



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 PM UTC

PDB ID : 3OHX / pdb_00003ohx
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 : 2010-08-18
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

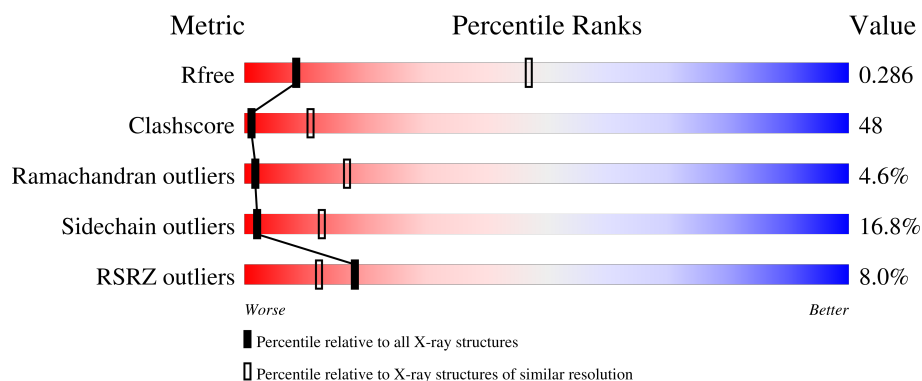
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	645	7% 44% 48% 7% ..
1	D	645	4% 43% 49% 6% ..
2	B	206	0% 36% 37% 16% 11%
2	E	206	2% 34% 40% 15% 11%
3	C	343	13% 24% 42% 17% 15%

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Mol	Chain	Length	Quality of chain
3	F	343	20%20%36%24%6%14%
4	M	88	38%47%11%5%
4	P	88	%38%47%11%5%

2 Entry composition

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			

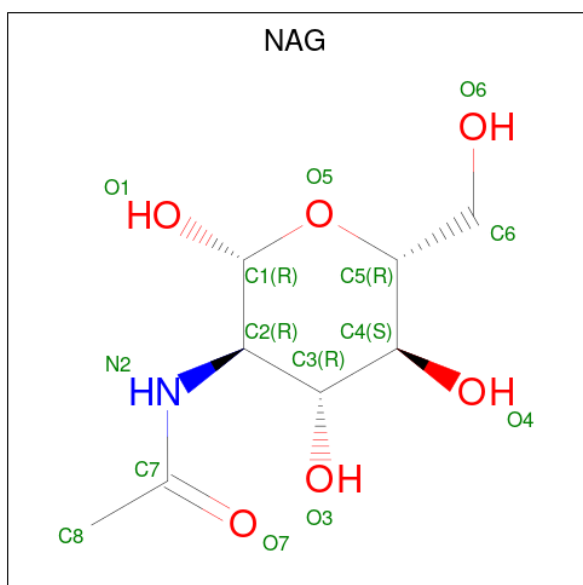
- Molecule 4 is a protein called Staphylococcal complement inhibitor.

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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

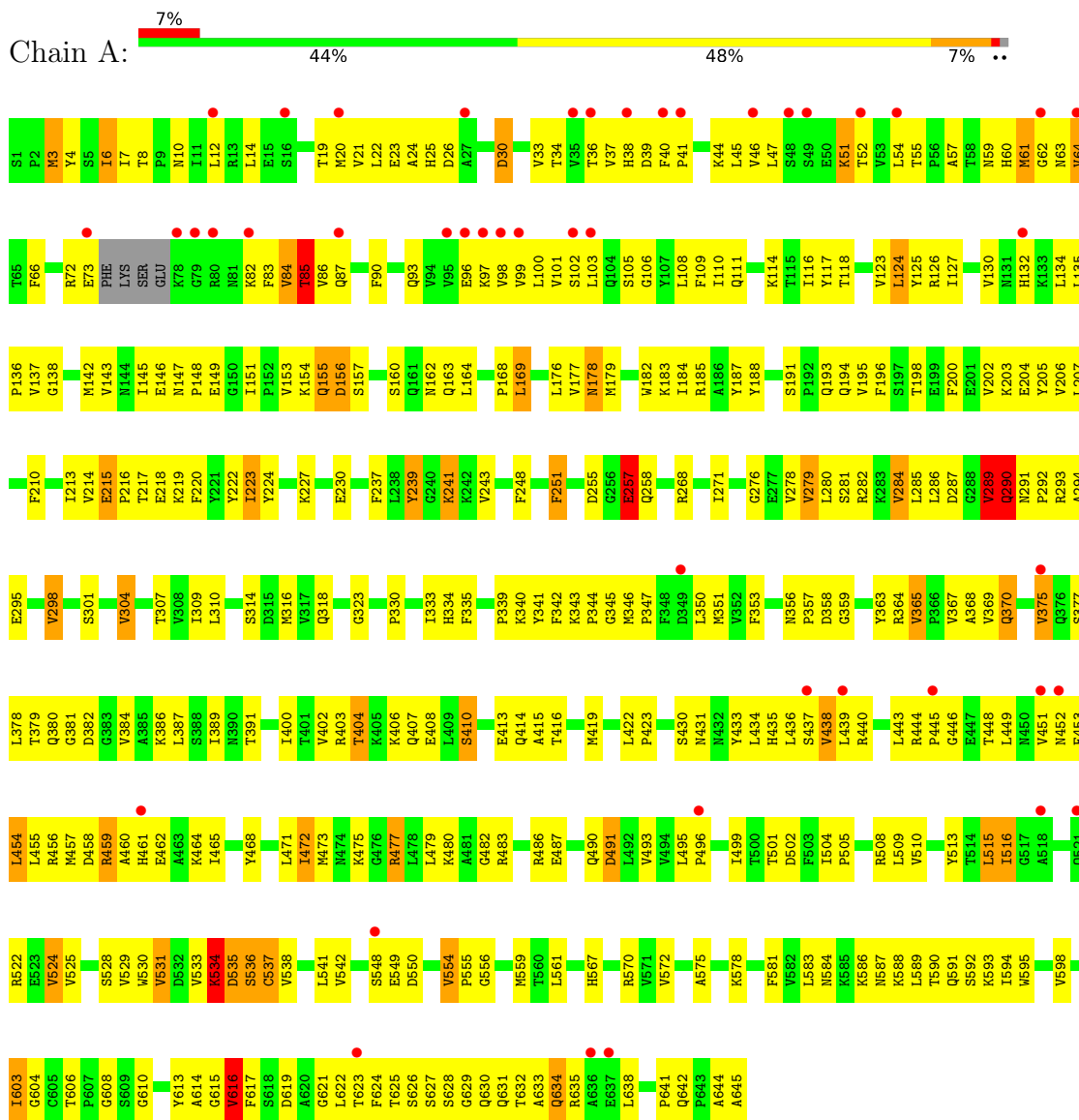


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

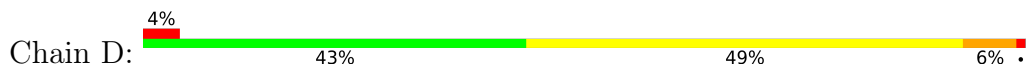
3 Residue-property plots

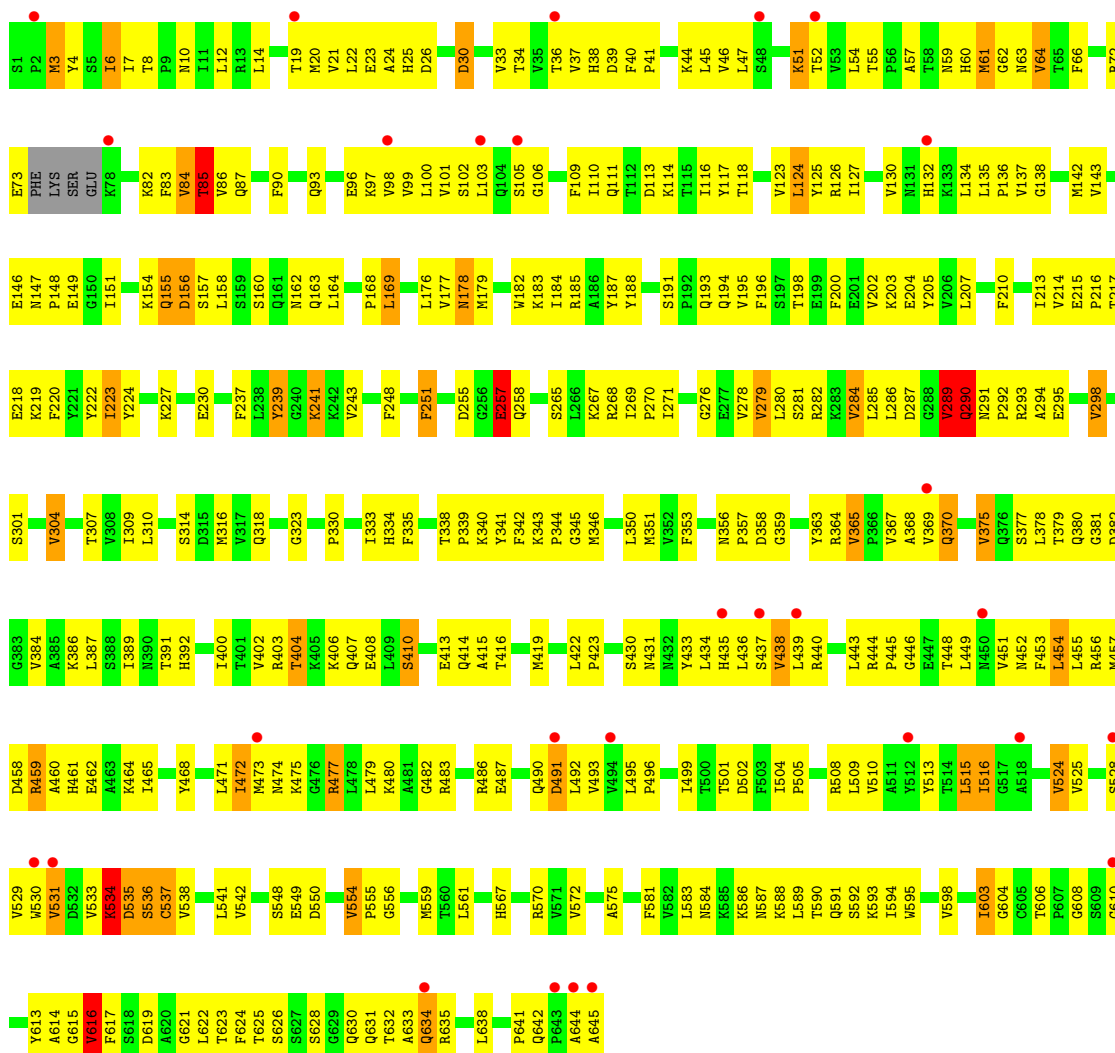
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

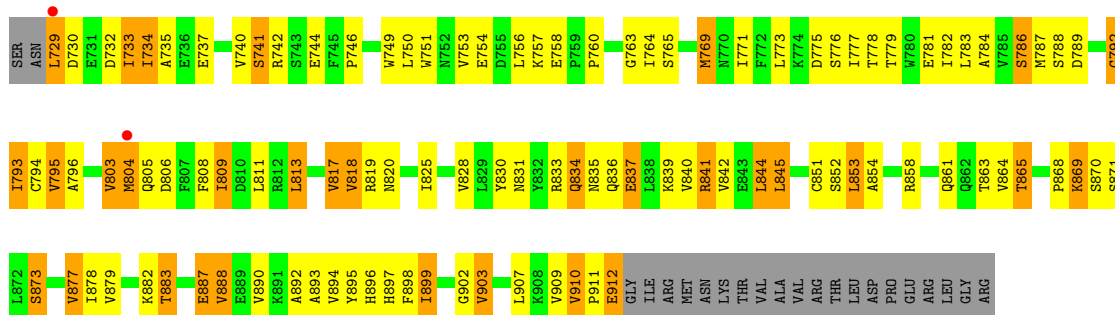


• Molecule 1: Complement C3



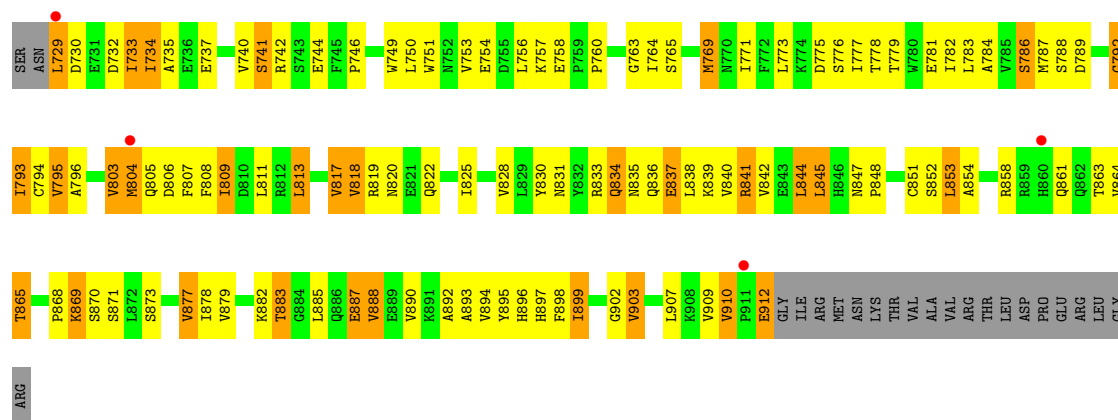


• Molecule 2: Complement C3

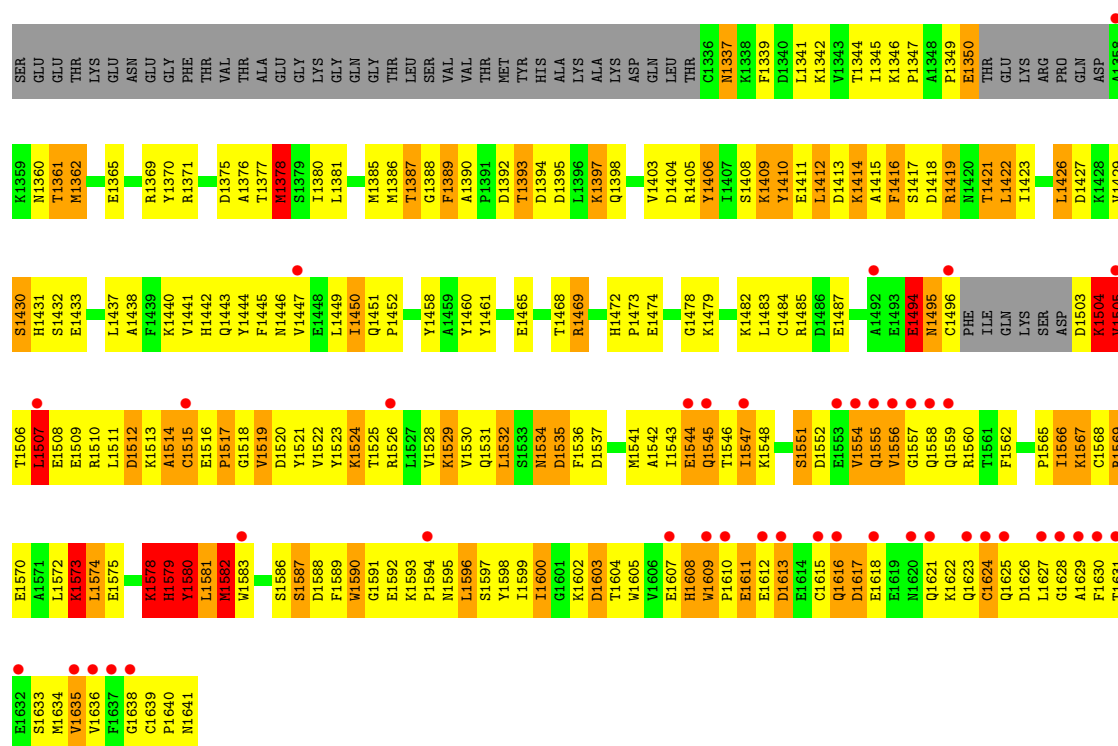
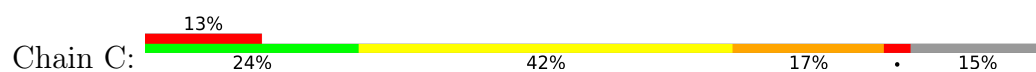


• Molecule 2: Complement C3

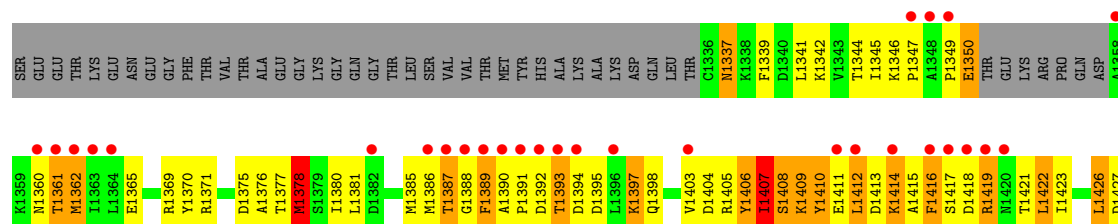
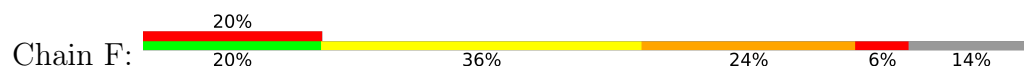


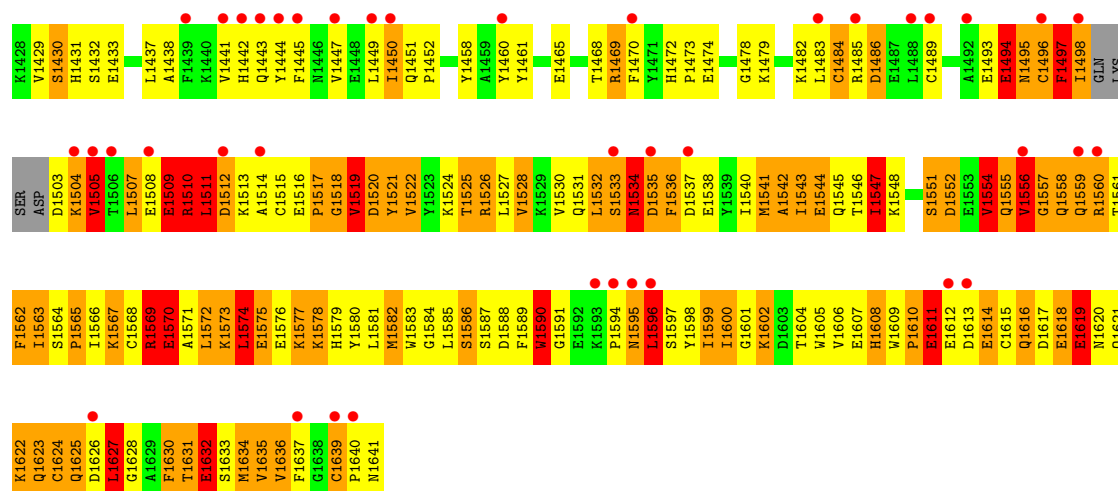


• Molecule 3: Complement C3

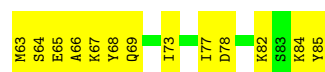


• Molecule 3: Complement C3

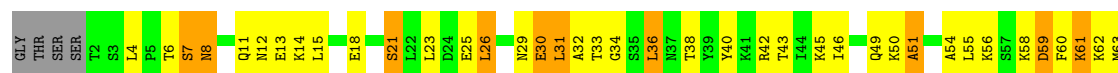




• Molecule 4: Staphylococcal complement inhibitor



• 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, α , β , γ	231.16Å 231.50Å 68.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.27 – 3.50 46.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (46.27-3.50) 93.1 (46.27-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.274 , 0.294 0.268 , 0.286	Depositor DCC
R_{free} test set	2017 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

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	0.57	0/5089	0.96	11/6916 (0.2%)
1	D	0.57	0/5089	0.96	11/6916 (0.2%)
2	B	0.63	0/1520	0.97	5/2066 (0.2%)
2	E	0.63	0/1520	0.97	5/2066 (0.2%)
3	C	0.63	1/2422 (0.0%)	1.04	9/3264 (0.3%)
3	F	0.70	0/2442	1.10	17/3291 (0.5%)
4	M	0.51	0/690	0.85	1/923 (0.1%)
4	P	0.51	0/690	0.84	1/923 (0.1%)
All	All	0.60	1/19462 (0.0%)	0.98	60/26365 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1515	CYS	CA-C	5.41	1.60	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1536	PHE	N-CA-C	-10.61	97.36	110.41
3	F	1512	ASP	N-CA-C	-9.59	101.13	113.12
3	C	1613	ASP	N-CA-C	-8.42	103.03	113.38
3	C	1582	MET	N-CA-C	8.14	120.96	108.42
3	F	1630	PHE	N-CA-C	-6.66	104.07	112.93
1	D	151	ILE	N-CA-C	6.65	114.14	107.55
1	A	151	ILE	N-CA-C	6.64	114.12	107.55
3	F	1505	VAL	N-CA-C	6.61	123.09	109.34
1	A	279	VAL	N-CA-C	6.60	118.22	108.45
1	D	279	VAL	N-CA-C	6.59	118.21	108.45
1	D	239	TYR	N-CA-C	-6.56	100.60	110.24
1	A	239	TYR	N-CA-C	-6.56	100.60	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1524	LYS	N-CA-C	-6.49	100.85	110.46
3	F	1562	PHE	N-CA-C	6.41	119.39	109.07
2	E	733	ILE	N-CA-C	6.36	116.78	107.75
2	B	733	ILE	N-CA-C	6.33	116.74	107.75
3	C	1609	TRP	N-CA-C	-6.31	94.98	107.91
2	B	887	GLU	N-CA-C	6.01	118.19	108.34
2	E	887	GLU	N-CA-C	6.01	118.19	108.34
3	F	1627	LEU	N-CA-C	-5.99	104.09	111.33
3	C	1514	ALA	N-CA-C	5.98	118.69	111.40
3	F	1407	ILE	CB-CA-C	-5.84	101.71	111.29
1	D	257	GLU	N-CA-C	-5.84	106.00	114.12
2	E	804	MET	N-CA-C	5.83	115.80	108.45
2	B	804	MET	N-CA-C	5.83	115.79	108.45
1	A	257	GLU	N-CA-C	-5.82	106.02	114.12
3	C	1592	GLU	N-CA-C	5.82	118.70	109.50
3	F	1575	GLU	N-CA-C	5.79	117.34	108.42
3	C	1409	LYS	N-CA-C	-5.78	103.97	111.02
3	F	1596	LEU	N-CA-C	5.73	115.96	107.88
1	D	531	VAL	O-C-N	-5.65	117.88	122.97
1	A	531	VAL	O-C-N	-5.65	117.89	122.97
1	D	333	ILE	N-CA-C	5.64	116.11	107.77
1	A	333	ILE	N-CA-C	5.63	116.10	107.77
3	F	1567	LYS	CA-C-N	-5.62	109.66	121.64
3	F	1567	LYS	C-N-CA	-5.62	109.66	121.64
3	F	1556	VAL	N-CA-C	5.62	121.03	109.34
3	F	1511	LEU	N-CA-C	-5.58	98.92	110.80
1	A	85	THR	CB-CA-C	-5.48	102.03	111.23
1	D	85	THR	CB-CA-C	-5.47	102.03	111.23
3	C	1557	GLY	N-CA-C	-5.41	108.26	115.40
4	M	46	ILE	CB-CA-C	-5.36	104.82	112.22
3	F	1569	ARG	N-CA-C	-5.35	99.40	110.80
4	P	46	ILE	CB-CA-C	-5.35	104.83	112.22
1	D	491	ASP	N-CA-C	-5.33	107.33	113.88
1	A	491	ASP	N-CA-C	-5.33	107.33	113.88
3	F	1406	TYR	N-CA-C	5.25	116.27	108.60
1	A	356	ASN	CA-C-N	-5.23	113.30	119.84
1	A	356	ASN	C-N-CA	-5.23	113.30	119.84
1	D	356	ASN	CA-C-N	-5.23	113.31	119.84
1	D	356	ASN	C-N-CA	-5.23	113.31	119.84
2	E	792	GLY	N-CA-C	5.21	121.29	112.22
2	B	792	GLY	N-CA-C	5.19	121.24	112.22
2	E	803	VAL	CB-CA-C	-5.12	104.76	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1478	GLY	N-CA-C	-5.09	107.06	114.90
3	F	1478	GLY	N-CA-C	-5.08	107.07	114.90
2	B	803	VAL	CB-CA-C	-5.07	104.83	110.96
1	A	289	VAL	N-CA-C	-5.04	98.86	109.34
1	D	289	VAL	N-CA-C	-5.03	98.88	109.34
3	F	1582	MET	N-CA-C	5.02	117.33	108.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4989	0	5051	387	0
1	D	4989	0	5051	391	0
2	B	1488	0	1512	126	0
2	E	1488	0	1512	123	0
3	C	2377	0	2279	333	0
3	F	2396	0	2299	490	0
4	M	682	0	697	62	0
4	P	682	0	697	56	0
5	A	14	0	13	4	0
5	D	14	0	13	3	0
All	All	19119	0	19124	1844	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 48.

All (1844) 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	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1581:LEU:HD12	3:C:1581:LEU:C	1.66	1.16
1:D:289:VAL:C	1:D:290:GLN:HG2	1.71	1.16
3:F:1507:LEU:HB3	3:F:1510:ARG:NH2	1.59	1.16
2:B:912:GLU:H	2:B:912:GLU:CD	1.52	1.15
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:1515:CYS:SG	3:C:1640:PRO:HD2	1.90	1.11
3:F:1558:GLN:C	3:F:1559:GLN:HG3	1.70	1.11
3:C:1349:PRO:O	3:C:1350:GLU:HB2	1.47	1.11
3:F:1558:GLN:O	3:F:1559:GLN:HG3	1.49	1.11
1:A:289:VAL:C	1:A:290:GLN:HG2	1.71	1.10
3:F:1497:PHE:CZ	3:F:1498:ILE:CG1	2.34	1.10
3:F:1507:LEU:CB	3:F:1510:ARG:HH21	1.62	1.10
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:1378:MET:HE3	1:D:268:ARG:HB2	1.30	1.08
3:F:1533:SER:HB2	3:F:1537:ASP:HA	1.19	1.08
3:F:1554:VAL:HG23	3:F:1558:GLN:OE1	1.52	1.08
1:D:590:THR:HG22	1:D:592:SER:H	1.13	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
2:E:912:GLU:H	2:E:912:GLU:CD	1.52	1.06
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:1569:ARG:HG2	3:F:1570:GLU:OE1	0.89	1.06
3:F:1574:LEU:HD23	3:F:1574:LEU:H	1.05	1.06
1:A:590:THR:HG22	1:A:592:SER:H	1.13	1.06
3:F:1572:LEU:C	3:F:1573:LYS:HG3	1.80	1.06
3:C:1507:LEU:HD21	3:C:1629:ALA:HB3	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1571:ALA:C	3:F:1572:LEU:CD2	2.29	1.04
3:F:1497:PHE:C	3:F:1497:PHE:CD2	2.34	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
2:E:841:ARG:HG2	2:E:841:ARG:HH11	1.22	1.02
3:F:1572:LEU:O	3:F:1573:LYS:CG	2.06	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
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:F:1572:LEU:O	3:F:1573:LYS:HG3	1.58	1.01
3:C:1360:ASN:ND2	3:C:1443:GLN:HB3	1.75	1.01
3:F:1574:LEU:H	3:F:1574:LEU:CD2	1.61	1.01
3:F:1360:ASN:ND2	3:F:1443:GLN:HB3	1.75	1.00
2:B:841:ARG:HH11	2:B:841:ARG:HG2	1.23	1.00
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
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:F:1595:ASN:C	3:F:1596:LEU:HG	1.88	0.97
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:HA	3:C:1578:LYS:HE3	1.48	0.94
3:C:1609:TRP:CZ3	3:C:1627:LEU:HD22	2.02	0.94
3:F:1509:GLU:HG2	3:F:1510:ARG:H	1.29	0.94
1:D:38:HIS:O	1:D:85:THR:HG23	1.67	0.94
2:E:853:LEU:HD11	3:F:1451:GLN:HB2	0.97	0.94
3:C:1495:ASN:H	3:C:1495:ASN:HD22	0.97	0.94
3:C:1578:LYS:CD	3:C:1608:HIS:HE1	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1495:ASN:H	3:C:1495:ASN:ND2	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
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:F:1535:ASP:CG	3:F:1536:PHE:H	1.77	0.92
3:F:1542:ALA:C	3:F:1543:ILE:HD12	1.94	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:1497:PHE:C	3:F:1497:PHE:HD2	1.74	0.92
3:F:1378:MET:CE	1:D:268:ARG:HB2	2.00	0.91
3:F:1495:ASN:ND2	3:F:1495:ASN:H	1.59	0.91
3:C:1609:TRP:CE3	3:C:1627:LEU:HD22	2.05	0.91
3:F:1590:TRP:HA	3:F:1590:TRP:CE3	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
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
3:F:1497:PHE:CD2	3:F:1498:ILE:CG1	2.54	0.90
1:D:634:GLN:HE21	1:D:635:ARG:H	0.91	0.90
2:B:912:GLU:CD	2:B:912:GLU:N	2.30	0.89
3:F:1450:ILE:HG13	3:F:1450:ILE:O	1.72	0.89
3:F:1519:VAL:H	3:F:1585:LEU:HD21	1.37	0.89
1:D:223:ILE:HD11	1:D:298:VAL:HG23	1.53	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
3:F:1543:ILE:CD1	3:F:1559:GLN:HA	2.02	0.89
1:D:634:GLN:NE2	1:D:635:ARG:H	1.66	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:H	3:C:1580:TYR:HD2	1.01	0.89
3:F:1572:LEU:HD22	3:F:1572:LEU:N	1.84	0.89
1:D:10:ASN:HB3	1:D:635:ARG:HH11	1.37	0.89
1:A:289:VAL:C	1:A:290:GLN:CG	2.44	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1504:LYS:C	3:F:1505:VAL:HG22	1.96	0.89
3:F:1569:ARG:HG2	3:F:1570:GLU:CD	1.98	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:HD22	3:F:1495:ASN:N	1.60	0.88
1:A:346:MET:O	1:A:391:THR:HG22	1.74	0.88
1:D:289:VAL:C	1:D:290:GLN:CG	2.44	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:F:1572:LEU:C	3:F:1574:LEU:HD23	1.99	0.88
3:C:1532:LEU:HB3	3:C:1569:ARG:NH1	1.90	0.87
3:F:1522:VAL:HG13	3:F:1583:TRP:HB3	1.55	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
3:F:1495:ASN:H	3:F:1495:ASN:HD22	0.90	0.86
3:F:1497:PHE:CD2	3:F:1498:ILE:N	2.42	0.86
3:F:1515:CYS:SG	3:F:1634:MET:HE1	2.14	0.86
3:F:1524:LYS:HD2	3:F:1525:THR:H	1.38	0.86
1:D:346:MET:O	1:D:391:THR:HG22	1.74	0.86
3:F:1574:LEU:N	3:F:1574:LEU:CD2	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:1526:ARG:HH21	3:F:1544:GLU:CD	1.84	0.86
3:F:1590:TRP:HA	3:F:1590:TRP:HE3	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:HA	3:F:1494:GLU:OE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1536:PHE:CD2	3:F:1566:ILE:HG12	2.11	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
2:B:853:LEU:CD1	3:C:1451:GLN:HB2	2.08	0.83
1:D:400:ILE:HD13	1:D:419:MET:HE3	1.60	0.83
3:F:1571:ALA:O	3:F:1572:LEU:HD22	1.77	0.83
3:F:1533:SER:CB	3:F:1536:PHE:O	2.27	0.82
1:D:590:THR:HB	1:D:593:LYS:HG3	1.61	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:1406:TYR:C	3:F:1407:ILE:CG1	2.53	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
3:F:1497:PHE:CE1	3:F:1498:ILE:CG1	2.62	0.81
1:D:8:THR:HG22	1:D:20:MET:HB2	1.60	0.81
3:C:1445:PHE:HE1	4:P:6:THR:HA	1.42	0.81
1:D:55:THR:HG22	1:D:57:ALA:H	1.45	0.81
3:F:1408:SER:OG	3:F:1410:TYR:HB3	1.81	0.81
3:F:1534:ASN:C	3:F:1534:ASN:HD22	1.85	0.81
1:A:400:ILE:HD13	1:A:419:MET:HE3	1.60	0.80
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
3:F:1572:LEU:C	3:F:1574:LEU:CD2	2.54	0.80
3:F:1509:GLU:O	3:F:1510:ARG:C	2.24	0.80
3:F:1572:LEU:O	3:F:1573:LYS:HD2	1.79	0.80
1:D:289:VAL:O	1:D:290:GLN:CG	2.30	0.80
2:E:912:GLU:CD	2:E:912:GLU:N	2.30	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
3:F:1525:THR:OG1	3:F:1541:MET:HE3	1.82	0.79
1:A:289:VAL:O	1:A:290:GLN:CG	2.30	0.79
3:F:1507:LEU:HD23	3:F:1507:LEU:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1569:ARG:CB	3:F:1570:GLU:OE1	2.30	0.79
3:F:1614:GLU:HG3	3:F:1614:GLU:O	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:1534:ASN:C	3:F:1534:ASN:ND2	2.40	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: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:HG2	2:B:841:ARG:NH1	1.95	0.78
3:F:1337:ASN:O	3:F:1371:ARG:HD2	1.84	0.78
4:M:4:LEU:HD13	3:F:1444:TYR:C	2.09	0.78
3:F:1536:PHE:HD2	3:F:1566:ILE:HG12	1.49	0.78
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:1573:LYS:HD3	3:F:1573:LYS:C	2.10	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
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:98:VAL:O	1:A:634:GLN:CG	2.33	0.76
1:A:365:VAL:HG13	1:A:379:THR:OG1	1.85	0.76
3:C:1548:LYS:HG2	3:C:1548:LYS:O	1.84	0.76
1:A:289:VAL:O	1:A:290:GLN:CD	2.29	0.76
1:D:22:LEU:HD11	1:D:64:VAL:HG23	1.67	0.76
1:D:289:VAL:O	1:D:290:GLN:CD	2.29	0.76
3:C:1506:THR:H	3:C:1509:GLU:HG2	1.49	0.76
1:A:98:VAL:O	1:A:634:GLN:CD	2.29	0.75
2:B:733:ILE:HG12	2:B:734:ILE:N	2.01	0.75
3:C:1581:LEU:C	3:C:1581:LEU:CD1	2.30	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:733:ILE:HG12	2:E:734:ILE:N	2.01	0.75
3:F:1483:LEU:CD1	3:F:1590:TRP:CZ2	2.69	0.75
3:F:1521:TYR:CE2	3:F:1584:GLY:N	2.55	0.75
1:D:98:VAL:O	1:D:634:GLN:CD	2.29	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
3:F:1521:TYR:HE2	3:F:1584:GLY:CA	2.00	0.74
3:F:1568:CYS:O	3:F:1569:ARG:C	2.30	0.74
1:D:117:TYR:CZ	1:D:123:VAL:HG13	2.22	0.74
1:D:365:VAL:HG13	1:D:379:THR:OG1	1.85	0.74
4:M:10:TYR:CE2	3:F:1417:SER:OG	2.34	0.74
1:D:610:GLY:HA3	1:D:616:VAL:N	2.03	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:F:1569:ARG:C	3:F:1570:GLU:OE1	2.30	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
3:F:1535:ASP:CG	3:F:1536:PHE:N	2.45	0.74
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
1:A:369:VAL:HG12	1:A:370:GLN:N	2.03	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
3:F:1497:PHE:CD2	3:F:1498:ILE:HG12	2.23	0.73
1:D:12:LEU:HB2	1:D:101:VAL:HG22	1.70	0.73
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:1605:TRP:C	3:F:1605:TRP:CD1	2.67	0.72
3:C:1504:LYS:HD3	3:C:1504:LYS:H	1.55	0.72
3:C:1504:LYS:HE2	3:C:1506:THR:HG23	1.70	0.72
3:F:1569:ARG:C	3:F:1570:GLU:CG	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1445:PHE:CE1	4:P:7:SER:N	2.58	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
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
3:C:1506:THR:C	3:C:1508:GLU:H	1.96	0.71
3:F:1388:GLY:O	3:F:1443:GLN:HA	1.89	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
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
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
1:A:257:GLU:CD	1:A:257:GLU:N	2.49	0.70
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:1508:GLU:O	3:C:1512:ASP:CG	2.34	0.70
3:C:1605:TRP:HE1	3:C:1607:GLU:HB2	1.56	0.70
3:F:1497:PHE:O	3:F:1498:ILE:C	2.33	0.70
3:F:1522:VAL:HG23	3:F:1548:LYS:HB3	1.71	0.70
1:A:85:THR:O	1:A:85:THR:OG1	2.03	0.70
1:A:281:SER:OG	1:A:284:VAL:HG23	1.90	0.70
3:F:1558:GLN:C	3:F:1559:GLN:CG	2.55	0.70
1:D:257:GLU:N	1:D:257:GLU:CD	2.49	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
1:D:6:ILE:HD11	1:D:20:MET:HE3	1.73	0.70
3:C:1526:ARG:CZ	3:C:1542:ALA:CB	2.70	0.70
1:D:85:THR:O	1:D:85:THR:OG1	2.03	0.70
1:D:223:ILE:CD1	1:D:298:VAL:HG23	2.21	0.70
1:D:237:PHE:CE2	1:D:243:VAL:HG22	2.27	0.70
1:A:237:PHE:CE2	1:A:243:VAL:HG22	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:P:36:LEU:HB3	4:P:40:TYR:CD2	2.27	0.69
3:F:1574:LEU:HB3	3:F:1580:TYR:CZ	2.26	0.69
1:D:504:ILE:HG12	1:D:533:VAL:HG11	1.73	0.69
1:A:504:ILE:HG12	1:A:533:VAL:HG11	1.73	0.69
3:F:1571:ALA:CA	3:F:1572:LEU:HD22	2.22	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
1:A:6:ILE:HD11	1:A:20:MET:HE3	1.73	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:1526:ARG:CG	3:C:1542:ALA:HB3	2.06	0.69
3:C:1535:ASP:HB2	3:C:1536:PHE:HD2	1.57	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:HG23	3:F:1530:VAL:O	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:38:HIS:CE1	1:A:45:LEU:HD12	2.28	0.68
1:A:223:ILE:CD1	1:A:298:VAL:HG23	2.21	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
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
2:E:781:GLU:OE2	1:D:588:LYS:NZ	2.27	0.68
1:D:330:PRO:O	1:D:357:PRO:HD3	1.93	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:1445:PHE:CE1	4:P:6:THR:C	2.72	0.68
3:C:1485:ARG:NH2	3:C:1591:GLY:HA3	2.09	0.68
3:F:1507:LEU:HD21	3:F:1622:LYS:HE3	1.76	0.68
3:F:1521:TYR:CG	3:F:1521:TYR:O	2.47	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1557:GLY:O	3:F:1558:GLN:O	2.12	0.68
3:C:1562:PHE:CE2	3:C:1582:MET:HE2	2.29	0.67
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:O	3:F:1570:GLU:HB2	1.93	0.67
3:F:1496:CYS:HA	3:F:1601:GLY:O	1.94	0.67
3:F:1568:CYS:C	3:F:1569:ARG:O	2.37	0.67
1:D:19:THR:HA	1:D:64:VAL: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:1551:SER:CB	3:C:1593:LYS:HZ1	2.06	0.67
3:C:1573:LYS:O	3:C:1573:LYS:HD2	1.95	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:F:1573:LYS:HB2	3:F:1573:LYS:HZ2	1.58	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:1406:TYR:C	3:F:1407:ILE:HG13	2.19	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
1:D:130:VAL:HG12	1:D:136:PRO:HA	1.78	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
3:F:1507:LEU:HD23	3:F:1507:LEU:N	2.10	0.66
1:D:407:GLN:O	1:D:408:GLU:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1445:PHE:HE1	4:P:6:THR:C	2.03	0.65
3:C:1581:LEU:CD1	3:C:1582:MET:N	2.41	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
1:D:624:PHE:O	1:D:631:GLN:HA	1.97	0.65
2:B:795:VAL:O	2:B:795:VAL:HG12	1.96	0.65
4:P:84:LYS:O	4:P:84:LYS:HG3	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
3:F:1532:LEU:CA	3:F:1569:ARG:HH12	2.08	0.65
1:D:8:THR:HG22	1:D:20:MET:CB	2.26	0.65
1:A:130:VAL:HG12	1:A:136:PRO:HA	1.78	0.65
1:D:554:VAL:HG13	1:D:555:PRO:HD2	1.78	0.65
2:B:839:LYS:NZ	4:P:12:ASN:OD1	2.30	0.65
3:C:1416:PHE:C	3:C:1416:PHE:CD2	2.75	0.65
4:M:84:LYS:O	4:M:84:LYS:HG3	1.96	0.65
3:F:1497:PHE:CE2	3:F:1498:ILE:CB	2.80	0.65
1:D:216:PRO:HB2	1:D:218:GLU:O	1.95	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
3:F:1520:ASP:OD1	3:F:1551:SER:HB2	1.97	0.65
1:D:93:GLN:OE1	1:D:93:GLN:HA	1.97	0.65
3:F:1556:VAL:O	3:F:1558:GLN:N	2.30	0.64
1:D:37:VAL:HG12	1:D:84:VAL:HG22	1.78	0.64
3:C:1582:MET:CB	3:C:1605:TRP:O	2.45	0.64
2:E:837:GLU:HG2	4:M:64:SER:OG	1.97	0.64
3:F:1485:ARG:CZ	3:F:1590:TRP:O	2.45	0.64
3:F:1570:GLU:OE1	3:F:1570:GLU:N	2.30	0.64
2:E:795:VAL:O	2:E:795:VAL:HG12	1.96	0.64
3:F:1416:PHE:C	3:F:1416:PHE:CD2	2.75	0.64
3:F:1595:ASN:C	3:F:1596:LEU:CG	2.67	0.64
1:A:37:VAL:HG12	1:A:84:VAL:HG22	1.78	0.64
3:C:1640:PRO:C	3:C:1641:ASN:HD22	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1600:ILE:HG22	3:F:1600:ILE:O	1.95	0.64
3:C:1612:GLU:O	3:C:1616:GLN:NE2	2.30	0.64
3:F:1536:PHE:CD2	3:F:1566:ILE:HG13	2.32	0.64
1:D:335:PHE:CD2	1:D:419:MET:HB3	2.33	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: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
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.78	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
1:D:6:ILE:HG22	1:D:625:THR:HB	1.80	0.64
3:C:1590:TRP:HA	3:C:1590:TRP:HE3	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
3:C:1634:MET:O	3:C:1635:VAL:C	2.42	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:ND2	3:F:1495:ASN:N	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:N	3:C:1580:TYR:HD2	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
2:E:760:PRO:HG3	1:D:567:HIS:ND1	2.13	0.63
3:F:1572:LEU:HB2	3:F:1574:LEU:CD2	2.24	0.63
1:D:307:THR:HG23	1:D:318:GLN:HG3	1.81	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
1:D:10:ASN:CG	1:D:635:ARG:HD2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:LYS:O	1:D:341:TYR:CD1	2.52	0.62
1:A:10:ASN:CG	1:A:635:ARG:HD2	2.24	0.62
1:A:114:LYS:HE3	1:A:116:ILE:O	1.99	0.62
1:A:286:LEU:HB3	1:A:291:ASN:ND2	2.14	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
1:D:286:LEU:HB3	1:D:291:ASN:ND2	2.15	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:93:GLN:OE1	1:A:93:GLN:HA	1.97	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:295:GLU:O	1:D:298:VAL:HB	2.00	0.62
3:F:1525:THR:HG1	3:F:1541:MET:HE3	1.63	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
3:F:1542:ALA:C	3:F:1543:ILE:CD1	2.71	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
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
1:D:142:MET:HG3	1:D:187:TYR:HE1	1.64	0.62
3:C:1506:THR:C	3:C:1508:GLU:N	2.58	0.61
3:C:1578:LYS:HE3	3:C:1578:LYS:CA	2.14	0.61
4:M:26:LEU:C	4:M:26:LEU:HD12	2.25	0.61
3:F:1408:SER:O	3:F:1409:LYS:C	2.42	0.61
3:F:1507:LEU:CD1	3:F:1626:ASP:CB	2.71	0.61
3:F:1554:VAL:HG22	3:F:1554:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:MET:HE1	1:D:454:LEU:HG	1.82	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:N	3:F:1572:LEU:HD23	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:A:346:MET:HE1	1:A:454:LEU:HG	1.82	0.61
3:F:1405:ARG:NE	3:F:1437:LEU:HD23	2.15	0.61
3:F:1460:TYR:CD1	1:D:248:PHE:CB	2.84	0.61
3:F:1526:ARG:NH2	3:F:1544:GLU:OE2	2.32	0.61
1:D:114:LYS:HE3	1:D:116:ILE:O	1.99	0.61
3:F:1409:LYS:O	3:F:1411:GLU:N	2.33	0.61
3:F:1543:ILE:C	3:F:1545:GLN:H	2.09	0.61
1:D:22:LEU:HB2	1:D:62:GLY:HA3	1.83	0.61
1:D:487:GLU:O	1:D:490:GLN:HB2	2.01	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
1:A:248:PHE:HD1	3:C:1378:MET:HE3	1.64	0.61
2:E:741:SER:HB3	2:E:902:GLY:C	2.26	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
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:N	2:E:912:GLU:OE1	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
4:M:14:LYS:HZ3	3:F:1415:ALA:CB	2.14	0.60
3:F:1408:SER:HG	3:F:1410:TYR:HB3	1.66	0.60
1:D:73:GLU:HB3	1:D:82:LYS:NZ	2.16	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:1526:ARG:HB2	3:F:1579:HIS:CD2	2.37	0.60
3:F:1526:ARG:NE	3:F:1579:HIS:NE2	2.48	0.60
3:F:1533:SER:O	3:F:1534:ASN:C	2.45	0.60
3:F:1577:LYS:O	3:F:1579:HIS:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:P:26:LEU:C	4:P:26:LEU:HD12	2.26	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
3:C:1623:GLN:C	3:C:1625:GLN:H	2.08	0.60
2:E:852:SER:C	2:E:854:ALA:H	2.10	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
2:B:741:SER:HB3	2:B:902:GLY:C	2.26	0.60
2:B:852:SER:C	2:B:854:ALA:H	2.10	0.60
3:C:1445:PHE:CE1	4:P:6:THR:HA	2.31	0.60
1:D:179:MET:HG3	1:D:203:LYS:HA	1.82	0.60
2:B:842:VAL:HG23	2:B:892:ALA:HB2	1.82	0.60
3:C:1565:PRO:C	3:C:1567:LYS:N	2.59	0.60
3:C:1608:HIS:CD2	3:C:1609:TRP:C	2.80	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
2:E:786:SER:HA	1:D:570:ARG:O	2.01	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
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
1:D:84:VAL:HG13	1:D:85:THR:N	2.14	0.59
1:D:606:THR:HG22	1:D:608:GLY:N	2.17	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
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:D:47:LEU:HD11	1:D:66:PHE:HB2	1.85	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
3:F:1526:ARG:NE	3:F:1544:GLU:OE2	2.36	0.59
1:D:99:VAL:HG12	1:D:100:LEU:N	2.18	0.59
1:A:117:TYR:CG	1:A:123:VAL:HG22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:117:TYR:CG	1:D:123:VAL:HG22	2.37	0.59
1:A:37:VAL:HG12	1:A:84:VAL:CG2	2.32	0.59
1:A:99:VAL:HG12	1:A:100:LEU:N	2.18	0.59
2:B:831:ASN:ND2	2:B:868:PRO:HA	2.18	0.59
4:M:10:TYR:CE2	3:F:1417:SER:CB	2.85	0.59
3:F:1377:THR:O	3:F:1378:MET:C	2.46	0.59
3:F:1495:ASN:O	3:F:1496:CYS:HB3	2.01	0.59
1:D:345:GLY:H	1:D:391:THR:HG23	1.68	0.59
1:D:534:LYS:CG	1:D:534:LYS:O	2.50	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
2:E:825:ILE:HD13	2:E:888:VAL:HG11	1.84	0.59
1:D:443:LEU:HD11	1:D:449:LEU:HD22	1.85	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
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
1:D:20:MET:HG2	1:D:64:VAL:HG21	1.84	0.58
1:A:61:MET:HE2	1:A:483:ARG:HG2	1.85	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:D:61:MET:HE2	1:D:483:ARG:HG2	1.85	0.58
1:A:6:ILE:CD1	1:A:22:LEU:HD23	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:SER:O	1:A:537:CYS:C	2.46	0.58
2:B:825:ILE:HD13	2:B:888:VAL:HG11	1.84	0.58
2:B:873:SER:HB3	3:C:1421:THR:HG21	1.86	0.58
3:C:1377:THR:O	3:C:1378:MET:C	2.46	0.58
3:F:1554:VAL:HB	3:F:1560:ARG:NH2	2.17	0.58
3:C:1341:LEU:HD23	3:C:1469:ARG:HB2	1.86	0.58
3:C:1397:LYS:O	3:C:1398:GLN:C	2.46	0.58
3:C:1525:THR:HA	3:C:1542:ALA:O	2.03	0.58
3:F:1345:ILE:HG23	3:F:1345:ILE:O	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
3:F:1631:THR:C	3:F:1633:SER:H	2.10	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
3:F:1397:LYS:O	3:F:1398:GLN:C	2.46	0.58
3:F:1409:LYS:C	3:F:1411:GLU:N	2.60	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:D:536:SER:O	1:D:537:CYS:C	2.46	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
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
3:C:1568:CYS:C	3:C:1570:GLU:H	2.11	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
1:D:6:ILE:CD1	1:D:22:LEU:HD23	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:TYR:CZ	1:D:525:VAL:HB	2.39	0.57
2:B:841:ARG:HH11	2:B:841:ARG:CG	2.06	0.57
3:C:1408:SER:O	3:C:1409:LYS:C	2.45	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: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:1589:PHE:HB3	3:C:1596:LEU:HD22	1.85	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
3:F:1585:LEU:O	3:F:1586:SER:C	2.47	0.57
1:D:97:LYS:HZ3	1:D:631:GLN:HB2	1.69	0.57
3:F:1341:LEU:HD23	3:F:1469:ARG:HB2	1.86	0.57
1:D:594:ILE:O	1:D:598:VAL:HG23	2.04	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
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:D:83:PHE:CD1	1:D:99:VAL:O	2.54	0.56
1:D:477:ARG:NH2	1:D:479:LEU:HD13	2.20	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:10:ASN:HB3	1:A:635:ARG:NH1	2.15	0.56
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.87	0.56
1:A:34:THR:HG22	1:A:51:LYS:HE2	1.88	0.56
1:A:570:ARG:O	2:B:786:SER:HA	2.05	0.56
3:C:1345:ILE:O	3:C:1345:ILE:HG23	2.04	0.56
3:C:1565:PRO:C	3:C:1567:LYS:H	2.11	0.56
4:M:84:LYS:O	4:M:85:TYR:HB2	2.05	0.56
3:F:1528:VAL:HG22	3:F:1542:ALA:H	1.69	0.56
1:D:34:THR:HG22	1:D:51:LYS:HE2	1.88	0.56
1:D:99:VAL:HG12	1:D:100:LEU:H	1.70	0.56
1:D:510:VAL:HG12	1:D:528:SER:CB	2.30	0.56
2:B:734:ILE:HD13	2:B:893:ALA:HB1	1.88	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
3:F:1544:GLU:OE2	3:F:1579:HIS:CE1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:LEU:O	1:D:509:LEU:HD12	2.06	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
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:1574:LEU:HB3	3:F:1580:TYR:OH	2.05	0.56
1:D:257:GLU:CD	1:D:257:GLU:H	2.14	0.56
1:A:471:LEU:O	1:A:509:LEU:HD12	2.06	0.56
3:C:1518:GLY:O	3:C:1519:VAL:C	2.48	0.56
4:P:84:LYS:O	4:P:85:TYR:HB2	2.05	0.56
3:F:1408:SER:C	3:F:1410:TYR:N	2.63	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:HD12	2:E:734:ILE:N	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
1:A:430:SER:O	1:A:431:ASN:HB2	2.06	0.56
2:B:819:ARG:HG2	2:B:820:ASN:CG	2.31	0.56
3:C:1578:LYS:HA	3:C:1578:LYS:CE	2.29	0.56
2:E:732:ASP:OD1	2:E:896:HIS:HA	2.06	0.56
2:E:851:CYS:HB3	2:E:879:VAL:HB	1.87	0.56
2:E:858:ARG:CZ	3:F:1449:LEU:CD1	2.84	0.56
3:F:1509:GLU:HB2	3:F:1512:ASP:HB3	1.87	0.56
3:F:1543:ILE:HD13	3:F:1559:GLN:CA	2.36	0.56
1:D:586:LYS:O	1:D:587:ASN:HB2	2.05	0.56
2:E:788:SER:O	2:E:792:GLY:N	2.35	0.55
3:F:1546:THR:O	3:F:1546:THR:HG23	2.06	0.55
1:D:364:ARG:HG2	1:D:378:LEU:HD23	1.87	0.55
3:C:1409:LYS:HG2	3:C:1413:ASP:OD2	2.06	0.55
2:E:883:THR:HA	2:E:909:VAL:HG12	1.88	0.55
3:F:1534:ASN:ND2	3:F:1534:ASN:O	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:SER:O	1:A:537:CYS:O	2.24	0.55
2:B:734:ILE:HD12	2:B:734:ILE:N	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
3:F:1607:GLU:O	3:F:1608:HIS:CB	2.54	0.55
1:D:406:LYS:H	1:D:414:GLN:HE22	1.53	0.55
1:A:142:MET:HG3	1:A:187:TYR:HE1	1.65	0.55
3:F:1444:TYR:CD1	3:F:1445:PHE:HB2	2.42	0.55
1:D:23:GLU:HG2	1:D:61:MET:HG2	1.87	0.55
1:A:440:ARG:NH2	1:A:529:VAL:HG23	2.22	0.55
3:C:1389:PHE:N	3:C:1389:PHE:CD2	2.75	0.55
2:E:741:SER:HB3	2:E:902:GLY:O	2.06	0.55
2:E:760:PRO:HG3	1:D:567:HIS:CG	2.41	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
1:A:257:GLU:CD	1:A:257:GLU:H	2.14	0.55
3:C:1546:THR:C	3:C:1548:LYS:H	2.15	0.55
3:C:1565:PRO:O	3:C:1567:LYS:N	2.39	0.55
3:F:1520:ASP:CG	3:F:1551:SER:HB2	2.32	0.55
1:A:293:ARG:O	1:A:294:ALA:C	2.50	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
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
2:E:808:PHE:C	2:E:808:PHE:CD1	2.85	0.55
3:F:1535:ASP:C	3:F:1566:ILE:HG23	2.30	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:A:610:GLY:N	1:A:616:VAL:HG23	2.22	0.54
3:F:1408:SER:OG	3:F:1410:TYR:CB	2.55	0.54
3:F:1409:LYS:O	3:F:1412:LEU:N	2.40	0.54
3:F:1574:LEU:CA	3:F:1580:TYR:OH	2.55	0.54
1:D:610:GLY:N	1:D:616:VAL:HG23	2.22	0.54
1:A:575:ALA:HB2	2:B:782:ILE:HG12	1.89	0.54
2:B:808:PHE:CD1	2:B:808:PHE:C	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:1562:PHE:HD2	3:F:1600:ILE:HD12	1.71	0.54
1:D:446:GLY:N	1:D:499:ILE:O	2.32	0.54
1:A:54:LEU:HB3	1:A:60:HIS:HA	1.89	0.54
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.72	0.54
2:B:844:LEU:C	2:B:844:LEU:HD12	2.33	0.54
3:F:1564:SER:HB2	3:F:1600:ILE:HB	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
1:A:147:ASN:HB2	1:A:148:PRO:HD3	1.90	0.54
1:A:286:LEU:C	1:A:291:ASN:ND2	2.65	0.54
3:F:1542:ALA:O	3:F:1543:ILE:CG1	2.56	0.54
3:F:1543:ILE:HD12	3:F:1543:ILE:N	2.21	0.54
3:F:1567:LYS:O	3:F:1567:LYS:HG2	2.08	0.54
1:D:286:LEU:C	1:D:291:ASN:ND2	2.65	0.54
3:F:1360:ASN:HD22	3:F:1443:GLN:CB	2.11	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
1:A:34:THR:CG2	1:A:51:LYS:HE2	2.38	0.54
1:A:287:ASP:N	1:A:291:ASN:HD21	2.05	0.54
3:C:1532:LEU:HD13	3:C:1532:LEU:N	2.21	0.54
4:M:14:LYS:HZ2	3:F:1415:ALA:CB	2.19	0.54
3:F:1522:VAL:C	3:F:1547:ILE:HD12	2.32	0.54
3:F:1532:LEU:HG	3:F:1569:ARG:HH22	1.73	0.54
1:D:536:SER:O	1:D:537:CYS:O	2.24	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
1:D:146:GLU:CD	1:D:185:ARG:HD2	2.33	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
3:F:1532:LEU:N	3:F:1532:LEU:CD1	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:THR:CG2	1:D:51:LYS:HE2	2.38	0.53
1:D:282:ARG:O	1:D:286:LEU:HD12	2.09	0.53
2:E:836:GLN:C	2:E:868:PRO:HG3	2.34	0.53
1:A:124:LEU:N	1:A:124:LEU:HD23	2.24	0.53
2:B:836:GLN:C	2:B:868:PRO:HG3	2.34	0.53
3:C:1568:CYS:C	3:C:1570:GLU:N	2.67	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
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
1:D:293:ARG:O	1:D:294:ALA:C	2.50	0.53
1:D:524:VAL:HB	1:D:613:TYR:CD1	2.43	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
2:E:763:GLY:O	2:E:764:ILE:HD13	2.09	0.53
1:D:534:LYS:O	1:D:534:LYS:HG3	2.05	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
2:B:907:LEU:HD23	2:B:907:LEU:H	1.73	0.53
3:C:1610:PRO:O	3:C:1611:GLU:C	2.51	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:39:ASP:OD1	1:A:44:LYS:HB2	2.09	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
3:C:1521:TYR:C	3:C:1521:TYR:CD1	2.86	0.53
2:E:844:LEU:C	2:E:844:LEU:HD12	2.33	0.53
3:F:1378:MET:CG	1:D:268:ARG:NH1	2.72	0.53
3:F:1570:GLU:CD	3:F:1570:GLU:N	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:907:LEU:HD23	2:E:907:LEU:O	2.10	0.52
3:C:1522:VAL:C	3:C:1523:TYR:CD1	2.87	0.52
4:M:59:ASP:C	4:M:59:ASP:OD1	2.52	0.52
3:F:1532:LEU:HA	3:F:1569:ARG:HH22	1.73	0.52
1:D:39:ASP:OD1	1:D:44:LYS:HB2	2.09	0.52
1:D:117:TYR:CD1	1:D:123:VAL:HG22	2.44	0.52
1:A:343:LYS:HD2	1:A:343:LYS:N	2.25	0.52
2:E:907:LEU:HD23	2:E:907:LEU:H	1.73	0.52
4:P:59:ASP:C	4:P:59:ASP:OD1	2.52	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:D:292:PRO:O	1:D:293:ARG:C	2.53	0.52
1:D:468:TYR:CE1	1:D:513:TYR:HD2	2.28	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
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:581:PHE:CE1	1:D:588:LYS:HD2	2.45	0.52
1:D:19:THR:HG23	1:D:64:VAL:O	2.10	0.52
1:D:343:LYS:N	1:D:343:LYS:HD2	2.25	0.52
1:D:468:TYR:HE1	1:D:513:TYR:HD2	1.57	0.52
3:C:1520:ASP:CG	3:C:1551:SER:HG	2.15	0.52
1:D:124:LEU:HD23	1:D:124:LEU:N	2.24	0.52
1:A:19:THR:HG23	1:A:64:VAL:O	2.10	0.52
1:A:146:GLU:CD	1:A:185:ARG:HD2	2.33	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
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:D:590:THR:HG21	1:D:592:SER:HB2	1.92	0.52
1:A:117:TYR:CD1	1:A:123:VAL:HG22	2.44	0.52
1:A:248:PHE:CD1	3:C:1378:MET:HE3	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
3:C:1543:ILE:C	3:C:1545:GLN:H	2.17	0.52
2:E:783:LEU:HD12	2:E:784:ALA:N	2.24	0.52
3:F:1403:VAL:C	3:F:1405:ARG:H	2.18	0.52
3:F:1497:PHE:CE2	3:F:1498:ILE:HB	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1563:ILE:HD11	3:F:1597:SER:OG	2.09	0.52
3:F:1578:LYS:O	3:F:1580:TYR:CE2	2.63	0.52
1:D:363:TYR:CE1	1:D:364:ARG:HG3	2.44	0.52
1:A:403:ARG:HG2	1:A:404:THR:O	2.10	0.52
1:A:404:THR:C	1:A:414:GLN:OE1	2.53	0.52
1:A:535:ASP:OD1	1:A:535:ASP:N	2.42	0.52
2:B:907:LEU:HD23	2:B:907:LEU:O	2.10	0.52
4:M:36:LEU:HB3	4:M:40:TYR:HD2	1.73	0.52
3:F:1519:VAL:N	3:F:1585:LEU:CD2	2.72	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
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
3:C:1551:SER:C	3:C:1593:LYS:NZ	2.67	0.52
3:F:1636:VAL:O	3:F:1637:PHE:C	2.51	0.52
1:D:193:GLN:HG2	1:D:194:GLN:N	2.24	0.52
1:D:404:THR:C	1:D:414:GLN:OE1	2.53	0.52
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
3:F:1639:CYS:C	3:F:1641:ASN:H	2.15	0.51
1:A:248:PHE:HD1	3:C:1378:MET:CE	2.23	0.51
3:F:1386:MET:O	3:F:1387:THR:C	2.54	0.51
3:F:1405:ARG:CZ	3:F:1437:LEU:HD23	2.41	0.51
3:F:1569:ARG:C	3:F:1570:GLU:CD	2.78	0.51
3:F:1622:LYS:O	3:F:1623:GLN:C	2.53	0.51
1:D:595:TRP:CE3	1:D:595:TRP:HA	2.45	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:CE	3:C:1531:GLN:HE21	2.22	0.51
3:C:1529:LYS:HE3	3:C:1531:GLN:HE21	1.76	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
2:B:793:ILE:HG13	2:B:794:CYS:N	2.23	0.51
3:C:1409:LYS:O	3:C:1412:LEU:N	2.42	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
3:F:1618:GLU:O	3:F:1619:GLU:C	2.54	0.51
1:D:365:VAL:CG1	1:D:379:THR:OG1	2.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:230:GLU:HA	1:A:279:VAL:HG22	1.92	0.51
1:A:357:PRO:O	1:A:358:ASP:C	2.53	0.51
3:C:1547:ILE:O	3:C:1547:ILE:HG22	2.11	0.51
3:C:1578:LYS:CB	3:C:1580:TYR:OH	2.58	0.51
4:P:49:GLN:O	4:P:50:LYS:C	2.52	0.51
4:P:66:ALA:O	4:P:67:LYS:C	2.53	0.51
3:F:1378:MET:CE	1:D:248:PHE:HD1	2.23	0.51
1:D:143:VAL:O	1:D:155:GLN:HA	2.10	0.51
1:D:477:ARG:HG2	1:D:477:ARG:HH11	1.72	0.51
1:A:97:LYS:HZ3	1:A:631:GLN:HB2	1.76	0.51
1:A:595:TRP:HA	1:A:595:TRP:CE3	2.45	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:D:495:LEU:HD12	1:D:496:PRO:CD	2.40	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
3:C:1451:GLN:HG3	3:C:1452:PRO:HD2	1.92	0.51
2:E:740:VAL:HB	4:P:42:ARG:HA	1.93	0.51
3:F:1378:MET:HE2	1:D:248:PHE:HD1	1.74	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:D:367:VAL:HG23	1:D:387:LEU:HD11	1.92	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
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:D:4:TYR:HB3	1:D:90:PHE:CE2	2.46	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
4:M:7:SER:O	4:M:8:ASN:C	2.54	0.51
3:F:1532:LEU:O	3:F:1534:ASN:N	2.43	0.51
3:F:1541:MET:HE1	3:F:1582:MET:SD	2.51	0.51
1:D:63:ASN:HD21	5:D:646:NAG:C1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:PRO:O	1:D:358:ASP:C	2.53	0.51
3:C:1386:MET:O	3:C:1387:THR:C	2.53	0.51
3:C:1626:ASP:C	3:C:1628:GLY:N	2.66	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:292:PRO:O	1:A:293:ARG:C	2.53	0.50
1:A:459:ARG:HH22	1:D:458:ASP:HA	1.76	0.50
1:A:590:THR:HG21	1:A:592:SER:HB2	1.92	0.50
2:E:744:GLU:C	2:E:746:PRO:HD3	2.37	0.50
4:M:49:GLN:O	4:M:50:LYS:C	2.53	0.50
4:P:18:GLU:O	4:P:21:SER:HB2	2.11	0.50
1:D:37:VAL:HB	1:D:46:VAL:HG23	1.93	0.50
1:D:590:THR:HB	1:D:593:LYS:CG	2.39	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
3:C:1405:ARG:CZ	3:C:1437:LEU:HD23	2.40	0.50
4:M:18:GLU:O	4:M:21:SER:HB2	2.12	0.50
4:P:7:SER:O	4:P:8:ASN:C	2.54	0.50
3:F:1510:ARG:NH1	3:F:1607:GLU:OE1	2.44	0.50
1:D:3:MET:HE2	1:D:626:SER:CB	2.41	0.50
1:D:472:ILE:HA	1:D:508:ARG:O	2.11	0.50
1:A:63:ASN:HD21	5:A:646:NAG:C1	2.24	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:286:LEU:HB3	1:A:291:ASN:HD22	1.76	0.50
1:A:402:VAL:HG12	1:A:403:ARG:N	2.27	0.50
3:C:1403:VAL:C	3:C:1405:ARG:H	2.18	0.50
3:C:1508:GLU:O	3:C:1512:ASP:OD2	2.29	0.50
3:F:1532:LEU:HA	3:F:1569:ARG:NH2	2.27	0.50
3:F:1536:PHE:CE2	3:F:1566:ILE:HG13	2.47	0.50
3:F:1537:ASP:CB	3:F:1569:ARG:HD2	2.42	0.50
3:F:1568:CYS:O	3:F:1569:ARG:O	2.29	0.50
1:D:351:MET:SD	1:D:440:ARG:HD3	2.52	0.50
3:F:1416:PHE:CE2	3:F:1444:TYR:HD2	2.25	0.50
1:D:438:VAL:HG13	1:D:449:LEU:HD11	1.92	0.50
1:A:3:MET:HE2	1:A:626:SER:CB	2.41	0.50
1:A:351:MET:SD	1:A:440:ARG:HD3	2.52	0.50
1:A:534:LYS:O	1:A:534:LYS:HG3	2.05	0.50
2:B:896:HIS:CB	4:P:61:LYS:HD3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:29:ASN:O	4:P:30:GLU:C	2.54	0.50
3:F:1524:LYS:C	3:F:1525:THR:CG2	2.85	0.50
3:C:1618:GLU:HA	3:C:1621:GLN:CD	2.37	0.50
4:M:4:LEU:HD13	3:F:1445:PHE:N	2.26	0.50
4:M:14:LYS:HZ3	3:F:1415:ALA:HB1	1.74	0.50
3:F:1444:TYR:CE1	3:F:1445:PHE:HB2	2.46	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
1:D:634:GLN:HE22	1:D:635:ARG:C	2.19	0.50
1:A:4:TYR:HB3	1:A:90:PHE:CE2	2.46	0.49
1:A:37:VAL:HB	1:A:46:VAL:HG23	1.93	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
4:M:29:ASN:O	4:M:30:GLU:C	2.55	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:D:406:LYS:N	1:D:414:GLN:HE22	2.10	0.49
1:A:459:ARG:NH2	1:D:458:ASP:HA	2.27	0.49
3:C:1546:THR:C	3:C:1548:LYS:N	2.70	0.49
2:E:787:MET:HG2	1:D:164:LEU:O	2.12	0.49
4:M:64:SER:O	4:M:65:GLU:C	2.55	0.49
4:P:30:GLU:OE2	4:P:45:LYS:HE3	2.13	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:472:ILE:HA	1:A:508:ARG:O	2.11	0.49
2:B:744:GLU:C	2:B:746:PRO:HD3	2.37	0.49
3:C:1337:ASN:C	3:C:1337:ASN:OD1	2.55	0.49
3:C:1482:LYS:O	3:C:1536:PHE:CE2	2.65	0.49
3:F:1337:ASN:C	3:F:1337:ASN:OD1	2.54	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: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
1:A:271:ILE:HD13	1:A:276:GLY:HA3	1.94	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
2:E:836:GLN:O	2:E:836:GLN:HG3	2.12	0.49
3:F:1393:THR:HG22	3:F:1419:ARG:HH22	1.78	0.49
1:D:179:MET:CG	1:D:203:LYS:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:PRO:HA	1:D:499:ILE:HG22	1.95	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:883:THR:HA	2:E:909:VAL:CG1	2.42	0.49
4:P:8:ASN:ND2	4:P:12:ASN:OD1	2.46	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
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
3:F:1612:GLU:C	3:F:1614:GLU:H	2.20	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
3:F:1510:ARG:O	3:F:1511:LEU:HB3	2.12	0.49
1:D:63:ASN:OD1	5:D:646:NAG:N2	2.46	0.49
1:D:138:GLY:HA2	1:D:160:SER:HG	1.75	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
4:M:8:ASN:ND2	4:M:12:ASN:OD1	2.46	0.49
3:F:1381:LEU:CD1	3:F:1426:LEU:HD11	2.43	0.49
3:F:1409:LYS:O	3:F:1410:TYR:C	2.56	0.49
3:F:1507:LEU:HD21	3:F:1622:LYS:CE	2.43	0.49
1:D:100:LEU:HD21	1:D:638:LEU:HD23	1.95	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
3:C:1416:PHE:C	3:C:1416:PHE:HD2	2.20	0.49
3:C:1611:GLU:HG2	3:C:1613:ASP:H	1.78	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:D:73:GLU:HB3	1:D:82:LYS:HZ3	1.78	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
1:A:63:ASN:OD1	5:A:646:NAG:N2	2.46	0.49
1:A:183:LYS:HD2	1:A:185:ARG:HD2	1.94	0.49
3:C:1393:THR:HG22	3:C:1419:ARG:HH22	1.78	0.49
3:C:1409:LYS:O	3:C:1410:TYR:C	2.56	0.49
3:F:1406:TYR:C	3:F:1406:TYR:CD2	2.88	0.49
3:F:1484:CYS:CB	3:F:1489:CYS:SG	3.01	0.49
1:D:83:PHE:HD1	1:D:99:VAL:C	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:HIS:HB3	4:P:61:LYS:HD3	1.95	0.48
3:C:1450:ILE:O	3:C:1450:ILE:CG1	2.55	0.48
3:C:1551:SER:C	3:C:1593:LYS:HZ3	2.18	0.48
4:P:64:SER:O	4:P:65:GLU:C	2.55	0.48
3:F:1416:PHE:C	3:F:1416:PHE:HD2	2.20	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
2:E:730:ASP:CG	2:E:730:ASP:O	2.56	0.48
4:M:26:LEU:HD12	4:M:26:LEU:O	2.13	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
1:D:183:LYS:HD2	1:D:185:ARG:HD2	1.94	0.48
1:A:25:HIS:O	1:A:26:ASP:HB2	2.12	0.48
1:A:445:PRO:HA	1:A:499:ILE:HG22	1.95	0.48
3:F:1514:ALA:HB2	3:F:1583:TRP:CE2	2.48	0.48
1:D:61:MET:HE2	1:D:483:ARG:CG	2.44	0.48
2:B:730:ASP:CG	2:B:730:ASP:O	2.55	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:D:291:ASN:N	1:D:292:PRO:CD	2.76	0.48
1:D:530:TRP:CD1	1:D:530:TRP:C	2.91	0.48
1:A:437:SER:O	1:A:452:ASN:HB2	2.13	0.48
1:A:458:ASP:HA	1:D:459:ARG:NH2	2.28	0.48
1:A:613:TYR:CE2	1:A:614:ALA:HB2	2.48	0.48
3:C:1444:TYR:CD1	3:C:1444:TYR:C	2.92	0.48
3:C:1530:VAL:HG12	3:C:1532:LEU:HD11	1.95	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:HB2	1.96	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
1:A:615:GLY:O	1:A:616:VAL:C	2.56	0.48
3:C:1360:ASN:OD1	3:C:1361:THR:N	2.47	0.48
3:C:1609:TRP:HZ3	3:C:1627:LEU:HD22	1.72	0.48
1:D:109:PHE:CZ	1:D:594:ILE:HG23	2.49	0.48
1:D:286:LEU:HB3	1:D:291:ASN:HD22	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1516:GLU:O	3:F:1517:PRO:C	2.55	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:F:1604:THR:HG23	3:F:1604:THR:O	2.13	0.48
1:A:83:PHE:HD1	1:A:99:VAL:C	2.21	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:20:MET:H	1:D:64:VAL:HB	1.79	0.48
1:D:25:HIS:O	1:D:26:ASP:HB2	2.12	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:A:439:LEU:HD12	1:A:439:LEU:O	2.12	0.48
3:C:1530:VAL:CG1	3:C:1532:LEU:HD11	2.44	0.48
2:E:822:GLN:NE2	3:F:1470:PHE:CD2	2.79	0.48
4:P:26:LEU:HD12	4:P:26:LEU:O	2.13	0.48
4:P:64:SER:O	4:P:67:LYS:N	2.47	0.48
3:F:1503:ASP:C	3:F:1505:VAL:N	2.71	0.48
3:F:1531:GLN:HG3	3:F:1531:GLN:O	2.14	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
2:E:809:ILE:HD12	2:E:903:VAL:HG23	1.96	0.47
2:E:839:LYS:HG2	2:E:895:TYR:HD1	1.79	0.47
4:M:66:ALA:O	4:M:67:LYS:C	2.53	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
1:A:458:ASP:HA	1:D:459:ARG:HH22	1.78	0.47
1:A:475:LYS:HG2	1:A:598:VAL:HG11	1.96	0.47
1:A:510:VAL:CG1	1:A:528:SER:HB3	2.33	0.47
1:A:530:TRP:CD1	1:A:530:TRP:C	2.91	0.47
3:C:1544:GLU:C	3:C:1545:GLN:HG3	2.36	0.47
3:F:1341:LEU:HD23	3:F:1469:ARG:N	2.29	0.47
3:F:1503:ASP:O	3:F:1504:LYS:C	2.58	0.47
3:F:1574:LEU:CB	3:F:1580:TYR:OH	2.62	0.47
3:F:1577:LYS:O	3:F:1579:HIS:CD2	2.64	0.47
1:A:7:ILE:HA	1:A:623:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:HE2	1:A:483:ARG:CG	2.44	0.47
1:A:403:ARG:CB	1:A:416:THR:HG22	2.44	0.47
2:B:809:ILE:HD12	2:B:903:VAL:HG23	1.96	0.47
2:B:839:LYS:HG2	2:B:895:TYR:HD1	1.79	0.47
3:F:1444:TYR:C	3:F:1444:TYR:CD1	2.92	0.47
3:F:1575:GLU:HG3	3:F:1576:GLU:N	2.29	0.47
1:D:287:ASP:N	1:D:291:ASN:ND2	2.63	0.47
1:A:97:LYS:NZ	1:A:631:GLN:HB2	2.29	0.47
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.50	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
4:M:64:SER:O	4:M:67:LYS:N	2.47	0.47
3:F:1376:ALA:HB3	3:F:1429:VAL:HG22	1.97	0.47
3:F:1409:LYS:O	3:F:1413:ASP:OD2	2.33	0.47
3:F:1631:THR:C	3:F:1633:SER:N	2.72	0.47
3:F:1634:MET:O	3:F:1635:VAL:C	2.58	0.47
1:A:214:VAL:HG11	1:A:304:VAL:CG2	2.45	0.47
3:C:1602:LYS:C	3:C:1604:THR:H	2.22	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:1609:TRP:CZ3	3:C:1627:LEU:HB3	2.50	0.47
3:F:1392:ASP:HB2	3:F:1442:HIS:NE2	2.30	0.47
3:F:1555:GLN:O	3:F:1556:VAL:O	2.33	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
1:A:135:LEU:HD22	2:B:789:ASP:O	2.14	0.47
1:A:251:PHE:CE1	1:A:304:VAL:CG1	2.98	0.47
1:A:549:GLU:O	1:A:550:ASP:HB2	2.14	0.47
2:B:877:VAL:HG13	3:C:1451:GLN:CD	2.39	0.47
3:C:1341:LEU:HD23	3:C:1469:ARG:N	2.29	0.47
3:C:1587:SER:O	3:C:1589:PHE:N	2.43	0.47
3:C:1608:HIS:CD2	3:C:1610:PRO:CG	2.97	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:1615:CYS:C	3:F:1617:ASP:N	2.72	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:222:TYR:CE2	1:D:224:TYR:HB2	2.50	0.47
1:D:351:MET:HE1	1:D:386:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.45	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
2:E:735:ALA:HB1	2:E:737:GLU:OE2	2.15	0.47
4:M:23:LEU:HD11	4:M:51:ALA:HB1	1.97	0.47
1:A:59:ASN:HB3	1:A:483:ARG:HH12	1.80	0.47
1:A:148:PRO:HG3	1:A:182:TRP:CD1	2.50	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:1508:GLU:O	3:C:1512:ASP:OD1	2.33	0.47
3:C:1573:LYS:O	3:C:1573:LYS:CD	2.63	0.47
3:F:1572:LEU:C	3:F:1574:LEU:HD21	2.32	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:462:GLU:HG3	1:D:486:ARG:NH2	2.29	0.47
1:D:475:LYS:HG2	1:D:598:VAL:CG1	2.45	0.47
1:D:510:VAL:HG21	1:D:622:LEU:HD12	1.95	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
3:C:1587:SER:C	3:C:1589:PHE:H	2.23	0.47
3:F:1624:CYS:O	3:F:1625:GLN:C	2.58	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
2:E:897:HIS:HB3	2:E:899:ILE:HG13	1.97	0.46
3:F:1450:ILE:O	3:F:1450:ILE:CG1	2.55	0.46
3:F:1527:LEU:HD12	3:F:1575:GLU:C	2.40	0.46
1:D:105:SER:O	1:D:132:HIS:CD2	2.68	0.46
1:D:294:ALA:O	1:D:295:GLU:C	2.58	0.46
1:D:301:SER:HB2	1:D:323:GLY:HA2	1.97	0.46
1:A:203:LYS:HG2	1:A:204:GLU:N	2.29	0.46
3:F:1483:LEU:CG	3:F:1590:TRP:CZ2	2.98	0.46
1:D:126:ARG:CZ	1:D:572:VAL:HB	2.45	0.46
1:D:148:PRO:HG3	1:D:182:TRP:CD1	2.50	0.46
1:D:271:ILE:HD13	1:D:271:ILE:HA	1.74	0.46
1:D:475:LYS:HG2	1:D:598:VAL:HG11	1.96	0.46
1:A:6:ILE:HD12	1:A:6:ILE:HA	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:MET:H	1:A:64:VAL:HB	1.79	0.46
1:A:215:GLU:HA	1:A:216:PRO:HD3	1.68	0.46
1:A:285:LEU:O	1:A:285:LEU:HG	2.14	0.46
1:A:634:GLN:HE22	1:A:635:ARG:C	2.19	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:1531:GLN:C	3:C:1532:LEU:HD13	2.40	0.46
3:C:1534:ASN:O	3:C:1566:ILE:CD1	2.64	0.46
1:D:47:LEU:HD23	1:D:47:LEU:C	2.41	0.46
1:D:615:GLY:O	1:D:616:VAL:C	2.56	0.46
1:A:59:ASN:HB3	1:A:483:ARG:NH1	2.29	0.46
1:A:287:ASP:N	1:A:291:ASN:ND2	2.63	0.46
2:E:852:SER:C	2:E:854:ALA:N	2.73	0.46
3:F:1600:ILE:C	3:F:1604:THR:HG21	2.41	0.46
1:D:6:ILE:HD12	1:D:6:ILE:HA	1.56	0.46
1:D:97:LYS:NZ	1:D:631:GLN:HB2	2.29	0.46
1:D:111:GLN:O	1:D:125:TYR:HA	2.16	0.46
1:D:285:LEU:O	1:D:285:LEU:HG	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: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
3:F:1543:ILE:C	3:F:1545:GLN:N	2.73	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
1:A:294:ALA:O	1:A:295:GLU:C	2.58	0.46
3:C:1392:ASP:HB2	3:C:1442:HIS:NE2	2.30	0.46
3:C:1525:THR:OG1	3:C:1541:MET:HE3	2.15	0.46
2:E:733:ILE:CG1	2:E:734:ILE:N	2.75	0.46
1:D:97:LYS:HG3	1:D:98:VAL:N	2.30	0.46
1:D:185:ARG:HA	1:D:196:PHE:O	2.16	0.46
3:C:1389:PHE:HD1	3:C:1441:VAL:CG2	2.26	0.46
4:P:36:LEU:N	4:P:36:LEU:CD2	2.78	0.46
3:F:1522:VAL:O	3:F:1547:ILE:HB	2.15	0.46
3:F:1524:LYS:C	3:F:1525:THR:HG22	2.39	0.46
3:F:1571:ALA:N	3:F:1572:LEU:HD23	2.30	0.46
1:D:214:VAL:HG11	1:D:304:VAL:CG2	2.45	0.46
1:A:40:PHE:CE2	1:A:41:PRO:HG3	2.51	0.46
1:A:47:LEU:HD23	1:A:47:LEU:C	2.41	0.46
2:B:877:VAL:HG13	3:C:1451:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1406:TYR:CZ	3:C:1408:SER:HA	2.50	0.46
3:C:1543:ILE:O	3:C:1543:ILE:HG22	2.16	0.46
3:F:1389:PHE:N	3:F:1389:PHE:HD2	2.14	0.46
3:F:1633:SER:O	3:F:1634:MET:C	2.56	0.46
1:D:309:ILE:HG12	1:D:316:MET:HG3	1.97	0.46
1:A:185:ARG:HA	1:A:196:PHE:O	2.16	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:1514:ALA:C	3:C:1516:GLU:H	2.23	0.46
3:C:1537:ASP:OD2	3:C:1569:ARG:HD3	2.16	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:D:40:PHE:CE2	1:D:41:PRO:HG3	2.51	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:H	3:C:1440:LYS:HG3	1.56	0.46
4:P:23:LEU:HD11	4:P:51:ALA:HB1	1.97	0.46
3:F:1409:LYS:C	3:F:1411:GLU:H	2.23	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
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.81	0.45
1:A:461:HIS:O	1:A:464:LYS:HB2	2.16	0.45
4:M:36:LEU:N	4:M:36:LEU:CD2	2.77	0.45
4:P:29:ASN:O	4:P:32:ALA:N	2.49	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
1:A:224:TYR:CD2	1:A:224:TYR:N	2.84	0.45
2:B:852:SER:C	2:B:854:ALA:N	2.73	0.45
3:C:1593:LYS:HA	3:C:1594:PRO:HA	1.71	0.45
4:M:29:ASN:O	4:M:32:ALA:N	2.49	0.45
1:D:20:MET:HG2	1:D:64:VAL:CB	2.47	0.45
1:D:118:THR:HG23	1:D:205:TYR:CE2	2.52	0.45
1:D:224:TYR:CD2	1:D:224:TYR:N	2.84	0.45
1:D:644:ALA:O	1:D:645:ALA:HB3	2.15	0.45
1:A:138:GLY:HA2	1:A:160:SER:HG	1.78	0.45
1:A:164:LEU:O	2:B:787:MET:HG2	2.15	0.45
2:E:863:THR:HB	4:M:7:SER:HB2	1.99	0.45
3:F:1389:PHE:HD1	3:F:1441:VAL:CG2	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1409:LYS:HA	3:F:1412:LEU:HB2	1.99	0.45
3:F:1605:TRP:C	3:F:1606:VAL:HG23	2.42	0.45
1:D:339:PRO:O	1:D:340:LYS:HD3	2.16	0.45
1:D:380:GLN:C	1:D:382:ASP:H	2.25	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
3:C:1508:GLU:O	3:C:1509:GLU:C	2.58	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
1:D:369:VAL:CG1	1:D:370:GLN:H	2.24	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:F:1406:TYR:CD2	3:F:1407:ILE:N	2.84	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
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
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
1:D:251:PHE:CD2	1:D:251:PHE:N	2.85	0.45
1:A:380:GLN:C	1:A:382:ASP:H	2.25	0.45
2:B:733:ILE:HB	2:B:895:TYR:CD2	2.51	0.45
3:C:1410:TYR:C	3:C:1410:TYR:CD2	2.95	0.45
3:C:1506:THR:O	3:C:1508:GLU:N	2.49	0.45
3:F:1615:CYS:O	3:F:1616:GLN:C	2.60	0.45
1:D:291:ASN:N	1:D:291:ASN:HD22	2.13	0.45
1:D:504:ILE:CG2	1:D:505:PRO:HA	2.47	0.45
1:A:295:GLU:H	1:A:295:GLU:CD	2.25	0.45
2:B:734:ILE:H	2:B:734:ILE:CD1	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
2:E:877:VAL:HG13	3:F:1451:GLN:CD	2.42	0.45
1:D:406:LYS:HG3	1:D:407:GLN:O	2.16	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:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.45
3:C:1341:LEU:HD23	3:C:1469:ARG:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1510:ARG:HG3	3:F:1583:TRP:HH2	1.81	0.45
3:F:1519:VAL:CG1	3:F:1520:ASP:N	2.76	0.45
1:A:37:VAL:CG1	1:A:84:VAL:CG2	2.94	0.45
1:A:101:VAL:CG1	1:A:102:SER:N	2.80	0.45
2:E:733:ILE:HB	2:E:895:TYR:CD2	2.51	0.45
1:D:434:LEU:HB2	1:D:513:TYR:HE2	1.81	0.45
1:D:634:GLN:NE2	1:D:635:ARG:C	2.75	0.45
1:A:97:LYS:NZ	1:A:632:THR:O	2.48	0.44
1:A:251:PHE:N	1:A:251:PHE:CD2	2.85	0.44
1:A:271:ILE:O	1:A:271:ILE:HG22	2.16	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
3:F:1472:HIS:CE1	3:F:1474:GLU:H	2.35	0.44
3:F:1497:PHE:HD2	3:F:1497:PHE:O	1.96	0.44
1:D:379:THR:HG22	1:D:384:VAL:N	2.31	0.44
1:A:38:HIS:HE1	1:A:45:LEU:CD1	2.30	0.44
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.52	0.44
1:A:406:LYS:HG3	1:A:407:GLN:O	2.16	0.44
1:A:641:PRO:O	1:A:642:GLN:C	2.59	0.44
3:C:1581:LEU:HD23	3:C:1627:LEU:HD21	1.99	0.44
3:F:1526:ARG:NH2	3:F:1544:GLU:OE1	2.48	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
1:D:641:PRO:O	1:D:642:GLN:C	2.59	0.44
1:A:136:PRO:CG	2:B:789:ASP:HA	2.48	0.44
1:A:590:THR:HB	1:A:593:LYS:CG	2.39	0.44
3:C:1375:ASP:CG	3:C:1430:SER:HA	2.43	0.44
3:C:1526:ARG:O	3:C:1526:ARG:HG3	2.18	0.44
3:C:1562:PHE:CE2	3:C:1598:TYR:HB3	2.53	0.44
3:C:1581:LEU:O	3:C:1581:LEU:CD1	2.60	0.44
4:P:29:ASN:C	4:P:31:LEU:N	2.76	0.44
1:A:30:ASP:OD1	1:A:30:ASP:N	2.50	0.44
1:A:97:LYS:HD3	1:A:625:THR:OG1	2.17	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.48	0.44
3:C:1504:LYS:O	3:C:1505:VAL:HG23	2.18	0.44
3:C:1626:ASP:C	3:C:1629:ALA:H	2.25	0.44
4:P:26:LEU:O	4:P:29:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1508:GLU:OE1	3:F:1508:GLU:HA	2.17	0.44
3:F:1575:GLU:CG	3:F:1576:GLU:N	2.80	0.44
1:D:516:ILE:C	1:D:516:ILE:HD12	2.42	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
1:A:516:ILE:C	1:A:516:ILE:HD12	2.42	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
3:C:1556:VAL:C	3:C:1558:GLN:H	2.25	0.44
2:E:817:VAL:HG22	2:E:907:LEU:HD12	1.99	0.44
3:F:1554:VAL:HG23	3:F:1558:GLN:CD	2.33	0.44
1:D:295:GLU:CD	1:D:295:GLU:H	2.25	0.44
1:D:541:LEU:HD12	1:D:541:LEU:HA	1.77	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
2:E:804:MET:HE2	1:D:239:TYR:HB2	1.99	0.44
1:A:351:MET:HE2	1:A:351:MET:HA	1.99	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
2:E:835:ASN:O	2:E:836:GLN:HB3	2.17	0.44
4:P:73:ILE:O	4:P:77:ILE:HG13	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
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.31	0.44
4:M:26:LEU:O	4:M:29:ASN:N	2.50	0.44
3:F:1460:TYR:CD1	1:D:248:PHE:CG	3.06	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
1:A:227:LYS:HE2	1:A:227:LYS:HB2	1.64	0.44
1:A:239:TYR:HB2	2:B:804:MET:HE2	2.00	0.44
2:B:863:THR:HB	4:P:7:SER:HB2	1.99	0.44
3:C:1565:PRO:O	3:C:1566:ILE:C	2.61	0.44
3:C:1641:ASN:HD22	3:C:1641:ASN:N	2.15	0.44
2:E:819:ARG:NH1	2:E:883:THR:HG23	2.32	0.44
3:F:1416:PHE:CD2	3:F:1417:SER:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:MET:HG2	1:D:64:VAL:CG2	2.47	0.44
1:D:147:ASN:HB2	1:D:148:PRO:CD	2.48	0.44
1:A:268:ARG:HB2	3:C:1378:MET:HE3	2.00	0.43
2:B:742:ARG:N	2:B:902:GLY:O	2.47	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:D:380:GLN:O	1:D:382:ASP:N	2.51	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:1610:PRO:C	3:C:1611:GLU:O	2.61	0.43
2:E:819:ARG:HG2	2:E:820:ASN:CG	2.43	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:D:86:VAL:O	1:D:86:VAL:HG12	2.10	0.43
1:D:465:ILE:HD11	1:D:515:LEU:HD13	2.00	0.43
1:D:492:LEU:HD12	1:D:492:LEU:HA	1.87	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:D:271:ILE:O	1:D:271:ILE:HG22	2.16	0.43
1:D:351:MET:HE2	1:D:351:MET:HA	1.99	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
2:E:833:ARG:HH22	2:E:899:ILE:CD1	2.24	0.43
4:M:15:LEU:HD22	4:M:60:PHE:CE1	2.53	0.43
4:P:14:LYS:O	4:P:15:LEU:C	2.61	0.43
4:P:33:THR:O	4:P:34:GLY:C	2.61	0.43
3:F:1562:PHE:CE1	3:F:1582:MET:HE1	2.54	0.43
1:D:36:THR:HA	1:D:47:LEU:O	2.17	0.43
1:D:584:ASN:OD1	1:D:584:ASN:C	2.61	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
2:E:773:LEU:O	1:D:556:GLY:HA2	2.18	0.43
3:F:1575:GLU:CD	3:F:1576:GLU:H	2.26	0.43
1:D:3:MET:HE2	1:D:626:SER:HB2	2.01	0.43
1:D:84:VAL:HG22	1:D:85:THR:H	1.84	0.43
1:D:97:LYS:HD3	1:D:625:THR:OG1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:VAL:HG12	1:D:403:ARG:H	1.84	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:446:GLY:O	1:D:378:LEU:HD13	2.19	0.43
1:A:458:ASP:OD2	1:A:460:ALA:HB3	2.18	0.43
1:A:634:GLN:NE2	1:A:635:ARG:C	2.75	0.43
3:C:1630:PHE:O	3:C:1631:THR:C	2.62	0.43
2:E:778:THR:HG23	2:E:779:THR:N	2.34	0.43
4:M:73:ILE:O	4:M:77:ILE:HG13	2.18	0.43
3:F:1375:ASP:CG	3:F:1430:SER:HA	2.43	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
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
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:1513:LYS:C	3:C:1516:GLU:HG3	2.43	0.43
3:C:1630:PHE:O	3:C:1633:SER:N	2.52	0.43
4:M:15:LEU:O	4:M:18:GLU:HB2	2.19	0.43
4:M:33:THR:O	4:M:34:GLY:C	2.61	0.43
1:D:453:PHE:CE2	1:D:495:LEU:HB2	2.53	0.43
1:D:455:LEU:HB2	1:D:468:TYR:OH	2.19	0.43
1:A:98:VAL:O	1:A:634:GLN:HG2	2.18	0.43
1:A:584:ASN:C	1:A:584:ASN:OD1	2.61	0.43
1:A:603:ILE:HB	1:A:635:ARG:HH12	1.84	0.43
4:M:14:LYS:O	4:M:15:LEU:C	2.61	0.43
4:P:15:LEU:HD22	4:P:60:PHE:CE1	2.53	0.43
4:P:68:TYR:O	4:P:69:GLN:C	2.61	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
3:F:1612:GLU:C	3:F:1614:GLU:N	2.76	0.43
1:D:404:THR:HG1	1:D:415:ALA:H	1.67	0.43
1:D:477:ARG:HH11	1:D:477:ARG:CG	2.31	0.43
1:A:3:MET:HE2	1:A:626:SER:HB2	2.01	0.43
1:A:177:VAL:HG22	1:A:178:ASN:N	2.34	0.43
5:A:646:NAG:O3	5:A:646:NAG:H62	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:1623:GLN:C	3:C:1625:GLN:N	2.77	0.43
1:D:454:LEU:HA	1:D:491:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:ASP:O	1:D:460:ALA:N	2.52	0.43
1:D:583:LEU:HA	1:D:583:LEU:HD23	1.76	0.43
2:B:865:THR:OG1	4:P:11:GLN:HG2	2.19	0.43
3:C:1616:GLN:O	3:C:1617:ASP:C	2.62	0.43
4:M:23:LEU:HA	4:M:23:LEU:HD23	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
3:F:1542:ALA:C	3:F:1543:ILE:CG1	2.92	0.43
3:F:1544:GLU:CD	3:F:1579:HIS:CE1	2.97	0.43
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
2:E:729:LEU:CD1	2:E:737:GLU:OE2	2.67	0.42
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:1532:LEU:C	3:F:1569:ARG:HH12	2.26	0.42
5:D:646:NAG:O3	5:D:646:NAG:H62	2.19	0.42
1:A:61:MET:HE1	1:A:482:GLY:HA2	2.01	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
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:D:286:LEU:C	1:D:291:ASN:HD22	2.27	0.42
1:D:289:VAL:O	1:D:290:GLN:CB	2.67	0.42
1:A:87:GLN:HG3	1:A:96:GLU:HB3	2.01	0.42
4:P:43:THR:HG21	4:P:73:ILE:HD13	2.01	0.42
3:F:1451:GLN:HA	3:F:1452:PRO:HD3	1.81	0.42
3:F:1562:PHE:CZ	3:F:1582:MET:HE1	2.54	0.42
1:D:298:VAL:O	1:D:298:VAL:HG12	2.18	0.42
1:A:454:LEU:HA	1:A:491:ASP:O	2.19	0.42
2:B:729:LEU:HD13	2:B:737:GLU:OE2	2.20	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:1569:ARG:C	3:F:1570:GLU:HG2	2.32	0.42
1:D:20:MET:HG2	1:D:64:VAL:HG11	2.02	0.42
3:C:1370:TYR:O	3:C:1431:HIS:HA	2.19	0.42
3:C:1575:GLU:H	3:C:1580:TYR:HH	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1635:VAL:HG12	3:F:1636:VAL:N	2.33	0.42
1:D:203:LYS:HG2	1:D:204:GLU:H	1.85	0.42
3:C:1378:MET:HA	3:C:1426:LEU:O	2.19	0.42
4:M:29:ASN:C	4:M:31:LEU:N	2.76	0.42
4:M:68:TYR:O	4:M:69:GLN:C	2.61	0.42
4:P:26:LEU:O	4:P:29:ASN:HB2	2.19	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
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
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
4:M:43:THR:HG21	4:M:73:ILE:HD13	2.01	0.42
3:F:1370:TYR:O	3:F:1431:HIS:HA	2.19	0.42
3:F:1631:THR:O	3:F:1633:SER:N	2.53	0.42
1:D:61:MET:CE	1:D:483:ARG:HG2	2.50	0.42
1:D:219:LYS:HD2	1:D:358:ASP:OD2	2.19	0.42
1:D:350:LEU:O	1:D:351:MET:HE2	2.19	0.42
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.54	0.42
1:A:402:VAL:HG12	1:A:403:ARG:H	1.84	0.42
3:C:1482:LYS:O	3:C:1536:PHE:CZ	2.72	0.42
2:E:778:THR:OG1	2:E:779:THR:N	2.52	0.42
4:P:82:LYS:C	4:P:84:LYS:H	2.27	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
1:A:33:VAL:HG22	1:A:90:PHE:HA	2.02	0.42
1:A:251:PHE:CD1	1:A:280:LEU:HB2	2.55	0.42
2:B:734:ILE:HD11	2:B:898:PHE:HA	2.02	0.42
2:E:885:LEU:HA	2:E:885:LEU:HD12	1.74	0.42
3:F:1497:PHE:CE1	3:F:1498:ILE:HD11	2.54	0.42
3:F:1628:GLY:C	3:F:1630:PHE:H	2.27	0.42
1:D:291:ASN:N	1:D:292:PRO:HD3	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:1415:ALA:O	3:F:1416:PHE:C	2.62	0.42
3:F:1541:MET:CE	3:F:1582:MET:SD	3.08	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
1:A:168:PRO:O	1:A:169:LEU:HG	2.20	0.41
1:A:220:PHE:HB3	1:A:357:PRO:HG2	2.01	0.41
1:A:298:VAL:O	1:A:298:VAL:HG12	2.18	0.41
4:M:26:LEU:O	4:M:29:ASN:HB2	2.19	0.41
4:M:58:LYS:C	4:M:63:MET:HE2	2.45	0.41
3:F:1437:LEU:C	3:F:1437:LEU:HD12	2.45	0.41
1:D:177:VAL:HG22	1:D:178:ASN:N	2.34	0.41
1:A:4:TYR:HB3	1:A:90:PHE:CZ	2.55	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:N	1:A:343:LYS:CD	2.83	0.41
1:A:350:LEU:O	1:A:351:MET:HE2	2.19	0.41
1:A:509:LEU:HB3	1:A:529:VAL:CG1	2.50	0.41
1:A:632:THR:O	1:A:633:ALA:C	2.63	0.41
2:B:898:PHE:CE2	4:M:50:LYS:HA	2.54	0.41
3:C:1414:LYS:HD3	3:C:1419:ARG:HG3	2.02	0.41
3:C:1437:LEU:C	3:C:1437:LEU:HD12	2.45	0.41
4:M:29:ASN:O	4:M:31:LEU:N	2.53	0.41
3:F:1552:ASP:O	3:F:1552:ASP:CG	2.61	0.41
3:F:1601:GLY:N	3:F:1604:THR:HG22	2.34	0.41
1:D:61:MET:HE1	1:D:482:GLY:HA2	2.01	0.41
1:D:220:PHE:HB3	1:D:357:PRO:HG2	2.01	0.41
1:D:400:ILE:HD12	1:D:400:ILE:N	2.35	0.41
1:D:502:ASP:OD1	1:D:502:ASP:N	2.54	0.41
1:A:400:ILE:N	1:A:400:ILE:HD12	2.35	0.41
2:E:733:ILE:CG1	2:E:734:ILE:H	2.28	0.41
2:E:734:ILE:HD11	2:E:898:PHE:HA	2.02	0.41
2:E:769:MET:HB2	1:D:561:LEU:HB3	2.02	0.41
3:F:1514:ALA:HB2	3:F:1583:TRP:CZ2	2.55	0.41
3:F:1548:LYS:HD2	3:F:1634:MET:HE3	2.03	0.41
1:D:106:GLY:HA2	1:D:132:HIS:CD2	2.55	0.41
1:A:73:GLU:HB3	1:A:82:LYS:HZ3	1.82	0.41
1:A:195:VAL:CG1	1:A:196:PHE:N	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:789:ASP:O	1:D:135:LEU:HD22	2.19	0.41
4:M:82:LYS:C	4:M:84:LYS:H	2.27	0.41
4:P:13:GLU:O	4:P:13:GLU:HG2	2.20	0.41
3:F:1378:MET:CE	1:D:248:PHE:CD1	3.03	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
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
1:D:632:THR:O	1:D:633:ALA:C	2.63	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
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
2:E:807:PHE:CD2	2:E:807:PHE:C	2.98	0.41
2:E:833:ARG:HD2	2:E:834:GLN:NE2	2.35	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
4:P:58:LYS:C	4:P:63:MET:HE2	2.45	0.41
1:D:33:VAL:HG22	1:D:90:PHE:HA	2.02	0.41
1:D:269:ILE:HA	1:D:270:PRO:HD3	1.93	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
3:C:1445:PHE:HZ	4:P:7:SER:HG	1.65	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
3:F:1545:GLN:HG3	3:F:1546:THR:H	1.86	0.41
3:F:1556:VAL:C	3:F:1558:GLN:H	2.27	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
1:A:37:VAL:CG1	1:A:84:VAL:HG21	2.51	0.41
1:A:286:LEU:C	1:A:291:ASN:HD22	2.27	0.41
1:A:292:PRO:O	1:A:294:ALA:N	2.54	0.41
1:A:453:PHE:HE2	1:A:495:LEU:HB2	1.86	0.41
1:A:615:GLY:C	1:A:617:PHE:N	2.79	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:1525:THR:CB	3:C:1541:MET:HE3	2.51	0.41
1:D:4:TYR:HB3	1:D:90:PHE:CZ	2.55	0.41
1:D:453:PHE:HE2	1:D:495:LEU:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:ND2	5:A:646:NAG:C1	2.84	0.41
1:A:378:LEU:HD13	1:D:446:GLY:O	2.20	0.41
2:E:869:LYS:O	2:E:870:SER:HB3	2.21	0.41
4:P:58:LYS:HA	4:P:58:LYS:HD2	1.75	0.41
3:F:1460:TYR:CE1	1:D:248:PHE:HB2	2.56	0.41
1:D:389:ILE:O	1:D:389:ILE:HG13	2.20	0.41
1:A:73:GLU:HB3	1:A:82:LYS:HZ1	1.82	0.41
1:A:342:PHE:HD1	1:A:391:THR:HG21	1.86	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
2:B:734:ILE:N	2:B:734:ILE:CD1	2.81	0.41
2:B:811:LEU:HD12	2:B:811:LEU:HA	1.85	0.41
3:C:1415:ALA:O	3:C:1416:PHE:C	2.62	0.41
3:C:1526:ARG:CZ	3:C:1542:ALA:HB2	2.51	0.41
3:C:1552:ASP:O	3:C:1554:VAL:HG12	2.20	0.41
3:C:1572:LEU:O	3:C:1573:LYS:C	2.62	0.41
2:E:786:SER:O	2:E:793:ILE:HA	2.21	0.41
2:E:838:LEU:HD23	2:E:838:LEU:HA	1.85	0.41
2:E:865:THR:OG1	4:M:11:GLN:HG2	2.21	0.41
3:F:1472:HIS:CE1	3:F:1473:PRO:HD2	2.55	0.41
1:D:14:LEU:HD11	1:D:103:LEU:CD2	2.51	0.41
1:D:98:VAL:O	1:D:634:GLN:HG2	2.17	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:N	1:D:343:LYS:CD	2.83	0.41
1:D:474:ASN:O	1:D:475:LYS:C	2.64	0.41
1:A:101:VAL:HG12	1:A:102:SER:N	2.35	0.41
1:A:241:LYS:HD3	1:A:241:LYS:HA	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
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:1378:MET:HE3	1:D:248:PHE:CD1	2.55	0.41
1:D:508:ARG:CZ	1:D:604:GLY:HA3	2.51	0.41
1:A:578:LYS:HB3	1:A:578:LYS:HE2	1.86	0.40
2:B:869:LYS:O	2:B:870:SER:HB3	2.21	0.40
3:C:1507:LEU:HB3	3:C:1508:GLU:OE1	2.21	0.40
4:P:61:LYS:HB3	4:P:62:LYS:H	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LYS:HE2	1:D:117:TYR:CD1	2.56	0.40
1:D:158:LEU:HD12	1:D:158:LEU:HA	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
1:A:286:LEU:O	1:A:287:ASP:C	2.64	0.40
1:A:627:SER:C	1:A:629:GLY:H	2.30	0.40
2:B:756:LEU:N	2:B:756:LEU:HD23	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
3:F:1556:VAL:CG1	3:F:1557:GLY:N	2.84	0.40
1:D:113:ASP:OD1	1:D:113:ASP:N	2.53	0.40
1:D:458:ASP:C	1:D:460:ALA:N	2.79	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:OD1	1:A:502:ASP:N	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:1555:GLN:O	3:C:1556:VAL:C	2.63	0.40
3:F:1507:LEU:HD12	3:F:1626:ASP:CG	2.46	0.40
3:F:1622:LYS:HG3	3:F:1623:GLN:H	1.78	0.40
1:D:434:LEU:HB2	1:D:513:TYR:CE2	2.57	0.40
1:A:389:ILE:O	1:A:389:ILE:HG13	2.20	0.40
1:A:458:ASP:C	1:A:460:ALA:N	2.79	0.40
1:A:487:GLU:HG3	1:D:392:HIS:HE1	1.86	0.40
2:B:863:THR:HB	4:P:7:SER:CB	2.52	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
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: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
1:D:615:GLY:C	1:D:617:PHE:N	2.79	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%)	7	35
1	D	637/645 (99%)	557 (87%)	69 (11%)	11 (2%)	7	35
2	B	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	11	43
2	E	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	11	43
3	C	287/343 (84%)	216 (75%)	44 (15%)	27 (9%)	0	6
3	F	289/343 (84%)	196 (68%)	42 (14%)	51 (18%)	0	1
4	M	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2	21
4	P	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2	21
All	All	2378/2564 (93%)	1970 (83%)	298 (12%)	110 (5%)	2	17

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	499 (89%)	64 (11%)	5	24
1	D	563/567 (99%)	499 (89%)	64 (11%)	5	24
2	B	172/191 (90%)	135 (78%)	37 (22%)	1	6
2	E	172/191 (90%)	135 (78%)	37 (22%)	1	6
3	C	266/309 (86%)	205 (77%)	61 (23%)	1	5
3	F	268/309 (87%)	191 (71%)	77 (29%)	0	2
4	M	76/79 (96%)	65 (86%)	11 (14%)	3	17
4	P	76/79 (96%)	65 (86%)	11 (14%)	3	17
All	All	2156/2292 (94%)	1794 (83%)	362 (17%)	2	13

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	6	ILE
1	A	21	VAL
1	A	30	ASP
1	A	51	LYS
1	A	52	THR

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Mol	Chain	Res	Type
1	A	61	MET
1	A	64	VAL
1	A	84	VAL
1	A	85	THR
1	A	110	ILE
1	A	124	LEU
1	A	127	ILE
1	A	137	VAL
1	A	149	GLU
1	A	155	GLN
1	A	156	ASP
1	A	157	SER
1	A	162	ASN
1	A	163	GLN
1	A	169	LEU
1	A	176	LEU
1	A	178	ASN
1	A	191	SER
1	A	198	THR
1	A	207	LEU
1	A	213	ILE
1	A	215	GLU
1	A	217	THR
1	A	223	ILE
1	A	241	LYS
1	A	251	PHE
1	A	257	GLU
1	A	278	VAL
1	A	284	VAL
1	A	289	VAL
1	A	290	GLN
1	A	298	VAL
1	A	304	VAL
1	A	314	SER
1	A	365	VAL
1	A	375	VAL
1	A	404	THR
1	A	410	SER
1	A	422	LEU
1	A	438	VAL
1	A	451	VAL
1	A	454	LEU

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Mol	Chain	Res	Type
1	A	472	ILE
1	A	477	ARG
1	A	501	THR
1	A	515	LEU
1	A	516	ILE
1	A	524	VAL
1	A	534	LYS
1	A	535	ASP
1	A	538	VAL
1	A	542	VAL
1	A	548	SER
1	A	554	VAL
1	A	559	MET
1	A	603	ILE
1	A	616	VAL
1	A	634	GLN
2	B	729	LEU
2	B	734	ILE
2	B	741	SER
2	B	753	VAL
2	B	757	LYS
2	B	765	SER
2	B	769	MET
2	B	771	ILE
2	B	776	SER
2	B	786	SER
2	B	793	ILE
2	B	795	VAL
2	B	809	ILE
2	B	813	LEU
2	B	817	VAL
2	B	818	VAL
2	B	828	VAL
2	B	834	GLN
2	B	837	GLU
2	B	841	ARG
2	B	844	LEU
2	B	845	LEU
2	B	861	GLN
2	B	864	VAL
2	B	865	THR
2	B	869	LYS

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Mol	Chain	Res	Type
2	B	871	SER
2	B	873	SER
2	B	877	VAL
2	B	882	LYS
2	B	887	GLU
2	B	888	VAL
2	B	890	VAL
2	B	899	ILE
2	B	903	VAL
2	B	910	VAL
2	B	912	GLU
3	C	1337	ASN
3	C	1342	LYS
3	C	1344	THR
3	C	1350	GLU
3	C	1361	THR
3	C	1362	MET
3	C	1378	MET
3	C	1387	THR
3	C	1389	PHE
3	C	1393	THR
3	C	1394	ASP
3	C	1397	LYS
3	C	1406	TYR
3	C	1412	LEU
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	1426	LEU
3	C	1430	SER
3	C	1433	GLU
3	C	1447	VAL
3	C	1450	ILE
3	C	1465	GLU
3	C	1468	THR
3	C	1469	ARG
3	C	1479	LYS
3	C	1484	CYS
3	C	1494	GLU

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Mol	Chain	Res	Type
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	1555	GLN
3	C	1567	LYS
3	C	1569	ARG
3	C	1573	LYS
3	C	1574	LEU
3	C	1578	LYS
3	C	1579	HIS
3	C	1580	TYR
3	C	1581	LEU
3	C	1582	MET
3	C	1587	SER
3	C	1590	TRP
3	C	1595	ASN
3	C	1599	ILE
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	753	VAL
2	E	757	LYS
2	E	765	SER
2	E	769	MET
2	E	771	ILE
2	E	776	SER
2	E	786	SER
2	E	793	ILE
2	E	795	VAL

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Mol	Chain	Res	Type
2	E	809	ILE
2	E	813	LEU
2	E	817	VAL
2	E	818	VAL
2	E	828	VAL
2	E	834	GLN
2	E	837	GLU
2	E	841	ARG
2	E	844	LEU
2	E	845	LEU
2	E	861	GLN
2	E	864	VAL
2	E	865	THR
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	888	VAL
2	E	890	VAL
2	E	899	ILE
2	E	903	VAL
2	E	910	VAL
2	E	912	GLU
4	M	7	SER
4	M	8	ASN
4	M	21	SER
4	M	25	GLU
4	M	26	LEU
4	M	31	LEU
4	M	36	LEU
4	M	38	THR
4	M	56	LYS
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

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Mol	Chain	Res	Type
4	P	36	LEU
4	P	38	THR
4	P	56	LYS
4	P	59	ASP
4	P	78	ASP
3	F	1337	ASN
3	F	1342	LYS
3	F	1344	THR
3	F	1350	GLU
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	1397	LYS
3	F	1408	SER
3	F	1412	LEU
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	1426	LEU
3	F	1430	SER
3	F	1433	GLU
3	F	1447	VAL
3	F	1450	ILE
3	F	1465	GLU
3	F	1468	THR
3	F	1469	ARG
3	F	1479	LYS
3	F	1484	CYS
3	F	1494	GLU
3	F	1495	ASN
3	F	1497	PHE
3	F	1498	ILE
3	F	1507	LEU
3	F	1509	GLU
3	F	1510	ARG

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Mol	Chain	Res	Type
3	F	1513	LYS
3	F	1519	VAL
3	F	1522	VAL
3	F	1525	THR
3	F	1526	ARG
3	F	1528	VAL
3	F	1532	LEU
3	F	1534	ASN
3	F	1540	ILE
3	F	1541	MET
3	F	1547	ILE
3	F	1551	SER
3	F	1552	ASP
3	F	1554	VAL
3	F	1555	GLN
3	F	1559	GLN
3	F	1560	ARG
3	F	1563	ILE
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	3	MET
1	D	6	ILE

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Mol	Chain	Res	Type
1	D	21	VAL
1	D	30	ASP
1	D	51	LYS
1	D	52	THR
1	D	61	MET
1	D	64	VAL
1	D	84	VAL
1	D	85	THR
1	D	110	ILE
1	D	124	LEU
1	D	127	ILE
1	D	137	VAL
1	D	149	GLU
1	D	155	GLN
1	D	156	ASP
1	D	157	SER
1	D	162	ASN
1	D	163	GLN
1	D	169	LEU
1	D	176	LEU
1	D	178	ASN
1	D	191	SER
1	D	198	THR
1	D	207	LEU
1	D	213	ILE
1	D	215	GLU
1	D	217	THR
1	D	223	ILE
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	298	VAL
1	D	304	VAL
1	D	314	SER
1	D	365	VAL
1	D	375	VAL
1	D	404	THR
1	D	410	SER

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Mol	Chain	Res	Type
1	D	422	LEU
1	D	438	VAL
1	D	451	VAL
1	D	454	LEU
1	D	472	ILE
1	D	477	ARG
1	D	501	THR
1	D	515	LEU
1	D	516	ILE
1	D	524	VAL
1	D	534	LYS
1	D	535	ASP
1	D	538	VAL
1	D	542	VAL
1	D	548	SER
1	D	554	VAL
1	D	559	MET
1	D	603	ILE
1	D	616	VAL
1	D	634	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	144	ASN
1	A	155	GLN
1	A	291	ASN
1	A	392	HIS
1	A	634	GLN
3	C	1431	HIS
3	C	1481	ASN
3	C	1495	ASN
3	C	1531	GLN
3	C	1608	HIS
3	C	1616	GLN
3	C	1641	ASN
4	M	8	ASN
4	M	29	ASN
4	M	69	GLN
4	P	8	ASN
4	P	29	ASN

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Mol	Chain	Res	Type
4	P	69	GLN
3	F	1495	ASN
3	F	1534	ASN
3	F	1545	GLN
3	F	1559	GLN
3	F	1616	GLN
3	F	1620	ASN
1	D	132	HIS
1	D	144	ASN
1	D	155	GLN
1	D	163	GLN
1	D	291	ASN
1	D	311	HIS
1	D	392	HIS
1	D	634	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	646	-	14,14,15	0.43	0	17,19,21	1.45	1 (5%)
5	NAG	A	646	-	14,14,15	0.44	0	17,19,21	1.46	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	646	-	-	4/6/23/26	0/1/1/1
5	NAG	A	646	-	-	4/6/23/26	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	A	646	NAG	C1-O5-C5	4.95	118.82	112.19
5	D	646	NAG	C1-O5-C5	4.92	118.78	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	641/645 (99%)	0.63	45 (7%)	22	14	18, 53, 106, 172	0
1	D	641/645 (99%)	0.61	28 (4%)	39	21	18, 53, 106, 172	0
2	B	184/206 (89%)	0.30	2 (1%)	78	54	19, 50, 80, 114	0
2	E	184/206 (89%)	0.43	4 (2%)	62	37	25, 57, 87, 120	0
3	C	293/343 (85%)	0.92	43 (14%)	6	5	35, 87, 198, 230	0
3	F	295/343 (86%)	1.34	69 (23%)	2	2	31, 93, 143, 194	0
4	M	84/88 (95%)	0.15	0	100	100	48, 68, 105, 175	0
4	P	84/88 (95%)	0.13	1 (1%)	76	52	43, 65, 101, 184	0
All	All	2406/2564 (93%)	0.67	192 (7%)	18	12	18, 63, 125, 230	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1557	GLY	7.0
1	A	78	LYS	6.4
3	C	1610	PRO	5.4
3	F	1391	PRO	5.2
3	F	1441	VAL	5.2
1	A	64	VAL	5.2
1	A	41	PRO	5.0
3	F	1559	GLN	4.8
1	A	48	SER	4.8
3	F	1412	LEU	4.8
3	F	1387	THR	4.7
3	F	1612	GLU	4.5
3	F	1420	ASN	4.5
3	C	1624	CYS	4.4
3	C	1627	LEU	4.4
3	C	1612	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	1632	GLU	4.3
3	F	1626	ASP	4.3
3	F	1417	SER	4.3
3	C	1631	THR	4.3
3	F	1594	PRO	4.2
3	F	1396	LEU	4.1
3	C	1628	GLY	4.0
3	C	1635	VAL	4.0
3	C	1609	TRP	4.0
1	A	99	VAL	4.0
3	F	1442	HIS	3.9
1	A	439	LEU	3.8
3	C	1594	PRO	3.8
3	C	1616	GLN	3.8
3	C	1637	PHE	3.8
3	C	1545	GLN	3.8
1	D	518	ALA	3.8
1	D	48	SER	3.7
3	F	1556	VAL	3.7
3	C	1526	ARG	3.7
3	F	1498	ILE	3.7
1	A	79	GLY	3.6
3	F	1483	LEU	3.6
3	F	1390	ALA	3.6
3	F	1449	LEU	3.6
1	A	461	HIS	3.5
3	F	1348	ALA	3.5
1	A	54	LEU	3.5
3	C	1544	GLU	3.5
3	F	1508	GLU	3.4
3	F	1411	GLU	3.4
1	A	80	ARG	3.4
3	F	1640	PRO	3.3
1	D	98	VAL	3.3
1	D	78	LYS	3.3
1	D	19	THR	3.3
1	A	46	VAL	3.3
3	F	1496	CYS	3.3
3	F	1361	THR	3.2
3	C	1547	ILE	3.2
3	C	1613	ASP	3.2
3	F	1419	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	530	TRP	3.1
3	F	1358	ALA	3.1
3	F	1450	ILE	3.1
1	A	49	SER	3.1
3	C	1358	ALA	3.1
3	C	1556	VAL	3.1
1	A	637	GLU	3.1
1	A	437	SER	3.0
1	D	491	ASP	3.0
1	A	82	LYS	3.0
3	F	1535	ASP	3.0
2	E	911	PRO	3.0
3	C	1623	GLN	3.0
3	F	1514	ALA	3.0
1	A	451	VAL	3.0
1	D	494	VAL	2.9
3	C	1559	GLN	2.9
1	A	103	LEU	2.9
1	A	452	ASN	2.9
3	C	1615	CYS	2.9
3	F	1363	ILE	2.9
3	F	1360	ASN	2.9
1	A	95	VAL	2.8
3	F	1460	TYR	2.8
3	F	1596	LEU	2.8
1	A	349	ASP	2.8
3	F	1492	ALA	2.8
3	F	1506	THR	2.8
1	A	102	SER	2.8
3	F	1470	PHE	2.8
3	F	1414	LYS	2.8
1	A	36	THR	2.7
3	C	1507	LEU	2.7
3	F	1533	SER	2.7
3	F	1489	CYS	2.7
3	F	1416	PHE	2.7
3	C	1555	GLN	2.7
1	D	439	LEU	2.7
3	F	1347	PRO	2.7
1	D	512	TYR	2.7
1	D	645	ALA	2.7
3	C	1625	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	1505	VAL	2.6
1	A	521	GLN	2.6
3	C	1618	GLU	2.6
1	D	105	SER	2.6
3	C	1638	GLY	2.6
3	F	1537	ASP	2.6
1	D	437	SER	2.6
3	C	1636	VAL	2.6
1	A	97	LYS	2.6
1	A	445	PRO	2.6
3	F	1447	VAL	2.6
3	C	1607	GLU	2.5
1	A	636	ALA	2.5
1	D	644	ALA	2.5
3	F	1389	PHE	2.5
3	F	1445	PHE	2.5
3	F	1444	TYR	2.5
3	F	1488	LEU	2.5
3	F	1386	MET	2.5
2	E	729	LEU	2.5
1	D	528	SER	2.5
1	D	435	HIS	2.4
2	B	729	LEU	2.4
3	F	1443	GLN	2.4
3	F	1362	MET	2.4
1	A	73	GLU	2.4
1	D	103	LEU	2.4
3	C	1621	GLN	2.4
1	A	40	PHE	2.4
1	A	27	ALA	2.4
3	C	1630	PHE	2.4
1	D	610	GLY	2.4
3	F	1418	ASP	2.4
3	F	1613	ASP	2.3
3	F	1388	GLY	2.3
1	D	132	HIS	2.3
1	A	35	VAL	2.3
3	C	1620	ASN	2.3
1	D	52	THR	2.3
1	A	375	VAL	2.3
3	F	1349	PRO	2.3
3	F	1504	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	1583	TRP	2.2
3	F	1637	PHE	2.2
2	B	804	MET	2.2
1	D	36	THR	2.2
1	D	473	MET	2.2
4	P	85	TYR	2.2
3	F	1639	CYS	2.2
3	F	1382	ASP	2.2
3	C	1554	VAL	2.2
2	E	804	MET	2.2
3	C	1492	ALA	2.1
1	A	132	HIS	2.1
3	F	1512	ASP	2.1
1	D	634	GLN	2.1
3	F	1560	ARG	2.1
1	D	369	VAL	2.1
2	E	860	HIS	2.1
1	D	531	VAL	2.1
3	C	1496	CYS	2.1
1	D	2	PRO	2.1
1	D	643	PRO	2.1
1	A	52	THR	2.1
1	A	623	THR	2.1
1	A	518	ALA	2.1
1	A	548	SER	2.1
1	A	87	GLN	2.1
3	C	1558	GLN	2.1
1	A	496	PRO	2.1
1	A	12	LEU	2.1
3	C	1553	GLU	2.1
3	F	1364	LEU	2.1
3	F	1403	VAL	2.1
1	A	20	MET	2.1
3	F	1394	ASP	2.0
3	F	1485	ARG	2.0
1	A	16	SER	2.0
3	C	1515	CYS	2.0
3	C	1447	VAL	2.0
1	D	450	ASN	2.0
3	F	1595	ASN	2.0
1	A	38	HIS	2.0
1	A	98	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	1505	VAL	2.0
1	A	62	GLY	2.0
3	F	1593	LYS	2.0
3	F	1393	THR	2.0
1	A	96	GLU	2.0
3	C	1629	ALA	2.0
3	F	1392	ASP	2.0
3	F	1439	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	D	646	14/15	0.58	0.20	62,87,108,108	0
5	NAG	A	646	14/15	0.61	0.22	62,87,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.