C:1574:LEU:HD23	3:C:1580:TYR:CD1	2.41	0.56
2:E:734:ILE:N	2:E:734:ILE:HD12	2.16	0.56
2:E:773:LEU:HD13	2:E:803:VAL:CG2	2.35	0.56
3:F:1605:TRP:CD1	3:F:1606:VAL:N	2.74	0.56
1:A:345:GLY:N	1:A:391:THR:HG23	2.20	0.56
3:C:1578:LYS:CE	3:C:1578:LYS:HA	2.29	0.56
1:D:586:LYS:O	1:D:587:ASN:HB2	2.05	0.56
2:E:732:ASP:OD1	2:E:896:HIS:HA	2.06	0.56
2:E:858:ARG:CZ	3:F:1449:LEU:CD1	2.84	0.56
2:E:851:CYS:HB3	2:E:879:VAL:HB	1.87	0.56
3:F:1509:GLU:HB2	3:F:1512:ASP:HB3	1.87	0.56
3:F:1533:SER:O	3:F:1534:ASN:C	2.45	0.56
3:F:1543:ILE:HD13	3:F:1559:GLN:CA	2.36	0.56
1:D:364:ARG:HG2	1:D:378:LEU:HD23	1.87	0.55
2:E:788:SER:O	2:E:792:GLY:N	2.35	0.55
3:C:1409:LYS:HG2	3:C:1413:ASP:OD2	2.06	0.55
3:C:1623:GLN:C	3:C:1625:GLN:H	2.08	0.55
1:D:345:GLY:N	1:D:391:THR:HG23	2.20	0.55
1:D:430:SER:O	1:D:431:ASN:HB2	2.06	0.55
2:E:883:THR:HA	2:E:909:VAL:HG12	1.88	0.55
3:F:1534:ASN:O	3:F:1534:ASN:ND2	2.31	0.55
4:P:26:LEU:C	4:P:26:LEU:HD12	2.26	0.55
1:A:536:SER:O	1:A:537:CYS:O	2.24	0.55
2:B:734:ILE:N	2:B:734:ILE:HD12	2.16	0.55
2:B:819:ARG:HH21	2:B:911:PRO:CB	2.19	0.55
2:B:883:THR:HA	2:B:909:VAL:HG12	1.88	0.55
3:C:1444:TYR:CD1	3:C:1445:PHE:HB2	2.42	0.55
1:D:406:LYS:H	1:D:414:GLN:HE22	1.53	0.55
3:F:1607:GLU:O	3:F:1608:HIS:CB	2.54	0.55
1:A:142:MET:HG3	1:A:187:TYR:HE1	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:852:SER:C	2:B:854:ALA:H	2.10	0.55
1:D:23:GLU:HG2	1:D:61:MET:HG2	1.87	0.55
2:E:852:SER:C	2:E:854:ALA:H	2.10	0.55
3:F:1444:TYR:CD1	3:F:1445:PHE:HB2	2.42	0.55
1:A:440:ARG:NH2	1:A:529:VAL:HG23	2.22	0.55
2:B:741:SER:HB3	2:B:902:GLY:C	2.26	0.55
3:C:1389:PHE:CD2	3:C:1389:PHE:N	2.75	0.55
2:E:760:PRO:HG3	1:D:567:HIS:CG	2.41	0.55
2:E:741:SER:HB3	2:E:902:GLY:O	2.06	0.55
3:F:1389:PHE:N	3:F:1389:PHE:CD2	2.75	0.55
3:F:1536:PHE:CE2	3:F:1566:ILE:CG1	2.90	0.55
3:F:1565:PRO:HD2	3:F:1568:CYS:HB3	1.89	0.55
3:C:1565:PRO:C	3:C:1567:LYS:N	2.59	0.55
3:C:1565:PRO:O	3:C:1567:LYS:N	2.39	0.55
3:C:1608:HIS:CD2	3:C:1609:TRP:C	2.80	0.55
1:A:406:LYS:H	1:A:414:GLN:HE22	1.53	0.55
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.32	0.55
1:D:440:ARG:NH2	1:D:529:VAL:HG23	2.22	0.55
3:F:1533:SER:HG	3:F:1538:GLU:HG3	1.65	0.55
2:E:782:ILE:HG12	1:D:575:ALA:HB2	1.88	0.55
3:F:1483:LEU:CG	3:F:1590:TRP:CH2	2.81	0.55
1:A:99:VAL:HG12	1:A:100:LEU:H	1.70	0.55
3:C:1537:ASP:OD2	3:C:1569:ARG:HB2	2.07	0.55
1:D:179:MET:HG3	1:D:202:VAL:O	2.06	0.55
1:D:210:PHE:CE2	1:D:310:LEU:HD21	2.41	0.55
2:B:741:SER:HB3	2:B:902:GLY:O	2.06	0.55
1:D:73:GLU:HB3	1:D:82:LYS:HZ3	1.72	0.55
1:A:610:GLY:N	1:A:616:VAL:HG23	2.22	0.54
1:D:610:GLY:N	1:D:616:VAL:HG23	2.22	0.54
3:F:1409:LYS:O	3:F:1412:LEU:N	2.40	0.54
3:F:1408:SER:OG	3:F:1410:TYR:CB	2.55	0.54
3:F:1574:LEU:CA	3:F:1580:TYR:OH	2.55	0.54
1:A:575:ALA:HB2	2:B:782:ILE:HG12	1.89	0.54
3:F:1411:GLU:O	3:F:1414:LYS:HG3	2.06	0.54
3:F:1533:SER:OG	3:F:1538:GLU:N	2.36	0.54
3:F:1416:PHE:HE2	3:F:1444:TYR:CD2	2.21	0.54
2:B:732:ASP:OD1	2:B:896:HIS:HA	2.06	0.54
1:D:446:GLY:N	1:D:499:ILE:O	2.32	0.54
3:F:1377:THR:O	3:F:1378:MET:C	2.46	0.54
3:F:1562:PHE:HD2	3:F:1600:ILE:HD12	1.71	0.54
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HB3	1:A:60:HIS:HA	1.89	0.54
1:D:38:HIS:HE1	1:D:45:LEU:HD12	1.73	0.54
1:D:54:LEU:HB3	1:D:60:HIS:HA	1.90	0.54
3:F:1564:SER:HB2	3:F:1600:ILE:HB	1.89	0.54
1:A:147:ASN:HB2	1:A:148:PRO:HD3	1.90	0.54
3:F:1542:ALA:O	3:F:1543:ILE:CG1	2.56	0.54
3:F:1543:ILE:N	3:F:1543:ILE:HD12	2.21	0.54
3:F:1567:LYS:O	3:F:1567:LYS:HG2	2.08	0.54
1:D:10:ASN:HB3	1:D:635:ARG:NH1	2.15	0.54
1:D:363:TYR:CZ	1:D:364:ARG:HG3	2.43	0.54
3:F:1360:ASN:HD22	3:F:1443:GLN:CB	2.11	0.54
1:A:287:ASP:N	1:A:291:ASN:HD21	2.05	0.54
1:A:34:THR:CG2	1:A:51:LYS:HE2	2.38	0.54
3:C:1532:LEU:HD13	3:C:1532:LEU:N	2.21	0.54
1:D:536:SER:O	1:D:537:CYS:O	2.24	0.54
3:F:1532:LEU:HG	3:F:1569:ARG:HH22	1.73	0.54
4:M:14:LYS:HZ2	3:F:1415:ALA:CB	2.19	0.54
1:A:363:TYR:CZ	1:A:364:ARG:HG3	2.43	0.54
3:C:1608:HIS:CD2	3:C:1610:PRO:HG3	2.43	0.54
1:D:147:ASN:HB2	1:D:148:PRO:HD3	1.90	0.54
1:D:287:ASP:N	1:D:291:ASN:HD21	2.05	0.54
3:C:1605:TRP:NE1	3:C:1607:GLU:HB2	2.22	0.54
1:D:634:GLN:NE2	1:D:635:ARG:O	2.34	0.54
1:A:524:VAL:HB	1:A:613:TYR:CD1	2.43	0.53
3:F:1505:VAL:HG21	3:F:1623:GLN:HG3	1.90	0.53
3:F:1572:LEU:O	3:F:1573:LYS:HD3	2.05	0.53
3:F:1631:THR:C	3:F:1633:SER:H	2.10	0.53
1:A:536:SER:O	1:A:537:CYS:C	2.46	0.53
3:C:1377:THR:O	3:C:1378:MET:C	2.46	0.53
3:C:1506:THR:N	3:C:1509:GLU:HG2	2.20	0.53
3:C:1522:VAL:HG23	3:C:1548:LYS:HD2	1.90	0.53
1:D:282:ARG:O	1:D:286:LEU:HD12	2.09	0.53
1:D:34:THR:CG2	1:D:51:LYS:HE2	2.38	0.53
3:F:1523:TYR:HE2	3:F:1598:TYR:HH	1.57	0.53
3:F:1532:LEU:CD1	3:F:1532:LEU:N	2.71	0.53
3:C:1397:LYS:O	3:C:1398:GLN:C	2.46	0.53
1:A:124:LEU:N	1:A:124:LEU:HD23	2.24	0.53
3:F:1409:LYS:C	3:F:1411:GLU:N	2.60	0.53
3:F:1503:ASP:O	3:F:1505:VAL:N	2.42	0.53
3:F:1530:VAL:O	3:F:1530:VAL:CG2	2.57	0.53
3:F:1533:SER:O	3:F:1535:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLN:HB2	2:B:795:VAL:HB	1.91	0.53
2:E:793:ILE:HG13	2:E:794:CYS:N	2.23	0.53
3:F:1404:ASP:HA	3:F:1427:ASP:HB2	1.88	0.53
3:F:1518:GLY:O	3:F:1519:VAL:O	2.26	0.53
3:F:1545:GLN:CG	3:F:1546:THR:N	2.71	0.53
3:C:1381:LEU:HD12	3:C:1426:LEU:HD11	1.91	0.53
3:C:1565:PRO:C	3:C:1567:LYS:H	2.11	0.53
3:C:1562:PHE:CE2	3:C:1582:MET:HE2	2.43	0.53
1:D:524:VAL:HB	1:D:613:TYR:CD1	2.43	0.53
3:F:1397:LYS:O	3:F:1398:GLN:C	2.46	0.53
2:B:808:PHE:CE1	2:B:830:TYR:HB2	2.44	0.53
3:C:1483:LEU:HD13	3:C:1536:PHE:CE2	2.44	0.53
1:D:534:LYS:HG3	1:D:534:LYS:O	2.05	0.53
2:E:763:GLY:O	2:E:764:ILE:HD13	2.09	0.53
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.91	0.53
3:C:1608:HIS:CD2	3:C:1610:PRO:N	2.76	0.53
1:D:536:SER:O	1:D:537:CYS:C	2.46	0.53
2:B:907:LEU:HD23	2:B:907:LEU:H	1.73	0.53
2:E:777:ILE:HD13	2:E:808:PHE:CD2	2.44	0.53
2:E:858:ARG:CZ	3:F:1449:LEU:HD11	2.39	0.53
3:F:1346:LYS:O	3:F:1362:MET:HB2	2.09	0.53
3:F:1527:LEU:HD11	3:F:1530:VAL:HG13	1.91	0.53
1:A:285:LEU:O	1:A:289:VAL:HG22	2.09	0.53
1:A:369:VAL:CG1	1:A:370:GLN:N	2.72	0.53
1:A:39:ASP:OD1	1:A:44:LYS:HB2	2.09	0.53
3:C:1568:CYS:C	3:C:1570:GLU:H	2.11	0.53
3:F:1378:MET:CG	1:D:268:ARG:NH1	2.72	0.53
1:D:285:LEU:O	1:D:289:VAL:HG22	2.09	0.53
1:D:535:ASP:N	1:D:535:ASP:OD1	2.42	0.53
2:B:740:VAL:HB	4:M:42:ARG:HA	1.92	0.52
2:B:783:LEU:HD12	2:B:784:ALA:N	2.24	0.52
3:C:1534:ASN:O	3:C:1566:ILE:HD12	2.09	0.52
2:E:907:LEU:O	2:E:907:LEU:HD23	2.10	0.52
1:D:117:TYR:CD1	1:D:123:VAL:HG22	2.44	0.52
1:D:39:ASP:OD1	1:D:44:LYS:HB2	2.09	0.52
3:F:1532:LEU:HA	3:F:1569:ARG:HH22	1.73	0.52
3:F:1542:ALA:C	3:F:1543:ILE:CD1	2.71	0.52
3:F:1548:LYS:HD2	3:F:1634:MET:HE2	1.92	0.52
1:A:343:LYS:HD2	1:A:343:LYS:N	2.25	0.52
3:C:1408:SER:O	3:C:1409:LYS:C	2.45	0.52
1:D:468:TYR:CE1	1:D:513:TYR:HD2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:907:LEU:HD23	2:E:907:LEU:H	1.73	0.52
3:F:1381:LEU:HD12	3:F:1426:LEU:HD11	1.91	0.52
3:F:1536:PHE:HA	3:F:1566:ILE:HG12	1.91	0.52
1:A:193:GLN:HG2	1:A:194:GLN:N	2.24	0.52
3:C:1346:LYS:O	3:C:1362:MET:HB2	2.09	0.52
1:D:581:PHE:CE1	1:D:588:LYS:HD2	2.45	0.52
2:E:808:PHE:CE1	2:E:830:TYR:HB2	2.44	0.52
3:F:1495:ASN:O	3:F:1496:CYS:CB	2.58	0.52
1:D:343:LYS:HD2	1:D:343:LYS:N	2.25	0.52
1:D:468:TYR:HE1	1:D:513:TYR:HD2	1.57	0.52
1:D:19:THR:HG23	1:D:64:VAL:O	2.10	0.52
3:F:1585:LEU:O	3:F:1586:SER:C	2.47	0.52
1:D:124:LEU:N	1:D:124:LEU:HD23	2.24	0.52
1:A:282:ARG:O	1:A:286:LEU:HD12	2.09	0.52
1:A:468:TYR:CE1	1:A:513:TYR:HD2	2.28	0.52
1:A:581:PHE:CE1	1:A:588:LYS:HD2	2.45	0.52
1:A:19:THR:HG23	1:A:64:VAL:O	2.10	0.52
1:D:590:THR:HG21	1:D:592:SER:HB2	1.92	0.52
2:E:896:HIS:CB	4:M:61:LYS:HD3	2.40	0.52
3:F:1451:GLN:HG3	3:F:1452:PRO:HD2	1.92	0.52
3:F:1581:LEU:HD12	3:F:1582:MET:H	1.73	0.52
1:A:117:TYR:CD1	1:A:123:VAL:HG22	2.44	0.52
1:A:468:TYR:HE1	1:A:513:TYR:CD2	2.28	0.52
1:A:541:LEU:CD2	2:B:786:SER:HB3	2.39	0.52
2:B:788:SER:O	2:B:792:GLY:N	2.35	0.52
1:D:363:TYR:CE1	1:D:364:ARG:HG3	2.44	0.52
2:E:783:LEU:HD12	2:E:784:ALA:N	2.24	0.52
3:F:1497:PHE:CE2	3:F:1498:ILE:HB	2.45	0.52
3:F:1578:LYS:O	3:F:1580:TYR:CE2	2.63	0.52
3:F:1563:ILE:HD11	3:F:1597:SER:OG	2.09	0.52
1:A:403:ARG:HG2	1:A:404:THR:O	2.10	0.52
1:A:535:ASP:N	1:A:535:ASP:OD1	2.42	0.52
2:B:907:LEU:O	2:B:907:LEU:HD23	2.10	0.52
1:D:230:GLU:HA	1:D:279:VAL:HG22	1.92	0.52
1:D:369:VAL:CG1	1:D:370:GLN:N	2.72	0.52
3:F:1519:VAL:N	3:F:1585:LEU:CD2	2.72	0.52
4:M:36:LEU:HB3	4:M:40:TYR:HD2	1.73	0.52
1:A:363:TYR:CE1	1:A:364:ARG:HG3	2.44	0.52
2:B:777:ILE:HD13	2:B:808:PHE:CD2	2.44	0.52
2:B:793:ILE:HG13	2:B:794:CYS:N	2.23	0.52
1:D:193:GLN:HG2	1:D:194:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:PRO:HG3	1:D:595:TRP:CE3	2.45	0.52
1:A:365:VAL:CG1	1:A:379:THR:OG1	2.56	0.51
2:E:773:LEU:HD13	2:E:803:VAL:HG22	1.92	0.51
1:D:595:TRP:HA	1:D:595:TRP:CE3	2.45	0.51
3:F:1405:ARG:CZ	3:F:1437:LEU:HD23	2.41	0.51
1:A:143:VAL:O	1:A:155:GLN:HA	2.10	0.51
1:A:472:ILE:HG13	1:A:480:LYS:HB3	1.92	0.51
2:B:763:GLY:O	2:B:764:ILE:HD13	2.09	0.51
3:C:1409:LYS:O	3:C:1411:GLU:N	2.43	0.51
3:C:1529:LYS:HE3	3:C:1531:GLN:HE21	1.76	0.51
3:C:1529:LYS:CE	3:C:1531:GLN:HE21	2.22	0.51
1:D:257:GLU:H	1:D:257:GLU:CD	2.14	0.51
2:E:734:ILE:H	2:E:734:ILE:CD1	2.16	0.51
2:B:773:LEU:HD13	2:B:803:VAL:HG22	1.92	0.51
3:C:1409:LYS:O	3:C:1412:LEU:N	2.42	0.51
1:D:365:VAL:CG1	1:D:379:THR:OG1	2.56	0.51
1:D:472:ILE:HG13	1:D:480:LYS:HB3	1.92	0.51
1:D:628:SER:HB2	1:D:630:GLN:OE1	2.11	0.51
3:F:1537:ASP:OD1	3:F:1538:GLU:N	2.43	0.51
3:F:1586:SER:O	3:F:1588:ASP:N	2.44	0.51
1:A:230:GLU:HA	1:A:279:VAL:HG22	1.92	0.51
3:C:1518:GLY:O	3:C:1519:VAL:C	2.48	0.51
3:C:1547:ILE:HG22	3:C:1547:ILE:O	2.11	0.51
3:C:1578:LYS:CB	3:C:1580:TYR:OH	2.58	0.51
1:D:143:VAL:O	1:D:155:GLN:HA	2.10	0.51
1:D:477:ARG:HH11	1:D:477:ARG:HG2	1.72	0.51
1:D:86:VAL:HG12	1:D:86:VAL:O	2.10	0.51
3:F:1378:MET:CE	1:D:248:PHE:HD1	2.23	0.51
3:F:1408:SER:C	3:F:1410:TYR:N	2.63	0.51
1:A:595:TRP:CE3	1:A:595:TRP:HA	2.45	0.51
1:A:97:LYS:HZ3	1:A:631:GLN:HB2	1.76	0.51
2:B:819:ARG:HG2	2:B:820:ASN:CG	2.31	0.51
1:D:351:MET:HE2	1:D:386:LYS:HA	1.91	0.51
1:D:495:LEU:HD12	1:D:496:PRO:CD	2.40	0.51
2:E:852:SER:HB3	2:E:878:ILE:HG22	1.91	0.51
2:E:896:HIS:HB3	4:M:61:LYS:HD3	1.93	0.51
3:F:1571:ALA:H	3:F:1572:LEU:CD2	2.24	0.51
1:A:468:TYR:HE1	1:A:513:TYR:HD2	1.57	0.51
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.45	0.51
2:B:819:ARG:NH1	3:C:1487:GLU:O	2.43	0.51
2:B:853:LEU:HD11	3:C:1451:GLN:CB	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1451:GLN:HG3	3:C:1452:PRO:HD2	1.92	0.51
1:D:367:VAL:HG23	1:D:387:LEU:HD11	1.92	0.51
2:E:740:VAL:HB	4:P:42:ARG:HA	1.93	0.51
3:F:1484:CYS:CB	3:F:1489:CYS:HB2	2.37	0.51
3:F:1507:LEU:N	3:F:1507:LEU:CD2	2.74	0.51
1:A:367:VAL:HG23	1:A:387:LEU:HD11	1.92	0.51
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.11	0.51
1:D:4:TYR:HB3	1:D:90:PHE:CE2	2.46	0.51
3:F:1560:ARG:HD3	3:F:1598:TYR:CE1	2.46	0.51
3:F:1572:LEU:CA	3:F:1574:LEU:HD21	2.41	0.51
3:F:1589:PHE:O	3:F:1590:TRP:CB	2.49	0.51
1:A:136:PRO:CD	2:B:789:ASP:HA	2.41	0.51
1:A:462:GLU:HG3	1:A:486:ARG:HH22	1.76	0.51
2:B:806:ASP:HB3	2:B:833:ARG:HH11	1.76	0.51
3:C:1444:TYR:CE1	3:C:1445:PHE:HB2	2.46	0.51
1:D:63:ASN:HD21	5:D:646:NAG:C1	2.24	0.51
3:F:1532:LEU:O	3:F:1534:ASN:N	2.43	0.51
3:F:1561:THR:O	3:F:1598:TYR:HB2	2.11	0.51
1:A:38:HIS:HE1	1:A:45:LEU:HD12	1.73	0.50
1:A:590:THR:HG21	1:A:592:SER:HB2	1.92	0.50
1:D:37:VAL:HB	1:D:46:VAL:HG23	1.93	0.50
1:A:459:ARG:HH22	1:D:458:ASP:HA	1.76	0.50
1:D:590:THR:HB	1:D:593:LYS:CG	2.39	0.50
4:P:18:GLU:O	4:P:21:SER:HB2	2.11	0.50
1:A:257:GLU:H	1:A:257:GLU:CD	2.14	0.50
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.92	0.50
3:C:1483:LEU:HD13	3:C:1536:PHE:CD2	2.46	0.50
1:D:462:GLU:HG3	1:D:486:ARG:HH22	1.76	0.50
1:D:468:TYR:HE1	1:D:513:TYR:CD2	2.28	0.50
1:A:248:PHE:HD1	3:C:1378:MET:CE	2.23	0.50
3:C:1405:ARG:CZ	3:C:1437:LEU:HD23	2.40	0.50
3:C:1546:THR:C	3:C:1548:LYS:H	2.15	0.50
1:D:472:ILE:HA	1:D:508:ARG:O	2.11	0.50
3:F:1510:ARG:NH1	3:F:1607:GLU:OE1	2.44	0.50
3:F:1520:ASP:CG	3:F:1551:SER:HB2	2.32	0.50
4:M:18:GLU:O	4:M:21:SER:HB2	2.12	0.50
1:A:184:ILE:HG13	1:A:200:PHE:HE2	1.77	0.50
1:A:440:ARG:HH22	1:A:529:VAL:HG23	1.77	0.50
1:A:63:ASN:HD21	5:A:646:NAG:C1	2.24	0.50
1:D:351:MET:HE1	1:D:386:LYS:HD3	1.92	0.50
3:F:1378:MET:HE3	1:D:248:PHE:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1568:CYS:O	3:F:1569:ARG:O	2.29	0.50
1:A:286:LEU:HB3	1:A:291:ASN:HD22	1.76	0.50
1:A:293:ARG:O	1:A:294:ALA:C	2.50	0.50
1:A:402:VAL:HG12	1:A:403:ARG:N	2.27	0.50
3:C:1508:GLU:O	3:C:1512:ASP:OD2	2.29	0.50
3:C:1581:LEU:CD1	3:C:1581:LEU:O	2.60	0.50
1:D:351:MET:SD	1:D:440:ARG:HD3	2.52	0.50
3:F:1532:LEU:HA	3:F:1569:ARG:NH2	2.27	0.50
3:F:1537:ASP:CB	3:F:1569:ARG:HD2	2.42	0.50
3:F:1536:PHE:CE2	3:F:1566:ILE:HG13	2.47	0.50
1:D:438:VAL:HG13	1:D:449:LEU:HD11	1.92	0.50
2:E:808:PHE:CD1	2:E:808:PHE:C	2.85	0.50
3:F:1416:PHE:CE2	3:F:1444:TYR:HD2	2.25	0.50
3:F:1535:ASP:C	3:F:1566:ILE:HG23	2.30	0.50
1:A:351:MET:SD	1:A:440:ARG:HD3	2.52	0.50
2:B:896:HIS:CB	4:P:61:LYS:HD3	2.41	0.50
1:A:25:HIS:O	1:A:26:ASP:HB2	2.12	0.50
2:B:808:PHE:CD1	2:B:808:PHE:C	2.85	0.50
4:M:14:LYS:HZ3	3:F:1415:ALA:HB1	1.74	0.50
4:M:4:LEU:HD13	3:F:1445:PHE:N	2.26	0.50
1:D:271:ILE:HD13	1:D:276:GLY:HA3	1.94	0.50
1:D:402:VAL:HG12	1:D:403:ARG:N	2.27	0.50
1:D:603:ILE:HD12	1:D:621:GLY:HA3	1.94	0.50
3:F:1444:TYR:CE1	3:F:1445:PHE:HB2	2.46	0.50
1:A:37:VAL:HB	1:A:46:VAL:HG23	1.93	0.49
1:A:4:TYR:HB3	1:A:90:PHE:CE2	2.46	0.49
3:C:1579:HIS:O	3:C:1580:TYR:O	2.30	0.49
3:C:1605:TRP:HE1	3:C:1607:GLU:CB	2.25	0.49
1:D:25:HIS:O	1:D:26:ASP:HB2	2.12	0.49
1:D:406:LYS:N	1:D:414:GLN:HE22	2.10	0.49
3:F:1493:GLU:O	3:F:1494:GLU:O	2.30	0.49
3:F:1532:LEU:HA	3:F:1569:ARG:CZ	2.42	0.49
1:A:351:MET:HE2	1:A:386:LYS:HA	1.94	0.49
1:D:184:ILE:HG13	1:D:200:PHE:HE2	1.77	0.49
1:D:403:ARG:HG2	1:D:404:THR:O	2.10	0.49
1:A:459:ARG:NH2	1:D:458:ASP:HA	2.27	0.49
2:E:787:MET:HG2	1:D:164:LEU:O	2.12	0.49
3:F:1520:ASP:O	3:F:1521:TYR:CB	2.45	0.49
4:P:30:GLU:OE2	4:P:45:LYS:HE3	2.13	0.49
1:A:472:ILE:HA	1:A:508:ARG:O	2.11	0.49
2:B:844:LEU:HD12	2:B:844:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1482:LYS:O	3:C:1536:PHE:CE2	2.65	0.49
1:D:439:LEU:HD12	1:D:439:LEU:O	2.13	0.49
1:D:440:ARG:HH22	1:D:529:VAL:HG23	1.77	0.49
3:F:1527:LEU:HA	3:F:1541:MET:HG3	1.94	0.49
3:F:1563:ILE:HD12	3:F:1598:TYR:O	2.12	0.49
3:F:1635:VAL:HG12	3:F:1636:VAL:HG23	1.95	0.49
1:A:271:ILE:HD13	1:A:276:GLY:HA3	1.94	0.49
1:A:286:LEU:C	1:A:291:ASN:ND2	2.65	0.49
1:A:291:ASN:N	1:A:292:PRO:CD	2.76	0.49
2:B:883:THR:HA	2:B:909:VAL:CG1	2.42	0.49
1:D:179:MET:CG	1:D:203:LYS:HA	2.42	0.49
1:D:286:LEU:C	1:D:291:ASN:ND2	2.65	0.49
1:D:445:PRO:HA	1:D:499:ILE:HG22	1.95	0.49
2:E:836:GLN:HG3	2:E:836:GLN:O	2.12	0.49
3:F:1393:THR:HG22	3:F:1419:ARG:HH22	1.78	0.49
3:F:1519:VAL:CG1	3:F:1520:ASP:N	2.76	0.49
1:A:403:ARG:NH1	1:A:416:THR:HG21	2.28	0.49
2:B:836:GLN:O	2:B:836:GLN:HG3	2.12	0.49
2:E:795:VAL:HB	1:D:591:GLN:HB2	1.94	0.49
2:E:806:ASP:HB3	2:E:833:ARG:HH11	1.76	0.49
2:E:844:LEU:C	2:E:844:LEU:HD12	2.33	0.49
2:E:883:THR:HA	2:E:909:VAL:CG1	2.42	0.49
3:F:1573:LYS:O	3:F:1574:LEU:O	2.29	0.49
3:F:1582:MET:HG2	3:F:1606:VAL:HG22	1.95	0.49
4:P:8:ASN:ND2	4:P:12:ASN:OD1	2.46	0.49
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.95	0.49
3:C:1504:LYS:HG2	3:C:1506:THR:CG2	2.42	0.49
3:F:1524:LYS:HD3	3:F:1609:TRP:CD1	2.48	0.49
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.95	0.49
3:C:1516:GLU:CB	3:C:1517:PRO:CD	2.76	0.49
1:D:403:ARG:NH1	1:D:416:THR:HG21	2.28	0.49
1:D:473:MET:HB2	1:D:508:ARG:HB2	1.95	0.49
1:D:63:ASN:OD1	5:D:646:NAG:N2	2.46	0.49
3:F:1510:ARG:O	3:F:1511:LEU:HB3	2.12	0.49
1:D:434:LEU:HD12	1:D:435:HIS:N	2.28	0.49
1:D:613:TYR:CE2	1:D:614:ALA:HB2	2.48	0.49
1:D:100:LEU:HD21	1:D:638:LEU:HD23	1.95	0.49
3:F:1381:LEU:CD1	3:F:1426:LEU:HD11	2.43	0.49
3:F:1507:LEU:HD21	3:F:1622:LYS:CE	2.43	0.49
4:M:8:ASN:ND2	4:M:12:ASN:OD1	2.46	0.49
3:C:1611:GLU:HG2	3:C:1613:ASP:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:CD	1:D:185:ARG:HD2	2.33	0.49
1:D:403:ARG:HB2	1:D:416:THR:HG22	1.95	0.49
1:D:509:LEU:HB3	1:D:529:VAL:HG13	1.94	0.49
2:E:822:GLN:HG2	3:F:1470:PHE:CZ	2.48	0.49
4:M:30:GLU:OE2	4:M:45:LYS:HE3	2.12	0.49
1:A:183:LYS:HD2	1:A:185:ARG:HD2	1.94	0.49
1:A:146:GLU:CD	1:A:185:ARG:HD2	2.33	0.49
1:A:63:ASN:OD1	5:A:646:NAG:N2	2.46	0.49
3:C:1393:THR:HG22	3:C:1419:ARG:HH22	1.78	0.49
3:F:1484:CYS:CB	3:F:1489:CYS:SG	3.01	0.49
3:F:1522:VAL:C	3:F:1547:ILE:HD12	2.32	0.49
2:B:896:HIS:HB3	4:P:61:LYS:HD3	1.95	0.48
3:C:1450:ILE:CG1	3:C:1450:ILE:O	2.55	0.48
2:E:836:GLN:C	2:E:868:PRO:HG3	2.34	0.48
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.49	0.48
1:A:406:LYS:N	1:A:414:GLN:HE22	2.10	0.48
1:A:434:LEU:HD12	1:A:435:HIS:N	2.28	0.48
1:D:183:LYS:HD2	1:D:185:ARG:HD2	1.94	0.48
3:F:1408:SER:O	3:F:1411:GLU:N	2.40	0.48
3:F:1536:PHE:CA	3:F:1566:ILE:HG12	2.42	0.48
3:F:1585:LEU:HD23	3:F:1585:LEU:HA	1.60	0.48
4:M:26:LEU:HD12	4:M:26:LEU:O	2.13	0.48
1:A:445:PRO:HA	1:A:499:ILE:HG22	1.95	0.48
2:B:836:GLN:C	2:B:868:PRO:HG3	2.34	0.48
3:F:1514:ALA:HB2	3:F:1583:TRP:CE2	2.48	0.48
1:D:291:ASN:N	1:D:292:PRO:CD	2.76	0.48
1:D:293:ARG:O	1:D:294:ALA:C	2.50	0.48
3:F:1360:ASN:OD1	3:F:1361:THR:N	2.47	0.48
3:F:1583:TRP:CH2	3:F:1605:TRP:CD2	3.01	0.48
1:A:437:SER:O	1:A:452:ASN:HB2	2.13	0.48
1:A:613:TYR:CE2	1:A:614:ALA:HB2	2.48	0.48
3:C:1530:VAL:HG12	3:C:1532:LEU:HD11	1.95	0.48
1:A:458:ASP:HA	1:D:459:ARG:NH2	2.28	0.48
3:F:1380:ILE:HG21	3:F:1458:TYR:CZ	2.48	0.48
3:F:1602:LYS:O	3:F:1602:LYS:HG2	2.13	0.48
1:A:351:MET:HE1	1:A:386:LYS:HD3	1.94	0.48
1:A:403:ARG:HB2	1:A:416:THR:HG22	1.95	0.48
1:A:477:ARG:HH22	1:A:479:LEU:HD13	1.78	0.48
3:C:1360:ASN:OD1	3:C:1361:THR:N	2.47	0.48
3:C:1568:CYS:C	3:C:1570:GLU:N	2.67	0.48
3:C:1609:TRP:HZ3	3:C:1627:LEU:HD22	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LEU:HB3	1:D:291:ASN:HD22	1.76	0.48
1:D:109:PHE:CZ	1:D:594:ILE:HG23	2.49	0.48
1:A:183:LYS:HD3	1:A:185:ARG:CD	2.44	0.48
1:A:509:LEU:HB3	1:A:529:VAL:HG13	1.94	0.48
3:C:1380:ILE:HG21	3:C:1458:TYR:CZ	2.49	0.48
3:C:1610:PRO:O	3:C:1611:GLU:C	2.51	0.48
1:D:183:LYS:HD3	1:D:185:ARG:CD	2.44	0.48
1:A:369:VAL:CG1	1:A:370:GLN:H	2.24	0.48
1:A:495:LEU:HD12	1:A:496:PRO:CD	2.40	0.48
1:A:603:ILE:HD12	1:A:621:GLY:HA3	1.94	0.48
3:C:1521:TYR:C	3:C:1521:TYR:CD1	2.86	0.48
3:F:1570:GLU:N	3:F:1570:GLU:CD	2.62	0.48
3:F:1604:THR:HG23	3:F:1604:THR:O	2.13	0.48
1:A:179:MET:CG	1:A:203:LYS:HA	2.42	0.48
1:A:606:THR:HG22	1:A:608:GLY:H	1.78	0.48
3:C:1581:LEU:CD2	3:C:1627:LEU:CD2	2.92	0.48
3:C:1630:PHE:O	3:C:1633:SER:HB3	2.13	0.48
2:E:789:ASP:HA	1:D:136:PRO:CD	2.43	0.48
1:D:477:ARG:HH22	1:D:479:LEU:HD13	1.78	0.48
1:D:549:GLU:O	1:D:550:ASP:HB2	2.14	0.48
1:D:20:MET:H	1:D:64:VAL:HB	1.79	0.48
1:A:439:LEU:HD12	1:A:439:LEU:O	2.12	0.48
3:C:1522:VAL:C	3:C:1523:TYR:CD1	2.87	0.48
3:C:1530:VAL:CG1	3:C:1532:LEU:HD11	2.44	0.48
3:C:1626:ASP:C	3:C:1628:GLY:N	2.66	0.48
2:E:822:GLN:NE2	3:F:1470:PHE:CD2	2.79	0.48
3:F:1531:GLN:O	3:F:1531:GLN:HG3	2.14	0.48
4:M:59:ASP:OD1	4:M:59:ASP:C	2.52	0.48
4:P:26:LEU:O	4:P:26:LEU:HD12	2.13	0.48
4:P:64:SER:O	4:P:67:LYS:N	2.47	0.48
1:A:634:GLN:NE2	1:A:635:ARG:O	2.34	0.47
3:C:1381:LEU:CD1	3:C:1426:LEU:HD11	2.43	0.47
3:C:1622:LYS:HD2	3:C:1622:LYS:O	2.14	0.47
1:D:203:LYS:HG2	1:D:204:GLU:N	2.29	0.47
1:D:606:THR:HG22	1:D:608:GLY:H	1.78	0.47
2:E:839:LYS:HG2	2:E:895:TYR:HD1	1.79	0.47
2:E:809:ILE:HD12	2:E:903:VAL:HG23	1.96	0.47
4:P:59:ASP:C	4:P:59:ASP:OD1	2.52	0.47
1:A:458:ASP:HA	1:D:459:ARG:HH22	1.78	0.47
1:A:510:VAL:CG1	1:A:528:SER:HB3	2.33	0.47
1:A:475:LYS:HG2	1:A:598:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:PRO:O	1:D:293:ARG:C	2.53	0.47
3:F:1341:LEU:HD23	3:F:1469:ARG:N	2.29	0.47
3:F:1577:LYS:O	3:F:1579:HIS:CD2	2.64	0.47
3:F:1574:LEU:CB	3:F:1580:TYR:OH	2.62	0.47
1:A:403:ARG:CB	1:A:416:THR:HG22	2.44	0.47
1:A:7:ILE:HA	1:A:623:THR:O	2.14	0.47
2:B:839:LYS:HG2	2:B:895:TYR:HD1	1.79	0.47
2:B:809:ILE:HD12	2:B:903:VAL:HG23	1.96	0.47
1:D:287:ASP:N	1:D:291:ASN:ND2	2.63	0.47
1:D:97:LYS:HG3	1:D:98:VAL:N	2.30	0.47
3:F:1575:GLU:HG3	3:F:1576:GLU:N	2.29	0.47
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.50	0.47
1:A:97:LYS:NZ	1:A:631:GLN:HB2	2.29	0.47
2:B:754:GLU:HG3	2:B:769:MET:SD	2.54	0.47
3:C:1507:LEU:O	3:C:1511:LEU:HG	2.14	0.47
3:F:1409:LYS:O	3:F:1413:ASP:OD2	2.33	0.47
3:F:1376:ALA:HB3	3:F:1429:VAL:HG22	1.97	0.47
4:M:64:SER:O	4:M:67:LYS:N	2.47	0.47
1:A:214:VAL:HG11	1:A:304:VAL:CG2	2.45	0.47
1:A:368:ALA:O	1:A:402:VAL:HG13	2.15	0.47
1:A:459:ARG:NH2	1:D:459:ARG:H	2.12	0.47
1:A:510:VAL:HG21	1:A:622:LEU:HD12	1.96	0.47
2:B:735:ALA:HB1	2:B:737:GLU:OE2	2.15	0.47
3:C:1543:ILE:C	3:C:1545:GLN:H	2.17	0.47
3:C:1609:TRP:CZ3	3:C:1627:LEU:HB3	2.50	0.47
1:D:403:ARG:CB	1:D:416:THR:HG22	2.44	0.47
1:D:437:SER:O	1:D:452:ASN:HB2	2.13	0.47
3:F:1392:ASP:HB2	3:F:1442:HIS:NE2	2.30	0.47
3:F:1403:VAL:C	3:F:1405:ARG:H	2.18	0.47
3:F:1555:GLN:O	3:F:1556:VAL:O	2.33	0.47
1:A:251:PHE:CE1	1:A:304:VAL:CG1	2.98	0.47
1:A:404:THR:C	1:A:414:GLN:OE1	2.53	0.47
3:C:1341:LEU:HD23	3:C:1469:ARG:N	2.29	0.47
3:C:1608:HIS:CD2	3:C:1610:PRO:CG	2.97	0.47
1:D:222:TYR:CE2	1:D:224:TYR:HB2	2.50	0.47
1:D:59:ASN:HB3	1:D:483:ARG:HH12	1.80	0.47
1:D:59:ASN:HB3	1:D:483:ARG:NH1	2.29	0.47
1:D:97:LYS:HZ3	1:D:631:GLN:HB2	1.79	0.47
1:A:135:LEU:HD22	2:B:789:ASP:O	2.14	0.47
1:A:549:GLU:O	1:A:550:ASP:HB2	2.14	0.47
3:C:1520:ASP:CG	3:C:1551:SER:HG	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1587:SER:O	3:C:1589:PHE:N	2.43	0.47
1:D:404:THR:C	1:D:414:GLN:OE1	2.53	0.47
2:E:754:GLU:HG3	2:E:769:MET:SD	2.55	0.47
2:E:756:LEU:HA	2:E:758:GLU:OE1	2.14	0.47
3:F:1636:VAL:O	3:F:1637:PHE:C	2.51	0.47
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.45	0.47
1:A:86:VAL:O	1:A:86:VAL:HG12	2.11	0.47
1:A:97:LYS:HG3	1:A:98:VAL:N	2.30	0.47
2:B:897:HIS:HB3	2:B:899:ILE:HG13	1.97	0.47
3:C:1337:ASN:O	3:C:1371:ARG:CD	2.60	0.47
3:C:1376:ALA:HB3	3:C:1429:VAL:HG22	1.97	0.47
3:C:1508:GLU:O	3:C:1512:ASP:OD1	2.33	0.47
3:C:1551:SER:C	3:C:1593:LYS:NZ	2.67	0.47
2:E:735:ALA:HB1	2:E:737:GLU:OE2	2.15	0.47
3:F:1639:CYS:C	3:F:1641:ASN:H	2.15	0.47
4:M:23:LEU:HD11	4:M:51:ALA:HB1	1.97	0.47
1:A:148:PRO:HG3	1:A:182:TRP:CD1	2.50	0.47
1:A:59:ASN:HB3	1:A:483:ARG:HH12	1.80	0.47
1:A:462:GLU:HG3	1:A:486:ARG:NH2	2.29	0.47
1:A:644:ALA:O	1:A:645:ALA:HB3	2.15	0.47
3:C:1573:LYS:CD	3:C:1573:LYS:O	2.63	0.47
1:D:251:PHE:CE1	1:D:304:VAL:CG1	2.98	0.47
1:D:368:ALA:O	1:D:402:VAL:HG13	2.15	0.47
1:D:475:LYS:HG2	1:D:598:VAL:CG1	2.45	0.47
1:D:462:GLU:HG3	1:D:486:ARG:NH2	2.29	0.47
1:D:510:VAL:HG21	1:D:622:LEU:HD12	1.95	0.47
3:F:1386:MET:O	3:F:1387:THR:C	2.54	0.47
3:F:1622:LYS:O	3:F:1623:GLN:C	2.53	0.47
1:A:291:ASN:HD22	1:A:291:ASN:N	2.13	0.47
1:A:459:ARG:H	1:D:459:ARG:NH2	2.13	0.47
1:A:475:LYS:HG2	1:A:598:VAL:CG1	2.45	0.46
3:C:1504:LYS:O	3:C:1505:VAL:O	2.33	0.46
3:C:1507:LEU:HD11	3:C:1629:ALA:HB3	1.97	0.46
3:C:1608:HIS:CD2	3:C:1610:PRO:CD	2.97	0.46
1:D:105:SER:O	1:D:132:HIS:CD2	2.68	0.46
1:D:301:SER:HB2	1:D:323:GLY:HA2	1.97	0.46
2:E:897:HIS:HB3	2:E:899:ILE:HG13	1.97	0.46
3:F:1450:ILE:CG1	3:F:1450:ILE:O	2.55	0.46
1:A:203:LYS:HG2	1:A:204:GLU:N	2.29	0.46
1:A:357:PRO:O	1:A:358:ASP:C	2.53	0.46
1:D:148:PRO:HG3	1:D:182:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ILE:HA	1:D:271:ILE:HD13	1.74	0.46
1:D:126:ARG:CZ	1:D:572:VAL:HB	2.45	0.46
1:D:475:LYS:HG2	1:D:598:VAL:HG11	1.96	0.46
3:F:1483:LEU:CG	3:F:1590:TRP:CZ2	2.98	0.46
3:F:1525:THR:OG1	3:F:1541:MET:CE	2.63	0.46
3:F:1618:GLU:O	3:F:1619:GLU:C	2.54	0.46
4:P:49:GLN:O	4:P:50:LYS:C	2.52	0.46
4:P:66:ALA:O	4:P:67:LYS:C	2.53	0.46
1:A:215:GLU:HA	1:A:216:PRO:HD3	1.68	0.46
1:A:285:LEU:HG	1:A:285:LEU:O	2.14	0.46
1:A:20:MET:H	1:A:64:VAL:HB	1.79	0.46
1:A:6:ILE:HA	1:A:6:ILE:HD12	1.56	0.46
2:B:756:LEU:HA	2:B:758:GLU:OE1	2.14	0.46
2:B:894:VAL:CG2	2:B:899:ILE:HB	2.45	0.46
3:C:1530:VAL:HG12	3:C:1532:LEU:CD1	2.45	0.46
3:C:1534:ASN:O	3:C:1566:ILE:CD1	2.64	0.46
1:A:287:ASP:N	1:A:291:ASN:ND2	2.63	0.46
1:A:59:ASN:HB3	1:A:483:ARG:NH1	2.29	0.46
1:D:111:GLN:O	1:D:125:TYR:HA	2.16	0.46
1:D:285:LEU:HG	1:D:285:LEU:O	2.14	0.46
1:D:375:VAL:CG2	1:D:387:LEU:HD22	2.46	0.46
1:D:461:HIS:O	1:D:464:LYS:HB2	2.16	0.46
1:D:97:LYS:NZ	1:D:631:GLN:HB2	2.29	0.46
1:D:6:ILE:HD12	1:D:6:ILE:HA	1.56	0.46
1:A:301:SER:HB2	1:A:323:GLY:HA2	1.97	0.46
3:C:1395:ASP:O	3:C:1398:GLN:HB3	2.15	0.46
1:D:7:ILE:HA	1:D:623:THR:O	2.14	0.46
1:A:105:SER:O	1:A:132:HIS:CD2	2.68	0.46
3:C:1392:ASP:HB2	3:C:1442:HIS:NE2	2.30	0.46
1:D:185:ARG:HA	1:D:196:PHE:O	2.16	0.46
1:D:357:PRO:O	1:D:358:ASP:C	2.53	0.46
2:E:733:ILE:CG1	2:E:734:ILE:N	2.75	0.46
4:M:7:SER:O	4:M:8:ASN:C	2.54	0.46
3:C:1386:MET:O	3:C:1387:THR:C	2.53	0.46
3:C:1389:PHE:HD1	3:C:1441:VAL:CG2	2.26	0.46
1:D:214:VAL:HG11	1:D:304:VAL:CG2	2.45	0.46
3:F:1522:VAL:O	3:F:1547:ILE:HB	2.15	0.46
3:F:1571:ALA:N	3:F:1572:LEU:HD23	2.30	0.46
4:P:36:LEU:N	4:P:36:LEU:CD2	2.78	0.46
1:A:40:PHE:CE2	1:A:41:PRO:HG3	2.51	0.46
3:C:1406:TYR:CZ	3:C:1408:SER:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:VAL:HG13	3:C:1451:GLN:NE2	2.31	0.46
3:C:1543:ILE:O	3:C:1543:ILE:HG22	2.16	0.46
1:D:309:ILE:HG12	1:D:316:MET:HG3	1.97	0.46
2:E:744:GLU:C	2:E:746:PRO:HD3	2.37	0.46
3:F:1389:PHE:HD2	3:F:1389:PHE:N	2.14	0.46
4:M:49:GLN:O	4:M:50:LYS:C	2.53	0.46
1:A:185:ARG:HA	1:A:196:PHE:O	2.16	0.46
1:A:292:PRO:O	1:A:293:ARG:C	2.53	0.46
1:A:339:PRO:O	1:A:340:LYS:HD3	2.16	0.46
1:A:375:VAL:CG2	1:A:387:LEU:HD22	2.46	0.46
2:B:833:ARG:HH22	2:B:899:ILE:CD1	2.24	0.46
3:C:1537:ASP:OD2	3:C:1569:ARG:HD3	2.16	0.46
1:D:40:PHE:CE2	1:D:41:PRO:HG3	2.51	0.46
2:E:796:ALA:HB2	1:D:541:LEU:HD23	1.98	0.46
3:F:1536:PHE:HD2	3:F:1566:ILE:CD1	2.24	0.46
1:A:111:GLN:O	1:A:125:TYR:HA	2.16	0.46
1:A:404:THR:HG1	1:A:415:ALA:H	1.62	0.46
1:A:541:LEU:HD23	2:B:796:ALA:HB2	1.98	0.46
3:C:1403:VAL:O	3:C:1404:ASP:HB2	2.15	0.46
3:C:1440:LYS:HG3	3:C:1440:LYS:H	1.56	0.46
1:D:97:LYS:NZ	1:D:632:THR:O	2.48	0.46
3:F:1569:ARG:CA	3:F:1570:GLU:OE1	2.64	0.46
3:F:1624:CYS:O	3:F:1627:LEU:N	2.48	0.46
4:P:23:LEU:HD11	4:P:51:ALA:HB1	1.97	0.46
4:P:7:SER:O	4:P:8:ASN:C	2.54	0.46
1:A:461:HIS:O	1:A:464:LYS:HB2	2.16	0.45
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.81	0.45
3:F:1395:ASP:O	3:F:1398:GLN:HB3	2.15	0.45
3:F:1403:VAL:O	3:F:1404:ASP:HB2	2.15	0.45
4:M:36:LEU:CD2	4:M:36:LEU:N	2.77	0.45
4:P:29:ASN:O	4:P:32:ALA:N	2.49	0.45
1:A:224:TYR:CD2	1:A:224:TYR:N	2.84	0.45
3:C:1593:LYS:HA	3:C:1594:PRO:HA	1.71	0.45
1:D:118:THR:HG23	1:D:205:TYR:CE2	2.52	0.45
1:D:20:MET:HG2	1:D:64:VAL:CB	2.47	0.45
1:D:224:TYR:N	1:D:224:TYR:CD2	2.84	0.45
1:D:644:ALA:O	1:D:645:ALA:HB3	2.15	0.45
4:M:29:ASN:O	4:M:32:ALA:N	2.49	0.45
1:A:164:LEU:O	2:B:787:MET:HG2	2.15	0.45
3:C:1403:VAL:C	3:C:1405:ARG:H	2.18	0.45
3:C:1562:PHE:CE2	3:C:1582:MET:HE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:PRO:O	1:D:340:LYS:HD3	2.16	0.45
3:F:1389:PHE:HD1	3:F:1441:VAL:CG2	2.26	0.45
3:F:1409:LYS:HA	3:F:1412:LEU:HB2	1.99	0.45
2:E:863:THR:HB	4:M:7:SER:HB2	1.99	0.45
1:A:36:THR:HA	1:A:47:LEU:O	2.17	0.45
2:B:804:MET:CG	2:B:805:GLN:H	2.29	0.45
3:C:1495:ASN:HB2	3:C:1496:CYS:H	1.62	0.45
1:D:369:VAL:CG1	1:D:370:GLN:H	2.24	0.45
2:E:894:VAL:CG2	2:E:899:ILE:HB	2.45	0.45
3:F:1341:LEU:HD23	3:F:1469:ARG:H	1.82	0.45
4:P:29:ASN:O	4:P:30:GLU:C	2.54	0.45
1:A:271:ILE:HD13	1:A:271:ILE:HA	1.74	0.45
1:A:504:ILE:CG2	1:A:505:PRO:HA	2.47	0.45
3:C:1472:HIS:CE1	3:C:1474:GLU:H	2.35	0.45
3:C:1618:GLU:HA	3:C:1621:GLN:CD	2.37	0.45
1:D:101:VAL:CG1	1:D:102:SER:N	2.80	0.45
1:D:210:PHE:HB3	1:D:237:PHE:HA	1.99	0.45
3:F:1406:TYR:CD2	3:F:1407:ILE:N	2.84	0.45
1:A:309:ILE:HG12	1:A:316:MET:HG3	1.97	0.45
1:A:541:LEU:HD12	1:A:541:LEU:HA	1.77	0.45
1:D:251:PHE:N	1:D:251:PHE:CD2	2.85	0.45
2:E:811:LEU:HG	2:E:813:LEU:HD13	1.98	0.45
3:F:1575:GLU:CG	3:F:1576:GLU:H	2.29	0.45
2:B:733:ILE:HB	2:B:895:TYR:CD2	2.51	0.45
3:C:1506:THR:O	3:C:1508:GLU:N	2.49	0.45
1:D:291:ASN:HD22	1:D:291:ASN:N	2.13	0.45
1:D:504:ILE:CG2	1:D:505:PRO:HA	2.47	0.45
4:M:29:ASN:O	4:M:30:GLU:C	2.55	0.45
2:B:734:ILE:CD1	2:B:734:ILE:H	2.16	0.45
3:C:1416:PHE:CD2	3:C:1417:SER:N	2.85	0.45
3:C:1416:PHE:CE2	3:C:1444:TYR:HD2	2.25	0.45
3:C:1451:GLN:HA	3:C:1452:PRO:HD3	1.81	0.45
3:C:1544:GLU:OE1	3:C:1579:HIS:NE2	2.50	0.45
3:C:1546:THR:C	3:C:1548:LYS:N	2.70	0.45
1:D:406:LYS:HG3	1:D:407:GLN:O	2.16	0.45
4:M:64:SER:O	4:M:65:GLU:C	2.55	0.45
1:A:20:MET:HG2	1:A:64:VAL:CB	2.47	0.45
1:A:379:THR:HG22	1:A:384:VAL:N	2.31	0.45
2:B:744:GLU:C	2:B:746:PRO:HD3	2.37	0.45
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.45
3:C:1337:ASN:C	3:C:1337:ASN:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1341:LEU:HD23	3:C:1469:ARG:H	1.82	0.45
3:C:1506:THR:CB	3:C:1509:GLU:HG2	2.46	0.45
2:E:786:SER:HB3	1:D:541:LEU:CD2	2.39	0.45
2:E:789:ASP:HA	1:D:136:PRO:CG	2.47	0.45
2:E:844:LEU:HD12	2:E:845:LEU:N	2.32	0.45
3:F:1337:ASN:OD1	3:F:1337:ASN:C	2.54	0.45
3:F:1510:ARG:HG3	3:F:1583:TRP:HH2	1.81	0.45
1:A:101:VAL:CG1	1:A:102:SER:N	2.80	0.45
1:A:37:VAL:CG1	1:A:84:VAL:CG2	2.94	0.45
1:D:434:LEU:HB2	1:D:513:TYR:HE2	1.81	0.45
2:E:733:ILE:HB	2:E:895:TYR:CD2	2.51	0.45
3:F:1582:MET:HB2	3:F:1582:MET:HE2	1.62	0.45
1:A:251:PHE:CD2	1:A:251:PHE:N	2.85	0.44
1:A:271:ILE:O	1:A:271:ILE:HG22	2.16	0.44
1:A:97:LYS:NZ	1:A:632:THR:O	2.48	0.44
3:C:1389:PHE:N	3:C:1389:PHE:HD2	2.14	0.44
3:C:1495:ASN:O	3:C:1496:CYS:HB3	2.17	0.44
1:D:379:THR:HG22	1:D:384:VAL:N	2.31	0.44
3:F:1472:HIS:CE1	3:F:1474:GLU:H	2.35	0.44
3:F:1497:PHE:O	3:F:1497:PHE:HD2	1.96	0.44
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.52	0.44
1:A:38:HIS:HE1	1:A:45:LEU:CD1	2.30	0.44
1:A:406:LYS:HG3	1:A:407:GLN:O	2.16	0.44
3:C:1581:LEU:HD23	3:C:1627:LEU:HD21	1.99	0.44
1:D:271:ILE:O	1:D:271:ILE:HG22	2.16	0.44
1:D:30:ASP:OD1	1:D:30:ASP:N	2.50	0.44
1:D:37:VAL:CG1	1:D:84:VAL:CG2	2.94	0.44
3:F:1524:LYS:C	3:F:1525:THR:CG2	2.85	0.44
3:F:1526:ARG:NH2	3:F:1544:GLU:OE1	2.48	0.44
1:A:590:THR:HB	1:A:593:LYS:CG	2.39	0.44
1:A:136:PRO:CG	2:B:789:ASP:HA	2.48	0.44
3:C:1526:ARG:HG3	3:C:1526:ARG:O	2.18	0.44
3:C:1562:PHE:CE2	3:C:1598:TYR:HB3	2.53	0.44
1:D:634:GLN:HE22	1:D:635:ARG:C	2.19	0.44
3:F:1612:GLU:C	3:F:1614:GLU:H	2.20	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.48	0.44
1:A:30:ASP:N	1:A:30:ASP:OD1	2.50	0.44
1:A:97:LYS:HD3	1:A:625:THR:OG1	2.17	0.44
3:C:1504:LYS:O	3:C:1505:VAL:HG23	2.18	0.44
3:F:1409:LYS:O	3:F:1410:TYR:C	2.56	0.44
3:F:1508:GLU:HA	3:F:1508:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1575:GLU:CG	3:F:1576:GLU:N	2.80	0.44
4:P:26:LEU:O	4:P:29:ASN:N	2.50	0.44
1:A:210:PHE:HB3	1:A:237:PHE:HA	1.99	0.44
1:A:410:SER:OG	1:A:413:GLU:HG3	2.18	0.44
2:B:817:VAL:HG22	2:B:907:LEU:HD12	1.99	0.44
3:C:1460:TYR:CG	3:C:1461:TYR:N	2.86	0.44
1:D:404:THR:HG1	1:D:415:ALA:H	1.66	0.44
1:D:541:LEU:HD12	1:D:541:LEU:HA	1.77	0.44
2:E:817:VAL:HG22	2:E:907:LEU:HD12	1.99	0.44
4:M:66:ALA:O	4:M:67:LYS:C	2.53	0.44
1:A:604:GLY:HA2	1:A:619:ASP:O	2.18	0.44
2:B:873:SER:HB3	3:C:1421:THR:CG2	2.48	0.44
3:C:1406:TYR:OH	3:C:1408:SER:HA	2.16	0.44
1:D:83:PHE:HD1	1:D:99:VAL:C	2.21	0.44
3:F:1406:TYR:CD2	3:F:1406:TYR:C	2.88	0.44
1:A:380:GLN:O	1:A:382:ASP:N	2.51	0.44
1:A:465:ILE:HD11	1:A:515:LEU:HD13	2.00	0.44
2:B:835:ASN:O	2:B:836:GLN:HB3	2.17	0.44
2:B:844:LEU:HD12	2:B:845:LEU:N	2.32	0.44
3:C:1409:LYS:O	3:C:1410:TYR:C	2.56	0.44
3:C:1551:SER:C	3:C:1593:LYS:HZ3	2.18	0.44
1:D:227:LYS:HE2	1:D:227:LYS:HB2	1.64	0.44
1:D:410:SER:OG	1:D:413:GLU:HG3	2.18	0.44
1:D:458:ASP:OD2	1:D:460:ALA:HB3	2.18	0.44
1:D:604:GLY:HA2	1:D:619:ASP:O	2.18	0.44
2:E:835:ASN:O	2:E:836:GLN:HB3	2.17	0.44
4:P:64:SER:O	4:P:65:GLU:C	2.55	0.44
4:P:73:ILE:O	4:P:77:ILE:HG13	2.18	0.44
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.31	0.44
1:D:255:ASP:O	1:D:258:GLN:HB3	2.18	0.44
1:D:468:TYR:CE1	1:D:513:TYR:CD2	3.05	0.44
1:D:510:VAL:CG1	1:D:528:SER:HB3	2.33	0.44
3:F:1460:TYR:CD1	1:D:248:PHE:CG	3.06	0.44
4:M:26:LEU:O	4:M:29:ASN:N	2.50	0.44
1:A:227:LYS:HE2	1:A:227:LYS:HB2	1.64	0.44
2:B:863:THR:HB	4:P:7:SER:HB2	1.99	0.44
3:C:1641:ASN:HD22	3:C:1641:ASN:N	2.15	0.44
1:D:147:ASN:HB2	1:D:148:PRO:CD	2.48	0.44
1:D:20:MET:HG2	1:D:64:VAL:CG2	2.47	0.44
2:E:730:ASP:CG	2:E:730:ASP:O	2.56	0.44
2:E:819:ARG:NH1	2:E:883:THR:HG23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1416:PHE:CD2	3:F:1417:SER:N	2.85	0.44
2:B:730:ASP:O	2:B:730:ASP:CG	2.55	0.43
2:B:742:ARG:N	2:B:902:GLY:O	2.47	0.43
1:D:380:GLN:O	1:D:382:ASP:N	2.51	0.43
1:D:530:TRP:CD1	1:D:530:TRP:C	2.91	0.43
3:F:1341:LEU:CD2	3:F:1469:ARG:HB2	2.48	0.43
3:F:1497:PHE:CE1	3:F:1498:ILE:CD1	3.00	0.43
1:A:124:LEU:HD12	2:B:751:TRP:CG	2.53	0.43
2:B:840:VAL:HG13	2:B:893:ALA:O	2.18	0.43
3:C:1444:TYR:CD1	3:C:1444:TYR:C	2.92	0.43
1:D:492:LEU:HA	1:D:492:LEU:HD12	1.87	0.43
1:D:465:ILE:HD11	1:D:515:LEU:HD13	2.00	0.43
2:E:840:VAL:HG13	2:E:893:ALA:O	2.18	0.43
3:F:1460:TYR:CG	3:F:1461:TYR:N	2.86	0.43
3:F:1483:LEU:CD1	3:F:1590:TRP:HZ2	2.26	0.43
1:A:615:GLY:O	1:A:616:VAL:C	2.56	0.43
3:F:1482:LYS:HB2	3:F:1489:CYS:SG	2.58	0.43
3:F:1509:GLU:CA	3:F:1512:ASP:HB3	2.48	0.43
3:F:1558:GLN:HG2	3:F:1559:GLN:H	1.83	0.43
1:A:20:MET:HG2	1:A:64:VAL:CG2	2.47	0.43
1:A:83:PHE:CD1	1:A:100:LEU:HA	2.54	0.43
1:A:84:VAL:HG22	1:A:85:THR:H	1.84	0.43
2:B:778:THR:OG1	2:B:779:THR:N	2.52	0.43
2:E:751:TRP:CG	1:D:124:LEU:HD12	2.53	0.43
1:D:36:THR:HA	1:D:47:LEU:O	2.17	0.43
2:E:833:ARG:HH22	2:E:899:ILE:CD1	2.24	0.43
3:F:1516:GLU:O	3:F:1517:PRO:C	2.55	0.43
4:M:15:LEU:HD22	4:M:60:PHE:CE1	2.53	0.43
1:A:455:LEU:CD1	1:A:457:MET:HG2	2.49	0.43
1:A:468:TYR:CE1	1:A:513:TYR:CD2	3.05	0.43
1:D:402:VAL:HG12	1:D:403:ARG:H	1.84	0.43
1:D:97:LYS:HD3	1:D:625:THR:OG1	2.17	0.43
1:D:84:VAL:HG22	1:D:85:THR:H	1.84	0.43
2:E:773:LEU:O	1:D:556:GLY:HA2	2.18	0.43
1:A:255:ASP:O	1:A:258:GLN:HB3	2.18	0.43
1:A:291:ASN:N	1:A:292:PRO:HD3	2.34	0.43
1:A:458:ASP:OD2	1:A:460:ALA:HB3	2.18	0.43
1:A:446:GLY:O	1:D:378:LEU:HD13	2.19	0.43
1:D:38:HIS:HE1	1:D:45:LEU:CD1	2.31	0.43
1:D:603:ILE:HB	1:D:635:ARG:HH12	1.84	0.43
2:E:778:THR:HG23	2:E:779:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:73:ILE:O	4:M:77:ILE:HG13	2.18	0.43
1:A:453:PHE:CE2	1:A:495:LEU:HB2	2.53	0.43
1:A:522:ARG:HA	1:A:522:ARG:HD3	1.94	0.43
1:A:83:PHE:HD1	1:A:99:VAL:C	2.21	0.43
2:B:733:ILE:CG1	2:B:734:ILE:H	2.28	0.43
3:C:1472:HIS:ND1	3:C:1473:PRO:HD2	2.34	0.43
3:C:1494:GLU:H	3:C:1494:GLU:HG2	1.49	0.43
3:C:1630:PHE:O	3:C:1633:SER:N	2.52	0.43
1:D:455:LEU:HB2	1:D:468:TYR:OH	2.19	0.43
1:D:453:PHE:CE2	1:D:495:LEU:HB2	2.53	0.43
3:F:1503:ASP:C	3:F:1505:VAL:N	2.71	0.43
4:M:15:LEU:O	4:M:18:GLU:HB2	2.19	0.43
1:A:603:ILE:HB	1:A:635:ARG:HH12	1.84	0.43
1:A:98:VAL:O	1:A:634:GLN:HG2	2.18	0.43
3:C:1575:GLU:H	3:C:1580:TYR:HH	1.62	0.43
1:D:477:ARG:CG	1:D:477:ARG:HH11	2.31	0.43
3:F:1349:PRO:O	3:F:1350:GLU:CB	2.35	0.43
3:F:1472:HIS:ND1	3:F:1473:PRO:HD2	2.34	0.43
4:P:15:LEU:HD22	4:P:60:PHE:CE1	2.53	0.43
1:A:177:VAL:HG22	1:A:178:ASN:N	2.34	0.43
5:A:646:NAG:H62	5:A:646:NAG:O3	2.19	0.43
2:B:729:LEU:CD1	2:B:737:GLU:OE2	2.67	0.43
3:C:1504:LYS:HG2	3:C:1506:THR:HG22	2.00	0.43
3:C:1544:GLU:C	3:C:1545:GLN:HG3	2.36	0.43
1:D:454:LEU:HA	1:D:491:ASP:O	2.19	0.43
1:D:458:ASP:O	1:D:460:ALA:N	2.52	0.43
1:D:583:LEU:HD23	1:D:583:LEU:HA	1.76	0.43
3:F:1503:ASP:O	3:F:1504:LYS:C	2.58	0.43
2:B:865:THR:OG1	4:P:11:GLN:HG2	2.19	0.43
3:F:1444:TYR:C	3:F:1444:TYR:CD1	2.92	0.43
4:M:23:LEU:HD23	4:M:23:LEU:HA	1.81	0.43
4:M:51:ALA:O	4:M:54:ALA:N	2.52	0.43
4:P:51:ALA:O	4:P:54:ALA:N	2.52	0.43
1:A:138:GLY:HA2	1:A:160:SER:HG	1.79	0.42
1:A:219:LYS:HD2	1:A:358:ASP:OD2	2.19	0.42
1:A:458:ASP:O	1:A:460:ALA:N	2.52	0.42
2:B:778:THR:HG23	2:B:779:THR:N	2.34	0.42
3:C:1607:GLU:O	3:C:1608:HIS:O	2.37	0.42
3:F:1378:MET:HE2	1:D:248:PHE:HD1	1.83	0.42
5:D:646:NAG:O3	5:D:646:NAG:H62	2.19	0.42
2:E:729:LEU:CD1	2:E:737:GLU:OE2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:804:MET:CG	2:E:805:GLN:H	2.29	0.42
2:E:847:ASN:HA	2:E:848:PRO:HD2	1.90	0.42
3:F:1631:THR:C	3:F:1633:SER:N	2.72	0.42
3:F:1634:MET:O	3:F:1635:VAL:C	2.58	0.42
1:A:455:LEU:HB2	1:A:468:TYR:OH	2.19	0.42
2:B:749:TRP:CE3	2:B:750:LEU:HB2	2.54	0.42
3:C:1555:GLN:O	3:C:1556:VAL:O	2.37	0.42
1:D:289:VAL:O	1:D:290:GLN:CB	2.67	0.42
2:E:729:LEU:HD13	2:E:737:GLU:OE2	2.20	0.42
4:P:15:LEU:O	4:P:18:GLU:HB2	2.19	0.42
1:A:87:GLN:HG3	1:A:96:GLU:HB3	2.01	0.42
2:B:877:VAL:HG13	3:C:1451:GLN:CD	2.39	0.42
3:C:1602:LYS:C	3:C:1604:THR:H	2.22	0.42
1:D:298:VAL:O	1:D:298:VAL:HG12	2.18	0.42
3:F:1451:GLN:HA	3:F:1452:PRO:HD3	1.81	0.42
4:P:43:THR:HG21	4:P:73:ILE:HD13	2.01	0.42
1:A:454:LEU:HA	1:A:491:ASP:O	2.19	0.42
1:A:530:TRP:CD1	1:A:530:TRP:C	2.91	0.42
2:B:729:LEU:HD13	2:B:737:GLU:OE2	2.20	0.42
3:C:1531:GLN:C	3:C:1532:LEU:HD13	2.40	0.42
1:D:20:MET:HG2	1:D:64:VAL:HG11	2.02	0.42
2:E:749:TRP:CE3	2:E:750:LEU:HB2	2.54	0.42
3:F:1378:MET:HA	3:F:1426:LEU:O	2.19	0.42
3:F:1460:TYR:HB2	1:D:248:PHE:CD2	2.55	0.42
3:F:1495:ASN:HD21	3:F:1602:LYS:HG3	1.83	0.42
3:F:1615:CYS:C	3:F:1617:ASP:N	2.72	0.42
1:A:61:MET:CE	1:A:483:ARG:HG2	2.50	0.42
3:C:1416:PHE:C	3:C:1416:PHE:HD2	2.20	0.42
3:C:1370:TYR:O	3:C:1431:HIS:HA	2.19	0.42
1:D:203:LYS:HG2	1:D:204:GLU:H	1.85	0.42
1:D:289:VAL:O	1:D:290:GLN:HG2	1.97	0.42
3:F:1635:VAL:HG12	3:F:1636:VAL:N	2.33	0.42
3:C:1378:MET:HA	3:C:1426:LEU:O	2.19	0.42
3:F:1416:PHE:C	3:F:1416:PHE:HD2	2.20	0.42
3:F:1414:LYS:HD3	3:F:1419:ARG:HG3	2.02	0.42
3:F:1496:CYS:O	3:F:1497:PHE:CB	2.50	0.42
3:F:1524:LYS:CD	3:F:1525:THR:N	2.75	0.42
3:F:1569:ARG:C	3:F:1570:GLU:CD	2.78	0.42
4:P:26:LEU:O	4:P:29:ASN:HB2	2.19	0.42
1:A:453:PHE:CB	1:A:493:VAL:HG23	2.41	0.42
2:B:833:ARG:HD2	2:B:834:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:852:SER:C	2:B:854:ALA:N	2.73	0.42
3:C:1513:LYS:O	3:C:1516:GLU:CG	2.57	0.42
3:C:1520:ASP:O	3:C:1521:TYR:HB3	2.20	0.42
1:D:219:LYS:HD2	1:D:358:ASP:OD2	2.19	0.42
1:D:61:MET:CE	1:D:483:ARG:HG2	2.50	0.42
3:F:1370:TYR:O	3:F:1431:HIS:HA	2.19	0.42
3:F:1572:LEU:C	3:F:1574:LEU:HD21	2.32	0.42
3:F:1631:THR:O	3:F:1633:SER:N	2.53	0.42
4:M:43:THR:HG21	4:M:73:ILE:HD13	2.01	0.42
1:A:402:VAL:HG12	1:A:403:ARG:H	1.84	0.42
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.54	0.42
3:C:1482:LYS:O	3:C:1536:PHE:CZ	2.72	0.42
3:C:1587:SER:C	3:C:1589:PHE:H	2.23	0.42
1:D:168:PRO:O	1:D:169:LEU:HG	2.20	0.42
1:D:251:PHE:CD1	1:D:280:LEU:HB2	2.55	0.42
1:D:495:LEU:HA	1:D:496:PRO:HD3	1.88	0.42
1:D:590:THR:HG22	1:D:591:GLN:N	2.35	0.42
2:E:778:THR:OG1	2:E:779:THR:N	2.52	0.42
2:E:852:SER:C	2:E:854:ALA:N	2.73	0.42
3:F:1624:CYS:O	3:F:1625:GLN:C	2.58	0.42
1:A:251:PHE:CD1	1:A:280:LEU:HB2	2.55	0.42
1:A:33:VAL:HG22	1:A:90:PHE:HA	2.02	0.42
2:B:734:ILE:HD11	2:B:898:PHE:HA	2.02	0.42
1:D:291:ASN:N	1:D:292:PRO:HD3	2.34	0.42
1:D:294:ALA:O	1:D:295:GLU:C	2.58	0.42
1:D:455:LEU:CD1	1:D:457:MET:HG2	2.49	0.42
1:D:509:LEU:HB3	1:D:529:VAL:CG1	2.50	0.42
1:D:613:TYR:CD2	1:D:614:ALA:N	2.88	0.42
2:E:885:LEU:HA	2:E:885:LEU:HD12	1.74	0.42
3:F:1409:LYS:C	3:F:1411:GLU:H	2.23	0.42
3:F:1497:PHE:CE1	3:F:1498:ILE:HD11	2.54	0.42
3:F:1543:ILE:C	3:F:1545:GLN:N	2.73	0.42
1:A:203:LYS:HG2	1:A:204:GLU:H	1.85	0.42
2:B:897:HIS:CB	2:B:899:ILE:HG13	2.50	0.42
3:C:1341:LEU:CD2	3:C:1469:ARG:HB2	2.48	0.42
1:D:83:PHE:CD1	1:D:100:LEU:HA	2.54	0.42
1:D:87:GLN:HG3	1:D:96:GLU:HB3	2.01	0.42
2:E:863:THR:HB	4:M:7:SER:CB	2.50	0.42
4:P:15:LEU:HD12	4:P:15:LEU:HA	1.82	0.42
1:A:168:PRO:O	1:A:169:LEU:HG	2.20	0.41
1:A:298:VAL:O	1:A:298:VAL:HG12	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:HB3	1:A:357:PRO:HG2	2.01	0.41
1:A:634:GLN:HE22	1:A:635:ARG:C	2.19	0.41
1:D:177:VAL:HG22	1:D:178:ASN:N	2.34	0.41
1:D:47:LEU:HD23	1:D:47:LEU:C	2.41	0.41
4:M:26:LEU:O	4:M:29:ASN:HB2	2.19	0.41
1:A:106:GLY:HA2	1:A:132:HIS:CD2	2.55	0.41
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.91	0.41
1:A:343:LYS:CD	1:A:343:LYS:N	2.83	0.41
1:A:4:TYR:HB3	1:A:90:PHE:CZ	2.55	0.41
1:A:509:LEU:HB3	1:A:529:VAL:CG1	2.50	0.41
3:C:1414:LYS:HD3	3:C:1419:ARG:HG3	2.02	0.41
1:D:220:PHE:HB3	1:D:357:PRO:HG2	2.01	0.41
1:D:400:ILE:N	1:D:400:ILE:HD12	2.35	0.41
1:D:502:ASP:OD1	1:D:502:ASP:N	2.54	0.41
1:D:615:GLY:O	1:D:616:VAL:C	2.56	0.41
3:F:1601:GLY:N	3:F:1604:THR:HG22	2.34	0.41
3:F:1600:ILE:C	3:F:1604:THR:HG21	2.41	0.41
4:M:29:ASN:O	4:M:31:LEU:N	2.53	0.41
2:B:898:PHE:CE2	4:M:50:LYS:HA	2.54	0.41
1:A:400:ILE:HD12	1:A:400:ILE:N	2.35	0.41
1:D:106:GLY:HA2	1:D:132:HIS:CD2	2.55	0.41
2:E:733:ILE:CG1	2:E:734:ILE:H	2.28	0.41
2:E:769:MET:HB2	1:D:561:LEU:HB3	2.02	0.41
2:E:734:ILE:HD11	2:E:898:PHE:HA	2.02	0.41
3:F:1514:ALA:HB2	3:F:1583:TRP:CZ2	2.55	0.41
1:A:195:VAL:CG1	1:A:196:PHE:N	2.82	0.41
1:A:294:ALA:O	1:A:295:GLU:C	2.58	0.41
1:A:73:GLU:HB3	1:A:82:LYS:HZ3	1.82	0.41
1:A:206:VAL:HG11	2:B:813:LEU:O	2.20	0.41
3:C:1472:HIS:CE1	3:C:1473:PRO:HD2	2.55	0.41
1:D:101:VAL:HG12	1:D:102:SER:N	2.35	0.41
1:D:195:VAL:CG1	1:D:196:PHE:N	2.82	0.41
1:D:241:LYS:HA	1:D:241:LYS:HD3	1.83	0.41
2:E:789:ASP:O	1:D:135:LEU:HD22	2.19	0.41
3:F:1390:ALA:HA	3:F:1391:PRO:HD3	1.92	0.41
3:F:1509:GLU:O	3:F:1512:ASP:N	2.53	0.41
3:F:1524:LYS:C	3:F:1525:THR:HG22	2.39	0.41
4:P:13:GLU:O	4:P:13:GLU:HG2	2.20	0.41
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.03	0.41
1:A:346:MET:O	1:A:391:THR:CG2	2.57	0.41
1:A:556:GLY:HA2	2:B:773:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:TYR:CD2	1:A:614:ALA:N	2.88	0.41
3:C:1611:GLU:HG2	3:C:1612:GLU:N	2.36	0.41
1:D:269:ILE:HA	1:D:270:PRO:HD3	1.93	0.41
1:D:33:VAL:HG22	1:D:90:PHE:HA	2.02	0.41
2:E:833:ARG:HD2	2:E:834:GLN:NE2	2.35	0.41
3:F:1527:LEU:HD12	3:F:1575:GLU:C	2.40	0.41
4:M:13:GLU:O	4:M:13:GLU:HG2	2.20	0.41
4:P:29:ASN:O	4:P:31:LEU:N	2.52	0.41
1:A:20:MET:HG2	1:A:64:VAL:HG11	2.01	0.41
1:A:436:LEU:HA	1:A:452:ASN:O	2.21	0.41
1:A:47:LEU:C	1:A:47:LEU:HD23	2.41	0.41
3:C:1514:ALA:O	3:C:1519:VAL:HG21	2.21	0.41
3:C:1537:ASP:OD2	3:C:1569:ARG:CB	2.68	0.41
1:D:37:VAL:CG1	1:D:84:VAL:HG21	2.51	0.41
1:D:436:LEU:HA	1:D:452:ASN:O	2.21	0.41
3:F:1545:GLN:HG3	3:F:1546:THR:H	1.86	0.41
3:F:1633:SER:O	3:F:1634:MET:C	2.56	0.41
3:C:1445:PHE:HZ	4:P:7:SER:HG	1.65	0.41
1:A:292:PRO:O	1:A:294:ALA:N	2.54	0.41
1:A:37:VAL:CG1	1:A:84:VAL:HG21	2.51	0.41
1:A:453:PHE:HE2	1:A:495:LEU:HB2	1.86	0.41
2:B:804:MET:HG2	2:B:805:GLN:N	2.35	0.41
2:B:818:VAL:HA	2:B:910:VAL:O	2.21	0.41
3:C:1514:ALA:C	3:C:1516:GLU:H	2.23	0.41
1:D:453:PHE:HE2	1:D:495:LEU:HB2	1.86	0.41
1:D:4:TYR:HB3	1:D:90:PHE:CZ	2.55	0.41
1:A:378:LEU:HD13	1:D:446:GLY:O	2.20	0.41
1:A:63:ASN:ND2	5:A:646:NAG:C1	2.84	0.41
1:D:389:ILE:O	1:D:389:ILE:HG13	2.20	0.41
2:E:869:LYS:O	2:E:870:SER:HB3	2.21	0.41
3:F:1460:TYR:CE1	1:D:248:PHE:HB2	2.56	0.41
4:P:58:LYS:HA	4:P:58:LYS:HD2	1.75	0.41
1:A:346:MET:HA	1:A:347:PRO:HD3	1.94	0.41
1:A:583:LEU:HA	1:A:583:LEU:HD23	1.76	0.41
1:A:590:THR:HG22	1:A:591:GLN:N	2.35	0.41
1:A:73:GLU:HB3	1:A:82:LYS:HZ1	1.82	0.41
2:B:811:LEU:HA	2:B:811:LEU:HD12	1.85	0.41
3:C:1552:ASP:O	3:C:1554:VAL:HG12	2.20	0.41
1:D:14:LEU:HD11	1:D:103:LEU:CD2	2.51	0.41
2:E:786:SER:O	2:E:793:ILE:HA	2.21	0.41
2:E:838:LEU:HA	2:E:838:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1472:HIS:CE1	3:F:1473:PRO:HD2	2.55	0.41
1:A:342:PHE:HD1	1:A:391:THR:HG21	1.86	0.41
2:B:734:ILE:N	2:B:734:ILE:CD1	2.81	0.41
3:C:1526:ARG:CZ	3:C:1542:ALA:HB2	2.51	0.41
1:D:265:SER:O	1:D:267:LYS:HG2	2.21	0.41
1:D:292:PRO:O	1:D:294:ALA:N	2.54	0.41
1:D:338:THR:HG23	1:D:339:PRO:HD2	2.03	0.41
1:D:343:LYS:CD	1:D:343:LYS:N	2.83	0.41
1:D:98:VAL:O	1:D:634:GLN:HG2	2.17	0.41
2:E:865:THR:OG1	4:M:11:GLN:HG2	2.21	0.41
1:A:101:VAL:HG12	1:A:102:SER:N	2.35	0.41
1:A:241:LYS:HA	1:A:241:LYS:HD3	1.83	0.41
1:A:508:ARG:CZ	1:A:604:GLY:HA3	2.51	0.41
3:C:1634:MET:CE	3:C:1638:GLY:O	2.69	0.41
1:D:380:GLN:C	1:D:382:ASP:H	2.25	0.41
1:D:508:ARG:CZ	1:D:604:GLY:HA3	2.51	0.41
2:E:839:LYS:HG2	2:E:895:TYR:CD1	2.56	0.41
2:E:897:HIS:CB	2:E:899:ILE:HG13	2.50	0.41
3:F:1337:ASN:O	3:F:1371:ARG:CD	2.60	0.41
3:F:1605:TRP:C	3:F:1606:VAL:HG23	2.42	0.41
1:A:578:LYS:HE2	1:A:578:LYS:HB3	1.86	0.40
2:B:869:LYS:O	2:B:870:SER:HB3	2.21	0.40
3:C:1508:GLU:O	3:C:1509:GLU:C	2.58	0.40
3:C:1507:LEU:HB3	3:C:1508:GLU:OE1	2.21	0.40
1:D:114:LYS:HE2	1:D:117:TYR:CD1	2.56	0.40
1:D:158:LEU:HA	1:D:158:LEU:HD12	1.89	0.40
1:D:342:PHE:HD1	1:D:391:THR:HG21	1.86	0.40
1:D:344:PRO:HG3	1:D:423:PRO:HB3	2.03	0.40
4:P:61:LYS:HB3	4:P:62:LYS:H	1.78	0.40
2:B:756:LEU:HD23	2:B:756:LEU:N	2.37	0.40
2:B:786:SER:O	2:B:793:ILE:HA	2.21	0.40
3:C:1532:LEU:HG	3:C:1569:ARG:NH1	2.35	0.40
1:D:113:ASP:OD1	1:D:113:ASP:N	2.53	0.40
3:F:1556:VAL:CG1	3:F:1557:GLY:N	2.84	0.40
1:A:14:LEU:HD11	1:A:103:LEU:CD2	2.51	0.40
1:A:108:LEU:HB2	1:A:196:PHE:CG	2.57	0.40
1:A:502:ASP:N	1:A:502:ASP:OD1	2.54	0.40
1:A:561:LEU:HB3	2:B:769:MET:HB2	2.02	0.40
2:B:858:ARG:HD3	3:C:1449:LEU:HD12	2.04	0.40
3:C:1556:VAL:C	3:C:1558:GLN:H	2.25	0.40
1:D:434:LEU:HB2	1:D:513:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1622:LYS:HG3	3:F:1623:GLN:H	1.78	0.40
1:A:389:ILE:O	1:A:389:ILE:HG13	2.20	0.40
1:A:487:GLU:HG3	1:D:392:HIS:HE1	1.86	0.40
3:C:1410:TYR:C	3:C:1410:TYR:CD2	2.95	0.40
3:C:1509:GLU:HA	3:C:1512:ASP:OD2	2.21	0.40
2:E:818:VAL:HA	2:E:910:VAL:O	2.20	0.40
3:F:1615:CYS:O	3:F:1616:GLN:C	2.60	0.40
2:B:863:THR:HB	4:P:7:SER:CB	2.52	0.40
1:A:145:ILE:O	1:A:153:VAL:HG22	2.22	0.40
1:A:183:LYS:CD	1:A:185:ARG:CD	3.00	0.40
1:A:380:GLN:C	1:A:382:ASP:H	2.25	0.40
1:A:248:PHE:CZ	3:C:1380:ILE:HD11	2.57	0.40
3:C:1526:ARG:CG	3:C:1542:ALA:CB	2.84	0.40
3:C:1568:CYS:O	3:C:1570:GLU:N	2.53	0.40
3:C:1574:LEU:HA	3:C:1580:TYR:CE1	2.56	0.40
2:E:793:ILE:CG1	2:E:794:CYS:N	2.85	0.40
3:F:1498:ILE:HG12	3:F:1498:ILE:H	1.66	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/645 (99%)	557 (87%)	69 (11%)	11 (2%)	11	49
1	D	637/645 (99%)	557 (87%)	69 (11%)	11 (2%)	11	49
2	B	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	17	59
2	E	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	17	59
3	C	287/343 (84%)	216 (75%)	44 (15%)	27 (9%)	1	9
3	F	289/343 (84%)	196 (68%)	42 (14%)	51 (18%)	0	2
4	M	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	4	32
All	All	2378/2564 (93%)	1970 (83%)	298 (12%)	110 (5%)	3	26

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	CYS
3	C	1505	VAL
3	C	1545	GLN
3	C	1578	LYS
3	C	1579	HIS
3	C	1580	TYR
3	C	1588	ASP
3	C	1611	GLU
3	C	1636	VAL
3	F	1407	ILE
3	F	1486	ASP
3	F	1494	GLU
3	F	1496	CYS
3	F	1497	PHE
3	F	1511	LEU
3	F	1519	VAL
3	F	1521	TYR
3	F	1533	SER
3	F	1542	ALA
3	F	1544	GLU
3	F	1554	VAL
3	F	1556	VAL
3	F	1557	GLY
3	F	1558	GLN
3	F	1587	SER
3	F	1590	TRP
3	F	1608	HIS
3	F	1616	GLN
3	F	1618	GLU
3	F	1619	GLU
3	F	1624	CYS
3	F	1625	GLN
1	D	537	CYS
1	A	290	GLN
3	C	1519	VAL
3	C	1547	ILE

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Mol	Chain	Res	Type
3	C	1556	VAL
3	C	1566	ILE
3	C	1635	VAL
4	M	51	ALA
4	P	51	ALA
3	F	1409	LYS
3	F	1410	TYR
3	F	1504	LYS
3	F	1505	VAL
3	F	1510	ARG
3	F	1518	GLY
3	F	1534	ASN
3	F	1543	ILE
3	F	1547	ILE
3	F	1570	GLU
3	F	1574	LEU
3	F	1610	PRO
3	F	1632	GLU
3	F	1635	VAL
1	D	290	GLN
1	A	534	LYS
2	B	853	LEU
2	B	883	THR
3	C	1410	TYR
3	C	1507	LEU
3	C	1544	GLU
3	C	1573	LYS
3	C	1608	HIS
2	E	853	LEU
2	E	883	THR
4	M	30	GLU
4	M	61	LYS
4	P	30	GLU
4	P	61	LYS
3	F	1509	GLU
3	F	1520	ASP
3	F	1569	ARG
3	F	1611	GLU
3	F	1640	PRO
1	D	534	LYS
3	C	1378	MET
3	C	1596	LEU

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Mol	Chain	Res	Type
3	C	1617	ASP
3	C	1624	CYS
3	F	1378	MET
3	F	1517	PRO
3	F	1595	ASN
3	F	1613	ASP
1	A	72	ARG
1	A	370	GLN
1	A	459	ARG
3	C	1494	GLU
3	C	1504	LYS
3	C	1517	PRO
3	C	1534	ASN
3	F	1535	ASP
3	F	1565	PRO
3	F	1631	THR
1	D	72	ARG
1	D	370	GLN
1	D	459	ARG
1	A	536	SER
3	C	1603	ASP
1	D	536	SER
1	A	289	VAL
3	F	1594	PRO
1	D	289	VAL
3	F	1636	VAL
1	A	381	GLY
1	D	381	GLY
1	A	359	GLY
1	A	616	VAL
1	D	359	GLY
1	D	616	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/567 (99%)	529 (94%)	34 (6%)	22	60
1	D	563/567 (99%)	529 (94%)	34 (6%)	22	60
2	B	172/191 (90%)	142 (83%)	30 (17%)	2	13
2	E	172/191 (90%)	142 (83%)	30 (17%)	2	13
3	C	266/309 (86%)	210 (79%)	56 (21%)	1	7
3	F	268/309 (87%)	202 (75%)	66 (25%)	1	4
4	M	76/79 (96%)	67 (88%)	9 (12%)	6	29
4	P	76/79 (96%)	66 (87%)	10 (13%)	5	24
All	All	2156/2292 (94%)	1887 (88%)	269 (12%)	5	26

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	30	ASP
1	A	61	MET
1	A	84	VAL
1	A	85	THR
1	A	137	VAL
1	A	149	GLU
1	A	155	GLN
1	A	157	SER
1	A	178	ASN
1	A	191	SER
1	A	213	ILE
1	A	215	GLU
1	A	217	THR
1	A	241	LYS
1	A	251	PHE
1	A	257	GLU
1	A	278	VAL
1	A	284	VAL
1	A	289	VAL
1	A	290	GLN
1	A	314	SER
1	A	320	GLU
1	A	410	SER
1	A	438	VAL
1	A	472	ILE
1	A	477	ARG

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Mol	Chain	Res	Type
1	A	502	ASP
1	A	515	LEU
1	A	534	LYS
1	A	535	ASP
1	A	548	SER
1	A	554	VAL
1	A	634	GLN
2	B	729	LEU
2	B	734	ILE
2	B	741	SER
2	B	757	LYS
2	B	765	SER
2	B	771	ILE
2	B	776	SER
2	B	786	SER
2	B	805	GLN
2	B	809	ILE
2	B	813	LEU
2	B	817	VAL
2	B	818	VAL
2	B	834	GLN
2	B	836	GLN
2	B	841	ARG
2	B	844	LEU
2	B	861	GLN
2	B	864	VAL
2	B	869	LYS
2	B	871	SER
2	B	873	SER
2	B	877	VAL
2	B	882	LYS
2	B	887	GLU
2	B	890	VAL
2	B	899	ILE
2	B	903	VAL
2	B	907	LEU
2	B	912	GLU
3	C	1337	ASN
3	C	1342	LYS
3	C	1344	THR
3	C	1361	THR
3	C	1362	MET

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Mol	Chain	Res	Type
3	C	1378	MET
3	C	1387	THR
3	C	1389	PHE
3	C	1393	THR
3	C	1394	ASP
3	C	1395	ASP
3	C	1406	TYR
3	C	1413	ASP
3	C	1414	LYS
3	C	1416	PHE
3	C	1418	ASP
3	C	1419	ARG
3	C	1421	THR
3	C	1422	LEU
3	C	1430	SER
3	C	1433	GLU
3	C	1437	LEU
3	C	1447	VAL
3	C	1450	ILE
3	C	1468	THR
3	C	1469	ARG
3	C	1479	LYS
3	C	1484	CYS
3	C	1494	GLU
3	C	1495	ASN
3	C	1503	ASP
3	C	1504	LYS
3	C	1505	VAL
3	C	1507	LEU
3	C	1512	ASP
3	C	1529	LYS
3	C	1532	LEU
3	C	1535	ASP
3	C	1551	SER
3	C	1554	VAL
3	C	1567	LYS
3	C	1569	ARG
3	C	1573	LYS
3	C	1574	LEU
3	C	1578	LYS
3	C	1580	TYR
3	C	1581	LEU

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Mol	Chain	Res	Type
3	C	1582	MET
3	C	1587	SER
3	C	1590	TRP
3	C	1595	ASN
3	C	1600	ILE
3	C	1603	ASP
3	C	1615	CYS
3	C	1616	GLN
3	C	1624	CYS
2	E	729	LEU
2	E	734	ILE
2	E	741	SER
2	E	757	LYS
2	E	765	SER
2	E	771	ILE
2	E	776	SER
2	E	786	SER
2	E	805	GLN
2	E	809	ILE
2	E	813	LEU
2	E	817	VAL
2	E	818	VAL
2	E	834	GLN
2	E	836	GLN
2	E	841	ARG
2	E	844	LEU
2	E	861	GLN
2	E	864	VAL
2	E	869	LYS
2	E	871	SER
2	E	873	SER
2	E	877	VAL
2	E	882	LYS
2	E	887	GLU
2	E	890	VAL
2	E	899	ILE
2	E	903	VAL
2	E	907	LEU
2	E	912	GLU
4	M	7	SER
4	M	8	ASN
4	M	21	SER

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Mol	Chain	Res	Type
4	M	25	GLU
4	M	26	LEU
4	M	31	LEU
4	M	38	THR
4	M	59	ASP
4	M	78	ASP
4	P	7	SER
4	P	8	ASN
4	P	21	SER
4	P	25	GLU
4	P	26	LEU
4	P	31	LEU
4	P	36	LEU
4	P	38	THR
4	P	59	ASP
4	P	78	ASP
3	F	1337	ASN
3	F	1342	LYS
3	F	1344	THR
3	F	1361	THR
3	F	1362	MET
3	F	1378	MET
3	F	1387	THR
3	F	1389	PHE
3	F	1393	THR
3	F	1394	ASP
3	F	1395	ASP
3	F	1408	SER
3	F	1413	ASP
3	F	1414	LYS
3	F	1416	PHE
3	F	1418	ASP
3	F	1419	ARG
3	F	1421	THR
3	F	1422	LEU
3	F	1430	SER
3	F	1433	GLU
3	F	1437	LEU
3	F	1447	VAL
3	F	1450	ILE
3	F	1468	THR
3	F	1469	ARG

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Mol	Chain	Res	Type
3	F	1479	LYS
3	F	1484	CYS
3	F	1493	GLU
3	F	1494	GLU
3	F	1495	ASN
3	F	1497	PHE
3	F	1498	ILE
3	F	1510	ARG
3	F	1522	VAL
3	F	1525	THR
3	F	1526	ARG
3	F	1528	VAL
3	F	1534	ASN
3	F	1541	MET
3	F	1551	SER
3	F	1552	ASP
3	F	1559	GLN
3	F	1560	ARG
3	F	1570	GLU
3	F	1572	LEU
3	F	1573	LYS
3	F	1574	LEU
3	F	1577	LYS
3	F	1578	LYS
3	F	1586	SER
3	F	1590	TRP
3	F	1596	LEU
3	F	1599	ILE
3	F	1600	ILE
3	F	1602	LYS
3	F	1611	GLU
3	F	1614	GLU
3	F	1619	GLU
3	F	1620	ASN
3	F	1622	LYS
3	F	1623	GLN
3	F	1627	LEU
3	F	1632	GLU
3	F	1634	MET
3	F	1639	CYS
1	D	6	ILE
1	D	30	ASP

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Mol	Chain	Res	Type
1	D	61	MET
1	D	84	VAL
1	D	85	THR
1	D	137	VAL
1	D	149	GLU
1	D	155	GLN
1	D	157	SER
1	D	178	ASN
1	D	191	SER
1	D	213	ILE
1	D	215	GLU
1	D	217	THR
1	D	241	LYS
1	D	251	PHE
1	D	257	GLU
1	D	278	VAL
1	D	284	VAL
1	D	289	VAL
1	D	290	GLN
1	D	314	SER
1	D	320	GLU
1	D	410	SER
1	D	438	VAL
1	D	472	ILE
1	D	477	ARG
1	D	502	ASP
1	D	515	LEU
1	D	534	LYS
1	D	535	ASP
1	D	548	SER
1	D	554	VAL
1	D	634	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	291	ASN
1	A	392	HIS
1	A	634	GLN
3	C	1495	ASN
3	C	1531	GLN

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Mol	Chain	Res	Type
3	C	1608	HIS
3	C	1616	GLN
3	C	1620	ASN
3	C	1641	ASN
4	P	8	ASN
3	F	1495	ASN
3	F	1534	ASN
3	F	1545	GLN
3	F	1616	GLN
3	F	1620	ASN
1	D	132	HIS
1	D	291	ASN
1	D	392	HIS
1	D	634	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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	0.43	0	15,19,21	1.49	1 (6%)
5	NAG	D	646	-	14,14,15	0.42	0	15,19,21	1.49	1 (6%)

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	-	-	0/6/23/26	0/1/1/1
5	NAG	D	646	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	646	NAG	C1-O5-C5	4.80	118.78	112.17
5	A	646	NAG	C1-O5-C5	4.83	118.82	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	646	NAG	4	0
5	D	646	NAG	3	0

## 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<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%)	-0.08	10 (1%) 72 64	18, 53, 106, 172	0
1	D	641/645 (99%)	-0.03	11 (1%) 70 62	18, 53, 106, 172	0
2	B	184/206 (89%)	-0.36	0 100 100	19, 50, 80, 114	0
2	E	184/206 (89%)	-0.31	0 100 100	25, 57, 87, 120	0
3	C	293/343 (85%)	0.28	24 (8%) 12 12	35, 87, 198, 230	0
3	F	295/343 (86%)	0.41	22 (7%) 15 14	31, 93, 143, 194	0
4	M	84/88 (95%)	-0.23	1 (1%) 79 71	48, 68, 105, 175	0
4	P	84/88 (95%)	-0.20	2 (2%) 59 50	43, 65, 101, 184	0
All	All	2406/2564 (93%)	-0.01	70 (2%) 52 43	18, 63, 125, 230	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1613	ASP	8.6
3	C	1624	CYS	7.4
4	P	85	TYR	6.1
3	F	1640	PRO	5.8
3	C	1610	PRO	5.3
3	C	1616	GLN	5.3
1	A	645	ALA	5.0
3	C	1617	ASP	4.8
3	C	1612	GLU	4.5
3	F	1359	LYS	4.4
3	C	1614	GLU	4.4
1	D	548	SER	4.0
4	M	85	TYR	3.9
3	F	1347	PRO	3.8
4	P	2	THR	3.8
1	A	48	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	49	SER	3.6
3	F	1559	GLN	3.6
3	F	1533	SER	3.5
1	D	87	GLN	3.3
3	C	1618	GLU	3.3
3	C	1619	GLU	3.3
3	F	1534	ASN	3.2
3	F	1596	LEU	3.2
3	F	1593	LYS	3.2
3	F	1349	PRO	3.2
3	C	1557	GLY	3.1
1	A	73	GLU	3.1
3	F	1592	GLU	3.1
3	C	1611	GLU	3.0
3	C	1640	PRO	2.8
1	D	518	ALA	2.8
3	C	1534	ASN	2.8
1	A	54	LEU	2.8
3	F	1641	ASN	2.8
1	D	48	SER	2.7
1	A	78	LYS	2.6
1	A	548	SER	2.6
3	C	1632	GLU	2.6
1	D	1	SER	2.6
3	C	1594	PRO	2.5
3	F	1391	PRO	2.5
3	C	1620	ASN	2.5
3	F	1551	SER	2.5
3	C	1503	ASP	2.5
1	D	52	THR	2.4
3	F	1476	GLU	2.4
1	A	644	ALA	2.4
3	C	1641	ASN	2.4
3	F	1360	ASN	2.3
3	F	1346	LYS	2.3
3	F	1488	LEU	2.3
1	A	79	GLY	2.3
1	A	461	HIS	2.3
1	D	92	THR	2.3
3	C	1627	LEU	2.3
3	F	1417	SER	2.2
1	D	49	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	1536	PHE	2.2
3	F	1440	LYS	2.2
3	C	1535	ASP	2.2
3	C	1559	GLN	2.2
3	C	1349	PRO	2.2
1	D	461	HIS	2.1
3	F	1443	GLN	2.1
3	F	1392	ASP	2.1
3	C	1623	GLN	2.1
1	D	489	GLY	2.1
3	F	1387	THR	2.1
1	D	36	THR	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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	D	646	14/15	0.70	0.32	-	62,87,108,108	0
5	NAG	A	646	14/15	0.74	0.34	-	62,87,108,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.