Full wwPDB X-ray Structure Validation Report (i)

Oct 29, 2024 – 09:51 AM EDT

PDB ID	:	3OHX
Title	:	Molecular Basis for Complement Recognition and Inhibition Determined by Crystallographic Studies of the Staphylococcal Complement Inhibitor (SCIN) Bound to C3c and C3b
Authors	:	Geisbrecht, B.V.; Garcia, B.L.
Deposited on	:	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 (i) 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 (i)) were used in the production of this report:

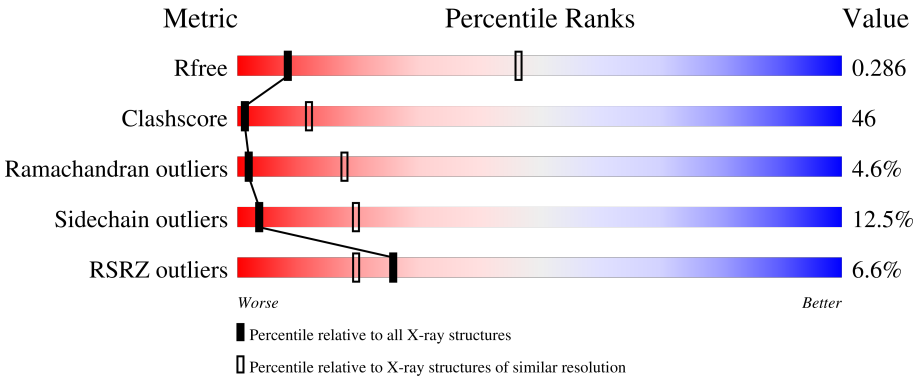
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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 <=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	6% 48% 47%
1	D	645	4% 48% 47%
2	B	206	% 37% 41% 10% 11%
2	E	206	% 36% 43% 10% 11%
3	C	343	10% 27% 41% 14% 15%

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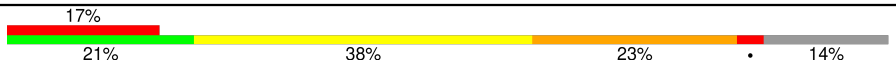
Mol	Chain	Length	Quality of chain
3	F	343	
4	M	88	
4	P	88	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19119 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Complement C3.

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

- Molecule 2 is a protein called Complement C3.

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

- Molecule 3 is a protein called Complement C3.

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

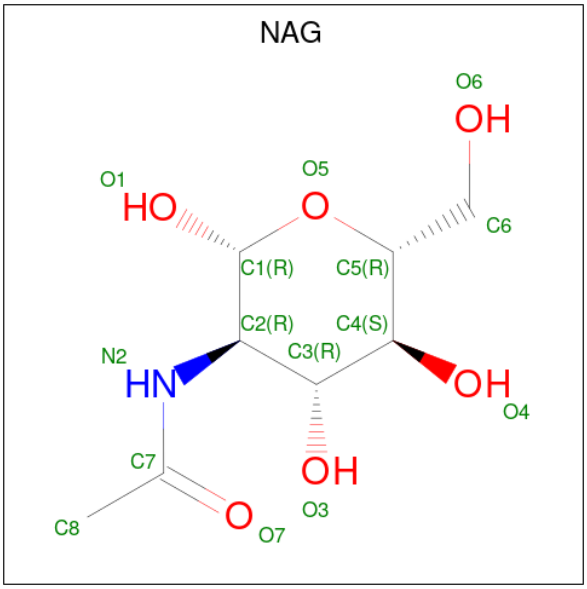
- Molecule 4 is a protein called Staphylococcal complement inhibitor.

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



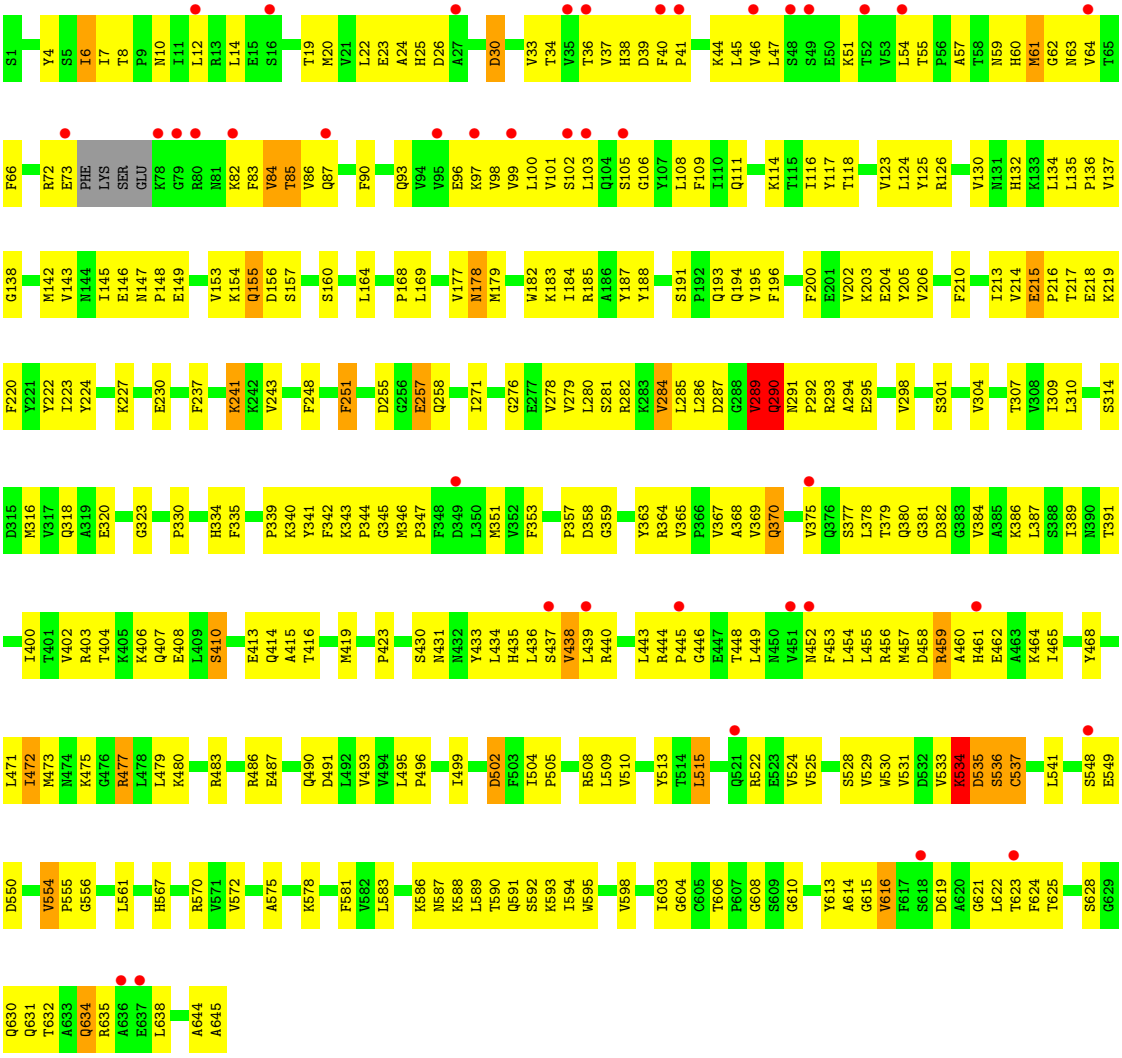
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

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.

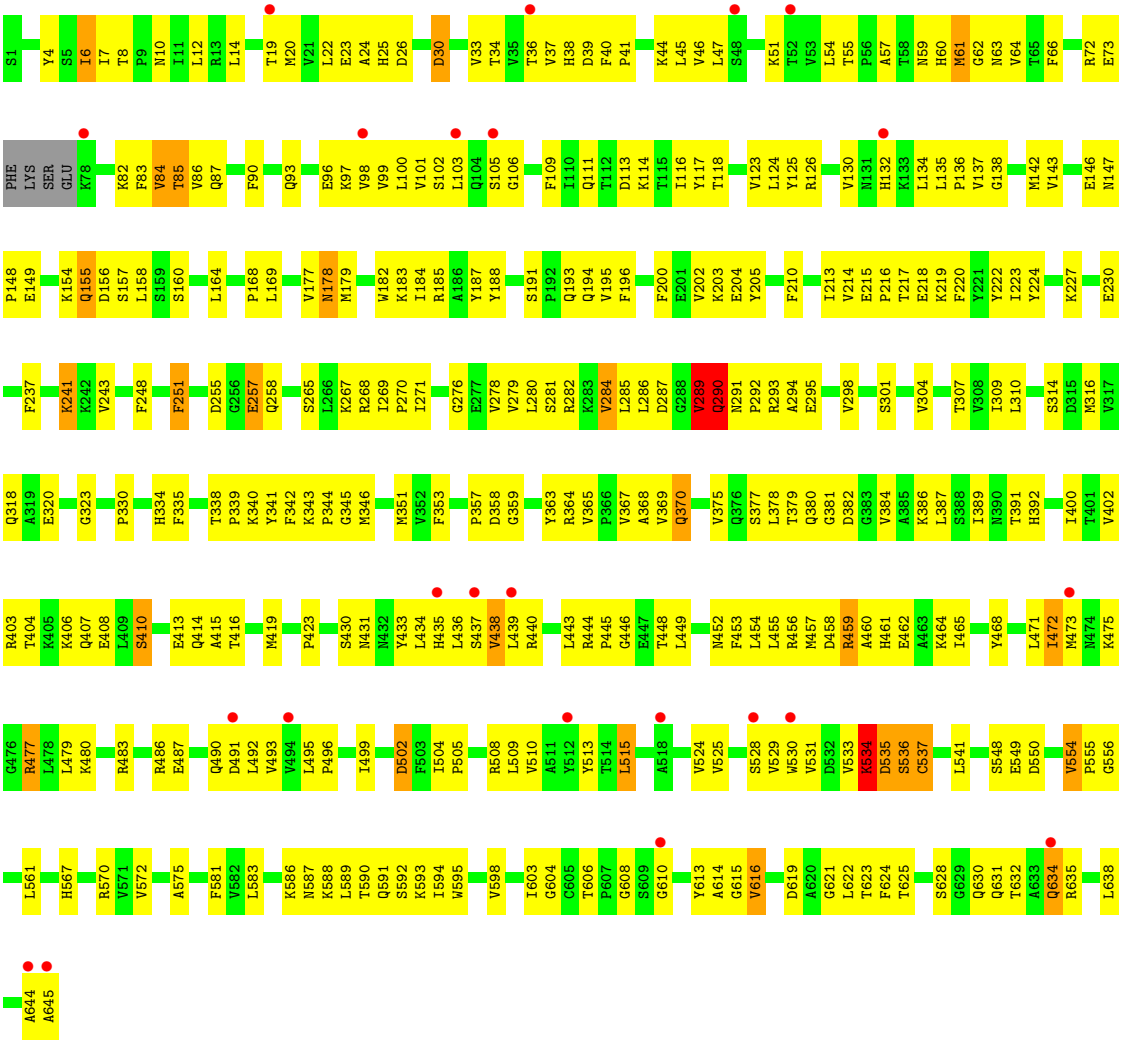
• Molecule 1: Complement C3

Chain A:



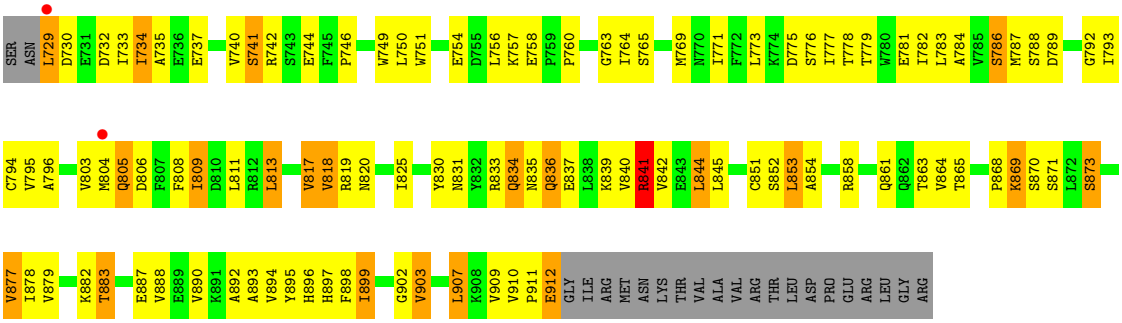
• Molecule 1: Complement C3

Chain D:



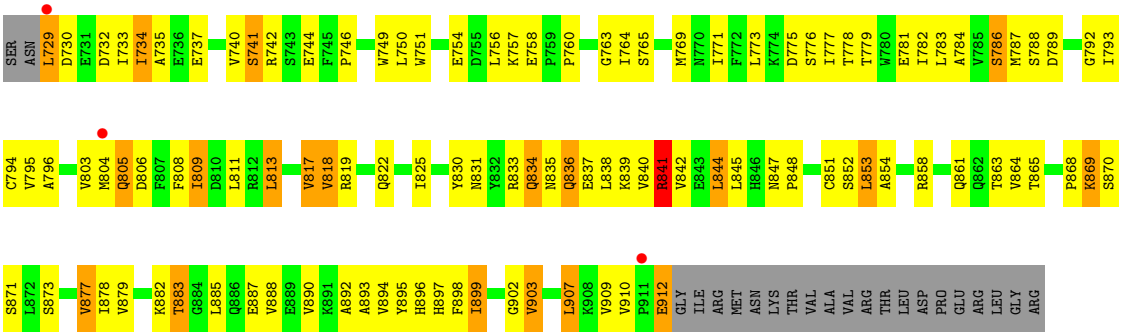
• Molecule 2: Complement C3

Chain B:



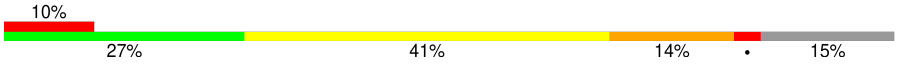
• Molecule 2: Complement C3

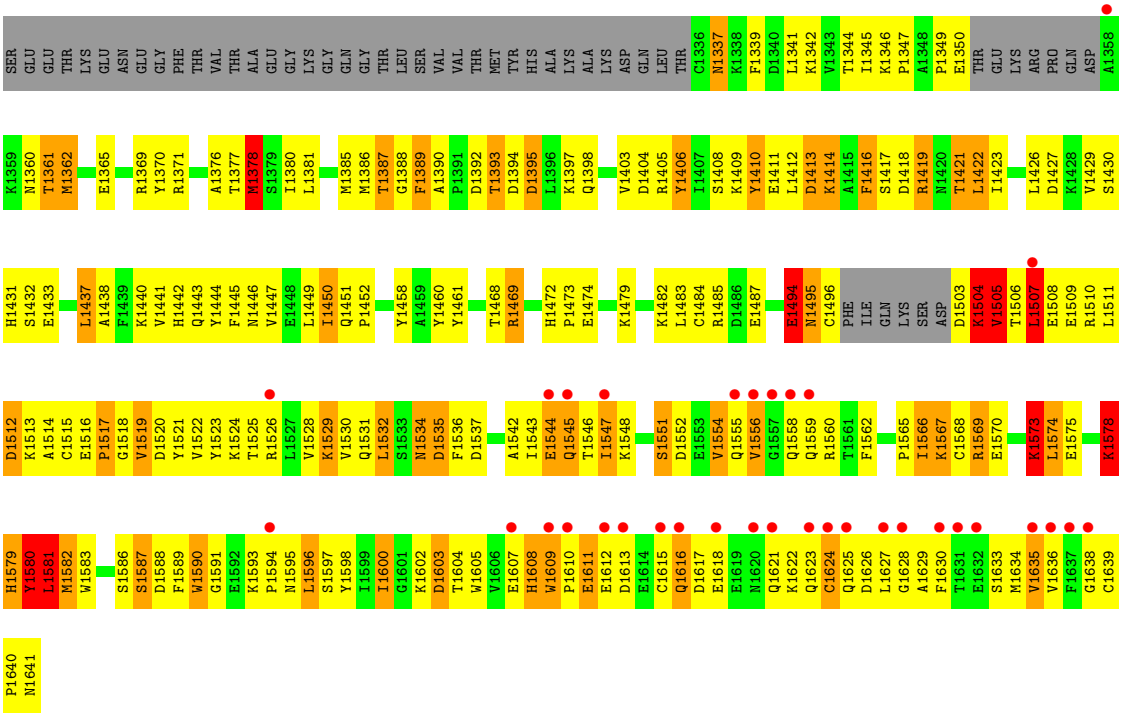
Chain E:



• Molecule 3: Complement C3

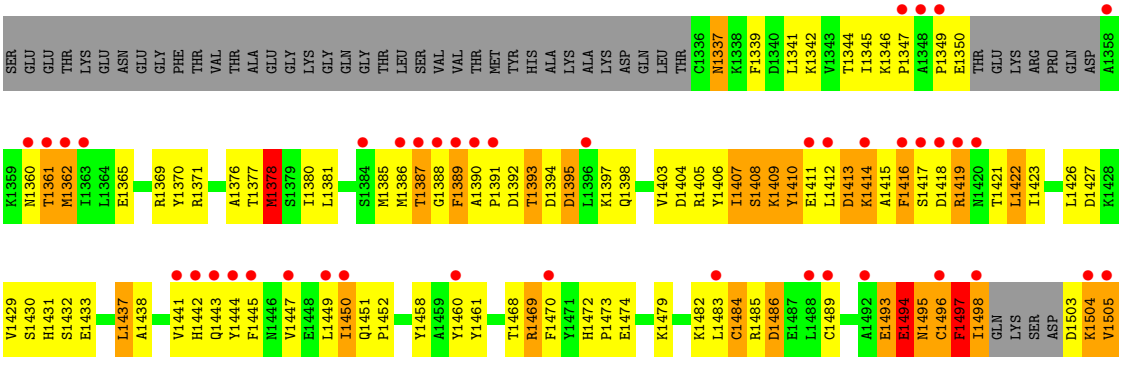
Chain C:

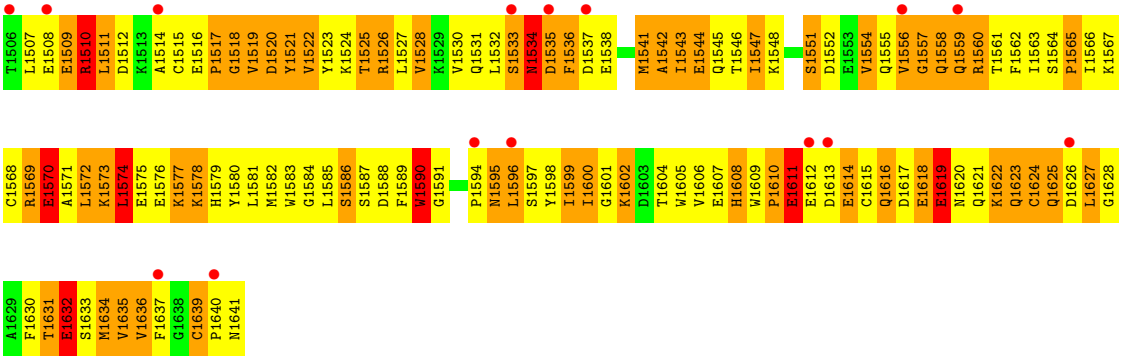




• Molecule 3: Complement C3

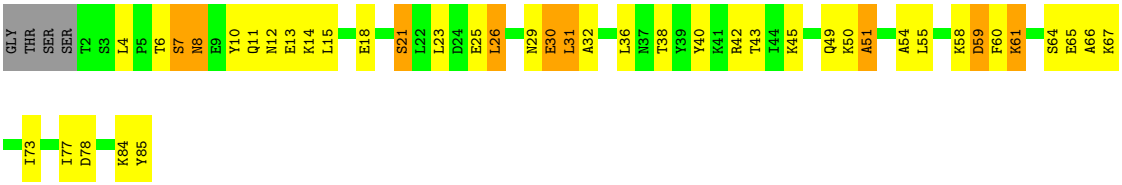
Chain F:





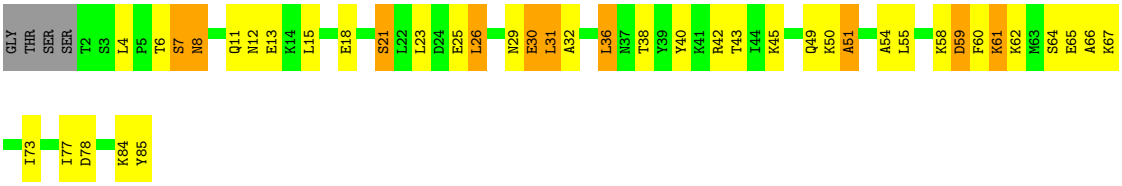
• Molecule 4: Staphylococcal complement inhibitor

Chain M:



• Molecule 4: Staphylococcal complement inhibitor

Chain P:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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 $< |L| >$, $< L^2 >$ 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	0.45	0/5089	0.63	0/6916
1	D	0.45	0/5089	0.63	0/6916
2	B	0.51	0/1520	0.70	1/2066 (0.0%)
2	E	0.51	0/1520	0.70	1/2066 (0.0%)
3	C	0.49	0/2422	0.73	2/3264 (0.1%)
3	F	0.56	0/2442	0.74	1/3291 (0.0%)
4	M	0.39	0/690	0.59	0/923
4	P	0.39	0/690	0.59	0/923
All	All	0.48	0/19462	0.67	5/26365 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4989	0	5051	367	0
1	D	4989	0	5051	372	0
2	B	1488	0	1512	125	0
2	E	1488	0	1512	119	0
3	C	2377	0	2279	319	0
3	F	2396	0	2299	474	0
4	M	682	0	697	56	0
4	P	682	0	697	50	0
5	A	14	0	13	4	0
5	D	14	0	13	3	0
All	All	19119	0	19124	1763	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1520:ASP:O	3:F:1521:TYR:HB3	1.60	0.98
3:F:1497:PHE:CE1	3:F:1498:ILE:HG13	1.98	0.98
3:C:1543:ILE:HD12	3:C:1554:VAL:HG21	1.47	0.97
3:C:1580:TYR:CD2	3:C:1580:TYR:N	2.30	0.96
3:C:1360:ASN:HD22	3:C:1443:GLN:HB3	1.30	0.96
3:C:1578:LYS:HB3	3:C:1580:TYR:HE2	1.12	0.95
3:C:1582:MET:HB2	3:C:1605:TRP:O	1.66	0.95
3:F:1507:LEU:HB3	3:F:1510:ARG:HH21	0.80	0.95
3:F:1536:PHE:CD2	3:F:1566:ILE:CG1	2.49	0.95
2:B:853:LEU:HD11	3:C:1451:GLN:HB2	1.45	0.95
1:D:510:VAL:HG12	1:D:528:SER:HB3	1.48	0.94
3:C:1578:LYS: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
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
3:F:1595:ASN:C	3:F:1596:LEU:HG	1.88	0.92
1:A:590:THR:HG22	1:A:592:SER:N	1.83	0.92
3:C:1543:ILE:O	3:C:1556:VAL:HG13	1.68	0.92
3:C:1581:LEU:C	3:C:1581:LEU:CD1	2.30	0.92
3:C:1522:VAL:O	3:C:1523:TYR:CD1	2.23	0.92
3:C:1526:ARG:HG2	3:C:1542:ALA:CB	2.00	0.92
3:F:1485:ARG:O	3:F:1486:ASP:HB2	1.68	0.92
3:F:1378:MET:CE	1:D:268:ARG:HB2	2.00	0.91
3:C:1609:TRP:CE3	3:C:1627:LEU:HD22	2.05	0.91
3:F:1590:TRP: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:912:GLU:CD	2:B:912:GLU:N	2.30	0.85
1:A:289:VAL:C	1:A:290:GLN:CG	2.44	0.84
3:F:1536:PHE:CD2	3:F:1566:ILE:HG12	2.11	0.84
3:F:1504:LYS:C	3:F:1505:VAL:HG22	1.96	0.84
3:F:1524:LYS:HD2	3:F:1525:THR:N	1.92	0.83
2:E:734:ILE:HD12	2:E:734:ILE:H	1.42	0.83
1:D:289:VAL:C	1:D:290:GLN:CG	2.44	0.83
2:B:853:LEU:CD1	3:C:1451:GLN:HB2	2.08	0.83
3:F:1571:ALA:O	3:F:1572:LEU:HD22	1.77	0.83
3:F:1572:LEU:C	3:F:1574:LEU:HD23	1.99	0.83
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:1526:ARG:HH21	3:F:1544:GLU:CD	1.84	0.81
1:A:8:THR:HG22	1:A:20:MET:HB2	1.60	0.81
3:C:1578:LYS:HG2	3:C:1580:TYR:CZ	2.16	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	3:F:1573:LYS:HD2	1.79	0.80
1:D:289:VAL:O	1:D:290:GLN:CG	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
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
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:1521:TYR:CE2	3:F:1584:GLY:CA	2.66	0.79
3:C:1522:VAL:O	3:C:1523:TYR:HD1	1.63	0.79
3:F:1406:TYR:O	3:F:1407:ILE:CG1	2.30	0.79
3:F:1521:TYR:CE2	3:F:1584:GLY:HA3	2.18	0.78
3:F:1533:SER:CB	3:F:1537:ASP:HA	2.10	0.78
3:F:1569:ARG:HG2	3:F:1570:GLU:CD	1.98	0.78
3:F:1569:ARG:O	3:F:1570:GLU:CG	2.30	0.78
3:C:1337:ASN:O	3:C:1371:ARG:HD2	1.84	0.78
3:C:1446:ASN:HB2	4:P:4:LEU:HB2	1.63	0.78
2:B:841:ARG:HG2	2:B:841:ARG:NH1	1.95	0.78
3:F:1337:ASN:O	3:F:1371:ARG:HD2	1.84	0.78
3:F:1536:PHE:HD2	3:F:1566:ILE:HG12	1.49	0.78
2:E:912:GLU:CD	2:E:912:GLU:N	2.30	0.77
3:F:1494:GLU:OE2	3:F:1494:GLU:CA	2.30	0.77
2:B:833:ARG:HH22	2:B:899:ILE:HD11	1.47	0.77
3:F:1543:ILE:HD13	3:F:1559:GLN:HA	1.65	0.77
2:B:819:ARG:HH21	2:B:911:PRO:HB3	1.49	0.77
3:F:1532:LEU:HA	3:F:1569:ARG:NH1	1.99	0.77
3:F:1601:GLY:H	3:F:1604:THR:CG2	1.97	0.77
1:A:22:LEU:HD11	1:A:64:VAL:HG23	1.67	0.77
3:C:1516:GLU:HB3	3:C:1517:PRO:HD2	1.65	0.77
3:F:1524:LYS:HE3	3:F:1579:HIS:HB3	1.67	0.77
1:D:98:VAL:O	1:D:634:GLN:CG	2.33	0.77
3:F:1558:GLN:O	3:F:1559:GLN:CG	2.29	0.76
3:F:1406:TYR:C	3:F:1407:ILE:CG1	2.53	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:786:SER:HB3	1:D:541:LEU:HD22	1.67	0.76
2:E:833:ARG:HH22	2:E:899:ILE:HD11	1.47	0.76
1:A: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
3:F:1534:ASN:C	3:F:1534:ASN:HD22	1.85	0.76
1:D:22:LEU:HD11	1:D:64:VAL:HG23	1.67	0.76
3:C:1506:THR:H	3:C:1509:GLU:HG2	1.49	0.76
3:F:1572:LEU:C	3:F:1574:LEU:CD2	2.54	0.76
2:B:733:ILE:HG12	2:B:734:ILE:N	2.01	0.75
3:F:1509:GLU:O	3:F:1510:ARG:C	2.24	0.75
2:E:733:ILE:HG12	2:E:734:ILE:N	2.01	0.75
3:F: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: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
1:D:117:TYR:CZ	1:D:123:VAL:HG13	2.22	0.74
3:F:1534:ASN:C	3:F:1534:ASN:ND2	2.40	0.74
1:D:365:VAL:HG13	1:D:379:THR:OG1	1.85	0.74
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:C:1416:PHE:HE2	3:C:1444:TYR:HD2	1.36	0.74
1:A:117:TYR:CZ	1:A:123:VAL:HG13	2.22	0.74
3:C:1634:MET:O	3:C:1638:GLY:N	2.21	0.74
1:A:369:VAL:HG12	1:A:370:GLN:N	2.03	0.73
1:D:530:TRP:HD1	1:D:531:VAL:N	1.85	0.73
1:A:610:GLY:HA3	1:A:616:VAL:N	2.02	0.73
3:F:1541:MET:HE1	3:F:1582:MET:SD	2.28	0.73
1:A:248:PHE:HD1	3:C:1378:MET:HE3	1.53	0.73
4:M:14:LYS:NZ	3:F:1415:ALA:CB	2.50	0.73
1:D:369:VAL:HG12	1:D:370:GLN:N	2.03	0.73
1:A:12:LEU:HB2	1:A:101:VAL:HG22	1.70	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:733:ILE:HD11	2:E:893:ALA:HB3	1.70	0.73
3:F:1535:ASP:OD2	3:F:1536:PHE:N	2.14	0.73
3:F:1510:ARG:O	3:F:1511:LEU:CB	2.37	0.72
3:F:1519:VAL:H	3:F:1585:LEU:CD2	2.01	0.72
3:F:1573:LYS:HD3	3:F:1573:LYS:C	2.10	0.72
3:C:1504:LYS: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: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
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
4:M:4:LEU:HD13	3:F:1444:TYR:C	2.09	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
1:D:6:ILE:HD11	1:D:20:MET:HE3	1.72	0.72
3:F:1388:GLY:O	3:F:1443:GLN:HA	1.89	0.71
1:A:289:VAL:O	1:A:290:GLN:CD	2.29	0.71
3:C:1608:HIS:NE2	3:C:1610:PRO:CA	2.53	0.71
1:D:6:ILE:HD11	1:D:22:LEU:HD23	1.72	0.71
3:C:1485:ARG:HH22	3:C:1591:GLY:HA3	1.55	0.71
3:C:1610:PRO:O	3:C:1611:GLU:O	2.09	0.71
3:C:1445:PHE:HE1	4:P:6:THR:CA	2.03	0.71
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:D:289:VAL:O	1:D:290:GLN:CD	2.29	0.71
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.72	0.71
1:A:98:VAL:O	1:A:634:GLN:CD	2.29	0.71
3:C:1629:ALA:O	3:C:1633:SER:HB2	1.91	0.71
1:D:24:ALA:HB3	1:D:60:HIS:HB3	1.72	0.71
3:C:1578:LYS:HB3	3:C:1580:TYR:CZ	2.25	0.71
3:F:1536:PHE:CD2	3:F:1566:ILE:HD11	2.24	0.71
3:C:1347:PRO:HA	3:C:1362:MET:HB3	1.71	0.71
3:F:1542:ALA:O	3:F:1543:ILE:HG13	1.91	0.71
2:B:733:ILE:HG12	2:B:734:ILE:H	1.55	0.70
2:B:840:VAL:HG11	2:B:892:ALA:HB1	1.72	0.70
3:C:1605:TRP:HE1	3:C:1607:GLU:HB2	1.56	0.70
3:F:1522:VAL:HG23	3:F:1548:LYS:HB3	1.71	0.70
1:D:98:VAL:O	1:D:634:GLN:CD	2.29	0.70
1:A:85:THR:O	1:A:85:THR:OG1	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:SER:OG	1:A:284:VAL:HG23	1.90	0.70
1:D:281:SER:OG	1:D:284:VAL:HG23	1.91	0.70
4:M:36:LEU:N	4:M:36:LEU:HD23	2.05	0.70
3:C:1526:ARG:CZ	3:C:1542:ALA:CB	2.70	0.70
1:D: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
3:C:1389:PHE:HD1	3:C:1441:VAL:HG23	1.57	0.70
3:C:1495:ASN:ND2	3:C:1495:ASN:N	2.33	0.70
3:F:1568:CYS:O	3:F:1569:ARG:C	2.30	0.70
4:P:36:LEU:N	4:P:36:LEU:HD23	2.07	0.70
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.74	0.69
1:A:589:LEU:HD12	1:A:590:THR:H	1.57	0.69
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:6:ILE:HD11	1:A:20:MET:HE3	1.73	0.69
3:F:1569:ARG:C	3:F:1570:GLU:OE1	2.30	0.69
1:A:504:ILE:HG12	1:A:533:VAL:HG11	1.73	0.69
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1544:GLU:OE1	3:C:1579:HIS:CE1	2.46	0.68
1:D:286:LEU:O	1:D:289:VAL:HG23	1.94	0.68
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: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
3:F:1557:GLY:O	3:F:1558:GLN:O	2.12	0.68
3:F:1605:TRP:C	3:F:1605:TRP:CD1	2.67	0.68
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:1569:ARG:C	3:F:1570:GLU:CG	2.62	0.67
3:F:1496:CYS:HA	3:F:1601:GLY:O	1.94	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:C:1506:THR:C	3:C:1508:GLU:H	1.96	0.67
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.77	0.67
3:C:1590:TRP:CE3	3:C:1590:TRP:HA	2.30	0.67
3:F:1526:ARG:NH2	3:F:1579:HIS:NE2	2.43	0.67
1:A:444:ARG:NH2	1:A:534:LYS:HD3	2.09	0.67
2:B:837:GLU:HG2	4:P:64:SER:OG	1.95	0.67
3:C:1504:LYS:CE	3:C:1506:THR:HG23	2.25	0.67
2:E:742:ARG:HB3	2:E:775:ASP:HB3	1.77	0.67
3:F:1558:GLN:C	3:F:1559:GLN:CG	2.55	0.66
3:F:1543:ILE:HD11	3:F:1559:GLN:HA	1.77	0.66
1:A:19:THR:HA	1:A:64:VAL:O	1.94	0.66
3:F:1601:GLY:N	3:F:1604:THR:CG2	2.58	0.66
3:C:1578:LYS:O	3:C:1579:HIS:CB	2.44	0.66
3:C:1510:ARG:HB3	3:C:1630:PHE:CE1	2.30	0.66
3:C:1508:GLU:O	3:C:1512:ASP:CG	2.34	0.66
3:F:1497:PHE:O	3:F:1498:ILE:C	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:VAL:HG12	1:D:136:PRO:HA	1.78	0.66
1:D:257:GLU:N	1:D:257:GLU:CD	2.49	0.66
1:A:8:THR:HG22	1:A:20:MET:CB	2.26	0.66
3:C:1546:THR:O	3:C:1548:LYS:N	2.28	0.66
2:E:793:ILE:HG13	2:E:794:CYS:H	1.61	0.66
2:B:793:ILE:HG13	2:B:794:CYS:H	1.61	0.66
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
3:F:1536:PHE:CE2	3:F:1566:ILE:CD1	2.79	0.65
3:C:1385:MET:HG3	3:C:1390:ALA:HA	1.79	0.65
3:C:1507:LEU:HD21	3:C:1629:ALA:CB	2.19	0.65
4:M:6:THR:HA	3:F:1445:PHE:CE1	2.29	0.65
3:F:1573:LYS:HB2	3:F:1573:LYS:HZ2	1.60	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:A:257:GLU:CD	1:A:257:GLU:N	2.49	0.65
1:D:554:VAL:HG13	1:D:555:PRO:HD2	1.78	0.65
2:B:839:LYS:NZ	4:P:12:ASN:OD1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:37:VAL:HG12	1:A:84:VAL:HG22	1.78	0.64
1:A:6:ILE:HG22	1:A:625:THR:HB	1.80	0.64
1:A:535:ASP:O	1:A:536:SER:HB3	1.97	0.64
3:F:1600:ILE: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
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
3:C:1445:PHE:CE1	4:P:6:THR:C	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:1568:CYS:C	3:F:1569:ARG:O	2.37	0.63
1:A:445:PRO:HA	1:A:499:ILE:O	1.98	0.62
3:C:1551:SER:HB3	3:C:1593:LYS:HZ1	1.63	0.62
3:C:1581:LEU:O	3:C:1581:LEU:CG	2.41	0.62
3:F:1535:ASP:CG	3:F:1536:PHE:N	2.45	0.62
1:D:84:VAL:HG13	1:D:85:THR:N	2.14	0.62
1:D:154:LYS:HE2	1:D:156:ASP:OD1	1.99	0.62
1:D:340:LYS:O	1:D:341:TYR:CD1	2.52	0.62
1: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
1:A:248:PHE:CD1	3:C:1378:MET:HE3	2.35	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
1:D:438:VAL:O	1:D:440:ARG:HG3	2.00	0.62
1:A:340:LYS:O	1:A:341:TYR:CD1	2.52	0.62
2:B:840:VAL:CG1	2:B:892:ALA:HB1	2.28	0.62
1:A:84:VAL:HG13	1:A:85:THR:N	2.14	0.62
3:F:1639:CYS:O	3:F:1641:ASN:N	2.29	0.62
1:D:455:LEU:HD11	1:D:457:MET:HG2	1.82	0.62
3:C:1516:GLU:HB3	3:C:1517:PRO:HD3	1.82	0.62
3:C:1520:ASP:CB	3:C:1586:SER:HB3	2.30	0.62
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:1578:LYS:HE3	3:C:1578:LYS:CA	2.14	0.61
3:F:1406:TYR:C	3:F:1407:ILE:HG13	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1507:LEU:CD1	3:F:1626:ASP:CB	2.71	0.61
3:F:1554:VAL: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
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
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
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
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
3:C:1445:PHE:HE1	4:P:6:THR:C	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1577:LYS:O	3:F:1579:HIS:HD2	1.84	0.60
1:A:334:HIS:HB2	1:A:353:PHE:HB3	1.83	0.60
3:C:1405:ARG:NE	3:C:1437:LEU:HD23	2.15	0.60
3:F:1408:SER:HG	3:F:1410:TYR:HB3	1.65	0.60
3:C:1416:PHE:C	3:C:1416:PHE:CD2	2.75	0.60
1:A:20:MET:HG2	1:A:64:VAL:HG21	1.84	0.60
1:A:73:GLU:HB3	1:A:82:LYS:NZ	2.16	0.60
2:B:833:ARG:NH2	2:B:899:ILE:HD11	2.17	0.60
1:D:134:LEU:HD11	1:D:598:VAL:HG21	1.84	0.60
3:C:1422:LEU:HD12	3:C:1423:ILE:N	2.17	0.60
1:D:37:VAL:HG12	1:D:84:VAL:CG2	2.32	0.60
1:D:513:TYR:CE1	1:D:525:VAL:HB	2.37	0.60
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
2:E:842:VAL:HG23	2:E:892:ALA:HB2	1.82	0.60
3:F:1483:LEU:CD2	3:F:1599:ILE:HG21	2.31	0.60
3:F:1571:ALA:N	3:F:1572:LEU:CD2	2.65	0.60
3:C:1640:PRO:C	3:C:1641:ASN:HD22	2.04	0.59
2:E:786:SER:HA	1:D:570:ARG:O	2.01	0.59
3:F:1416:PHE:C	3:F:1416:PHE:CD2	2.75	0.59
3:F:1533:SER:OG	3:F:1538:GLU:CG	2.34	0.59
2:B:841:ARG:HG2	2:B:841:ARG:O	2.01	0.59
1:A:534:LYS:CG	1:A:534:LYS:O	2.50	0.59
2:E:831:ASN:ND2	2:E:868:PRO:HA	2.18	0.59
3:F:1497:PHE:CD1	3:F:1498:ILE:HG12	2.36	0.59
3:F:1595:ASN:C	3:F:1596:LEU:CG	2.67	0.59
1: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
3:C:1360:ASN:HD22	3:C:1443:GLN:CB	2.11	0.59
3:C:1593:LYS:HG2	3:C:1596:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:TYR:CG	1:D:123:VAL:HG22	2.37	0.59
1:A: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: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:C:1634:MET:O	3:C:1635:VAL:C	2.42	0.59
3:F:1341:LEU:O	3:F:1469:ARG:HG2	2.03	0.59
1:A:136:PRO:HD2	2:B:789:ASP:HA	1.83	0.58
3:C:1341:LEU:O	3:C:1469:ARG:HG2	2.03	0.58
3:F:1422:LEU:HD12	3:F:1423:ILE:N	2.17	0.58
1:A:47:LEU:HD11	1:A:66:PHE:HB2	1.85	0.58
3:C:1532:LEU:HB3	3:C:1569:ARG:HH12	1.68	0.58
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
3:C:1608:HIS:HD2	3:C:1610:PRO:HG3	1.68	0.58
1:D:444:ARG:CZ	1:D:534:LYS:HD3	2.33	0.58
1:D:589:LEU:HD12	1:D:590:THR:N	2.18	0.58
3:F:1406:TYR:CD1	3:F:1407:ILE:N	2.72	0.58
3:F:1560:ARG:HD3	3:F:1598:TYR:HE1	1.68	0.58
1:A: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
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:F:1554:VAL:HB	3:F:1560:ARG:NH2	2.17	0.58
1:D:10:ASN:CG	1:D:635:ARG:HD2	2.24	0.58

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1589:PHE:HB3	3:C:1596:LEU:HD22	1.85	0.57
4:M:26:LEU:C	4:M:26:LEU:HD12	2.25	0.57
3:F:1408:SER:O	3:F:1409:LYS:C	2.42	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: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
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
3:F:1543:ILE:C	3:F:1545:GLN:H	2.09	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
2:E:741:SER:HB3	2:E:902:GLY:C	2.26	0.56
4:M:4:LEU:HB3	3:F:1444:TYR:O	2.05	0.56
3:F:1483:LEU:HG	3:F:1590:TRP:CZ2	2.40	0.56
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1411:GLU:O	3:C:1414:LYS:HG3	2.06	0.56
3:C:1581:LEU:CD2	3:C:1627:LEU:HD21	2.36	0.56
3:C:1608:HIS:CD2	3:C:1610:PRO:CA	2.88	0.56
3:F:1546:THR:O	3:F:1546:THR:HG23	2.06	0.56
3:F:1574:LEU:HB3	3:F:1580:TYR:OH	2.05	0.56
1:A:430:SER:O	1:A:431:ASN:HB2	2.06	0.56
1:A:471:LEU:O	1:A:509:LEU:HD12	2.06	0.56
4:P:84:LYS:O	4:P:85:TYR:HB2	2.05	0.56
2:B:851:CYS:HB3	2:B:879:VAL:HB	1.87	0.56
3:C:1349:PRO:O	3:C:1350:GLU:CB	2.34	0.56
3:C:1524:LYS:O	3:C:1525:THR:HG23	2.06	0.56
3:C:1574:LEU:HD23	3:C:1580:TYR:CD1	2.41	0.56
2:E:734:ILE: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
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:1533:SER:O	3:F:1534:ASN:C	2.45	0.56
3:F:1543:ILE:HD13	3:F:1559:GLN:CA	2.36	0.56
1:D: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
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
3:C:1623:GLN:C	3:C:1625:GLN:H	2.08	0.55
2:E:883:THR:HA	2:E:909:VAL:HG12	1.88	0.55
4:P:26:LEU:C	4:P:26:LEU:HD12	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:852:SER:C	2:B:854:ALA:H	2.10	0.55
2:E:852:SER:C	2:E:854:ALA:H	2.10	0.55
3:F:1444:TYR:CD1	3:F:1445:PHE:HB2	2.42	0.55
1: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
2:B:741:SER:HB3	2:B:902:GLY:C	2.26	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
3:C:1565:PRO:C	3:C:1567:LYS:N	2.59	0.55
3:C:1565:PRO:O	3:C:1567:LYS:N	2.39	0.55
3:C:1608:HIS:CD2	3:C:1609:TRP:C	2.80	0.55
1:A:406:LYS:H	1:A:414:GLN:HE22	1.53	0.55
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.32	0.55
3:F:1533:SER:HG	3:F:1538:GLU:HG3	1.65	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
1:D:179:MET:HG3	1:D:202:VAL:O	2.06	0.55
1:D:210:PHE:CE2	1:D:310:LEU:HD21	2.41	0.55
2:B:741:SER:HB3	2:B:902:GLY:O	2.06	0.55
1:D:73:GLU:HB3	1:D:82:LYS:HZ3	1.72	0.55
1:A:610:GLY:N	1:A:616:VAL:HG23	2.22	0.54
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
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:1377:THR:O	3:F:1378:MET:C	2.46	0.54
3:F:1562:PHE:HD2	3:F:1600:ILE:HD12	1.71	0.54
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.72	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
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
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: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
3:F:1631:THR:C	3:F:1633:SER:H	2.10	0.53
1:A:536:SER:O	1:A:537:CYS:C	2.46	0.53
3:C:1377:THR:O	3:C:1378:MET:C	2.46	0.53
3:C:1506:THR:N	3:C:1509:GLU:HG2	2.20	0.53
3:C:1522:VAL:HG23	3:C:1548:LYS:HD2	1.90	0.53
3:F:1523:TYR:HE2	3:F:1598:TYR:HH	1.57	0.53
3:F:1532:LEU:N	3:F:1532:LEU:CD1	2.71	0.53
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
3:C:1397:LYS:O	3:C:1398:GLN:C	2.46	0.53
1:A:124:LEU:N	1:A:124:LEU:HD23	2.24	0.53
3:F:1409:LYS:C	3:F:1411:GLU:N	2.60	0.53
3:F:1503:ASP:O	3:F:1505:VAL:N	2.42	0.53
3:F:1530:VAL:O	3:F:1530:VAL:CG2	2.57	0.53
3:F:1533:SER:O	3:F:1535:ASP:N	2.42	0.53

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:F:1585:LEU:O	3:F:1586:SER:C	2.47	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
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: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: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
2:E:783:LEU:HD12	2:E:784:ALA:N	2.24	0.52
3:F:1497:PHE:CE2	3:F:1498:ILE:HB	2.45	0.52
3:F: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: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
2:B:793:ILE:HG13	2:B:794:CYS:N	2.23	0.52
1:D:193:GLN:HG2	1:D:194:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:PRO:HG3	1:D:595:TRP:CE3	2.45	0.52
1:A:365:VAL:CG1	1:A:379:THR:OG1	2.56	0.51
2:E:773:LEU:HD13	2:E:803:VAL:HG22	1.92	0.51
3:F:1405:ARG:CZ	3:F:1437:LEU:HD23	2.41	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
1:D:257:GLU:CD	1:D:257:GLU:H	2.14	0.51
2:B:773:LEU:HD13	2:B:803:VAL:HG22	1.92	0.51
3:C:1409:LYS:O	3:C:1412:LEU:N	2.42	0.51
3:F:1537:ASP:OD1	3:F:1538:GLU:N	2.43	0.51
3:F:1586:SER:O	3:F:1588:ASP:N	2.44	0.51
1:D:365:VAL:CG1	1:D:379:THR:OG1	2.56	0.51
1:D:472:ILE:HG13	1:D:480:LYS:HB3	1.92	0.51
1:D:628:SER:HB2	1:D:630:GLN:OE1	2.11	0.51
1:A:230:GLU:HA	1:A:279:VAL:HG22	1.92	0.51
3:C:1518:GLY:O	3:C:1519:VAL:C	2.48	0.51
3:C:1547:ILE:O	3:C:1547:ILE:HG22	2.11	0.51
3:C:1578:LYS:CB	3:C:1580:TYR:OH	2.58	0.51
3:F:1378:MET:CE	1:D:248:PHE:HD1	2.23	0.51
3:F:1408:SER:C	3:F:1410:TYR:N	2.63	0.51
1:D:86:VAL:O	1:D:86:VAL:HG12	2.10	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:B:819:ARG:HG2	2:B:820:ASN:CG	2.31	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:351:MET:HE2	1:D:386:LYS:HA	1.91	0.51
1:D:495:LEU:HD12	1:D:496:PRO:CD	2.40	0.51
1:A:468:TYR:HE1	1:A:513:TYR:HD2	1.57	0.51
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.45	0.51
2:B:819:ARG:NH1	3:C:1487:GLU:O	2.43	0.51
2:B:853:LEU:HD11	3:C:1451:GLN:CB	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1451:GLN:HG3	3:C:1452:PRO:HD2	1.92	0.51
2:E:740:VAL:HB	4:P:42:ARG:HA	1.93	0.51
3:F:1484:CYS:CB	3:F:1489:CYS:HB2	2.37	0.51
3:F:1507:LEU:N	3:F:1507:LEU:CD2	2.74	0.51
1: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
3:F:1532:LEU:O	3:F:1534:ASN:N	2.43	0.51
1:D:63:ASN:HD21	5:D:646:NAG:C1	2.24	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: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
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:257:GLU:CD	1:A:257:GLU:H	2.14	0.50
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.92	0.50
3:C:1483:LEU:HD13	3:C:1536:PHE:CD2	2.46	0.50
1:D:462:GLU:HG3	1:D:486:ARG:HH22	1.76	0.50
1:D:468:TYR:HE1	1:D:513:TYR:CD2	2.28	0.50
1:A:248:PHE:HD1	3:C:1378:MET:CE	2.23	0.50
3:C:1405:ARG:CZ	3:C:1437:LEU:HD23	2.40	0.50
3:C:1546:THR:C	3:C:1548:LYS:H	2.15	0.50
4:M:18:GLU:O	4:M:21:SER:HB2	2.12	0.50
3:F:1510:ARG:NH1	3:F:1607:GLU:OE1	2.44	0.50
3:F:1520:ASP:CG	3:F:1551:SER:HB2	2.32	0.50
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
3:F:1378:MET:HE3	1:D:248:PHE:CD1	2.46	0.50
3:F:1568:CYS:O	3:F:1569:ARG:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:MET:HE1	1:D:386:LYS:HD3	1.92	0.50
1:A:286:LEU:HB3	1:A:291:ASN:HD22	1.76	0.50
1:A:293:ARG:O	1:A:294:ALA:C	2.50	0.50
1:A:402:VAL:HG12	1:A:403:ARG:N	2.27	0.50
3:C:1508:GLU:O	3:C:1512:ASP:OD2	2.29	0.50
3:C:1581:LEU:CD1	3:C:1581:LEU:O	2.60	0.50
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
1:D:351:MET:SD	1:D:440:ARG:HD3	2.52	0.50
2:E:808:PHE:C	2:E:808:PHE:CD1	2.85	0.50
3:F:1416:PHE:CE2	3:F:1444:TYR:HD2	2.25	0.50
3:F:1535:ASP:C	3:F:1566:ILE:HG23	2.30	0.50
1:D:438:VAL:HG13	1:D:449:LEU:HD11	1.92	0.50
1:A:351:MET:SD	1:A:440:ARG:HD3	2.52	0.50
2:B:896:HIS:CB	4:P:61:LYS:HD3	2.41	0.50
1:A:25:HIS:O	1:A:26:ASP:HB2	2.12	0.50
2:B:808:PHE:CD1	2:B:808:PHE:C	2.85	0.50
4:M: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: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
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:25:HIS:O	1:D:26:ASP:HB2	2.12	0.49
1:D:406:LYS:N	1:D:414:GLN:HE22	2.10	0.49
1:A:351:MET:HE2	1:A:386:LYS:HA	1.94	0.49
1:A:459:ARG:NH2	1:D:458:ASP:HA	2.27	0.49
2:E:787:MET:HG2	1:D:164:LEU:O	2.12	0.49
4:P:30:GLU:OE2	4:P:45:LYS:HE3	2.13	0.49
3:F:1520:ASP:O	3:F:1521:TYR:CB	2.45	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:844:LEU:C	2:B:844:LEU:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1482:LYS:O	3:C:1536:PHE:CE2	2.65	0.49
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:286:LEU:C	1:A:291:ASN:ND2	2.65	0.49
1:A:291:ASN:N	1:A:292:PRO:CD	2.76	0.49
2:B:883:THR:HA	2:B:909:VAL:CG1	2.42	0.49
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
3:F:1519:VAL:CG1	3:F:1520:ASP:N	2.76	0.49
1:D:179:MET:CG	1:D:203:LYS:HA	2.42	0.49
1:D:286:LEU:C	1:D:291:ASN:ND2	2.65	0.49
1:D:445:PRO:HA	1:D:499:ILE:HG22	1.95	0.49
1:A:403:ARG:NH1	1:A:416:THR:HG21	2.28	0.49
2:B:836:GLN:HG3	2:B:836:GLN:O	2.12	0.49
2:E:795:VAL:HB	1:D:591:GLN:HB2	1.94	0.49
2:E:806:ASP:HB3	2:E:833:ARG:HH11	1.76	0.49
2:E:844:LEU:C	2:E:844:LEU:HD12	2.33	0.49
2:E:883:THR:HA	2:E:909:VAL:CG1	2.42	0.49
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
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: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: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:1611:GLU:HG2	3:C:1613:ASP:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:GLU:CD	1:D:185:ARG:HD2	2.33	0.49
1:D:403:ARG:HB2	1:D:416:THR:HG22	1.95	0.49
1:D:509:LEU:HB3	1:D:529:VAL:HG13	1.94	0.49
1:A:63:ASN:OD1	5:A:646:NAG:N2	2.46	0.49
1:A:146:GLU:CD	1:A:185:ARG:HD2	2.33	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:F:1484:CYS:CB	3:F:1489:CYS:SG	3.01	0.49
3:F:1522:VAL:C	3:F:1547:ILE:HD12	2.32	0.49
2:B:896:HIS:HB3	4:P:61:LYS:HD3	1.95	0.48
3:C:1450:ILE:O	3:C:1450:ILE:CG1	2.55	0.48
2:E:836:GLN:C	2:E:868:PRO:HG3	2.34	0.48
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.49	0.48
1:A:406:LYS:N	1:A:414:GLN:HE22	2.10	0.48
1:A:434:LEU:HD12	1:A:435:HIS:N	2.28	0.48
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:445:PRO:HA	1:A:499:ILE:HG22	1.95	0.48
2:B:836:GLN:C	2:B:868:PRO:HG3	2.34	0.48
3:F:1514:ALA:HB2	3:F:1583:TRP:CE2	2.48	0.48
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:293:ARG:O	1:D:294:ALA:C	2.50	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: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:HD3	1.94	0.48
1:A:403:ARG:HB2	1:A:416:THR:HG22	1.95	0.48
1:A:477:ARG:HH22	1:A:479:LEU:HD13	1.78	0.48
3:C:1360:ASN:OD1	3:C:1361:THR:N	2.47	0.48
3:C:1568:CYS:C	3:C:1570:GLU:N	2.67	0.48
3:C:1609:TRP:HZ3	3:C:1627:LEU:HD22	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D: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
3:C:1610:PRO:O	3:C:1611:GLU:C	2.51	0.48
1:D:183:LYS:HD3	1:D:185:ARG:CD	2.44	0.48
1:A:369:VAL:CG1	1:A:370:GLN:H	2.24	0.48
1:A:495:LEU:HD12	1:A:496:PRO:CD	2.40	0.48
1:A:603:ILE:HD12	1:A:621:GLY:HA3	1.94	0.48
3:C:1521:TYR:C	3:C:1521:TYR:CD1	2.86	0.48
3:F:1570:GLU:CD	3:F:1570:GLU:N	2.62	0.48
3:F:1604:THR:HG23	3:F:1604:THR:O	2.13	0.48
1:A:179:MET:CG	1:A:203:LYS:HA	2.42	0.48
1:A:606:THR:HG22	1:A:608:GLY:H	1.78	0.48
3:C:1581:LEU:CD2	3:C:1627:LEU:CD2	2.92	0.48
3:C:1630:PHE:O	3:C:1633:SER:HB3	2.13	0.48
2:E:789:ASP:HA	1:D:136:PRO:CD	2.43	0.48
1:D:20:MET:H	1:D:64:VAL:HB	1.79	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:1522:VAL:C	3:C:1523:TYR:CD1	2.87	0.48
3:C:1530:VAL:CG1	3:C:1532:LEU:HD11	2.44	0.48
3:C:1626:ASP:C	3:C:1628:GLY:N	2.66	0.48
2:E:822:GLN:NE2	3:F:1470:PHE:CD2	2.79	0.48
4:M:59:ASP:C	4:M:59:ASP:OD1	2.52	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: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:P:59:ASP:C	4:P:59:ASP:OD1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1341:LEU:HD23	3:F:1469:ARG:N	2.29	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:D:292:PRO:O	1:D:293:ARG:C	2.53	0.47
1:A:7:ILE:HA	1:A:623:THR:O	2.14	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:1575:GLU:HG3	3:F:1576:GLU:N	2.29	0.47
1:D:97:LYS:HG3	1:D:98:VAL:N	2.30	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
1:A:214:VAL:HG11	1:A:304:VAL:CG2	2.45	0.47
1:A:368:ALA:O	1:A:402:VAL:HG13	2.15	0.47
1:A:459:ARG:NH2	1:D:459:ARG:H	2.12	0.47
1:A:510:VAL:HG21	1:A:622:LEU:HD12	1.96	0.47
2:B:735:ALA:HB1	2:B:737:GLU:OE2	2.15	0.47
3:C:1543:ILE:C	3:C:1545:GLN:H	2.17	0.47
3:C:1609:TRP:CZ3	3:C:1627:LEU:HB3	2.50	0.47
3:F:1392:ASP:HB2	3:F:1442:HIS:NE2	2.30	0.47
3:F:1403:VAL:C	3:F:1405:ARG:H	2.18	0.47
3:F:1555:GLN:O	3:F:1556:VAL:O	2.33	0.47
1: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:404:THR:C	1:A:414:GLN:OE1	2.53	0.47
1:A:549:GLU:O	1:A:550:ASP:HB2	2.14	0.47
3:C:1341:LEU:HD23	3:C:1469:ARG:N	2.29	0.47
3:C:1520:ASP:CG	3:C:1551:SER:HG	2.16	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:1636:VAL:O	3:F:1637:PHE:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ASN:HB3	1:D:483:ARG:NH1	2.29	0.47
1:D:59:ASN:HB3	1:D:483:ARG:HH12	1.80	0.47
1:D:97:LYS:HZ3	1:D:631:GLN:HB2	1.79	0.47
1:D:222:TYR:CE2	1:D:224:TYR:HB2	2.50	0.47
1:D:404:THR:C	1:D:414:GLN:OE1	2.53	0.47
1:A:86:VAL:O	1:A:86:VAL:HG12	2.11	0.47
1:A:97:LYS:HG3	1:A:98:VAL:N	2.30	0.47
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
3:C:1508:GLU:O	3:C:1512:ASP:OD1	2.33	0.47
3:C:1551:SER:C	3:C:1593:LYS:NZ	2.67	0.47
2:E:735:ALA:HB1	2:E:737:GLU:OE2	2.15	0.47
4:M:23:LEU:HD11	4:M:51:ALA:HB1	1.97	0.47
3:F:1639:CYS:C	3:F:1641:ASN:H	2.15	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:1573:LYS:O	3:C:1573:LYS:CD	2.63	0.47
3:F:1386:MET:O	3:F:1387:THR:C	2.54	0.47
3:F:1622:LYS:O	3:F:1623:GLN:C	2.53	0.47
1: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
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
1:D:105:SER:O	1:D:132:HIS:CD2	2.68	0.46
1:D:301:SER:HB2	1:D:323:GLY:HA2	1.97	0.46
1:A:203:LYS:HG2	1:A:204:GLU:N	2.29	0.46
1:A:357:PRO:O	1:A:358:ASP:C	2.53	0.46
4:P:49:GLN:O	4:P:50:LYS:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:66:ALA:O	4:P:67:LYS:C	2.53	0.46
3:F:1483:LEU:CG	3:F:1590:TRP:CZ2	2.98	0.46
3:F:1525:THR:OG1	3:F:1541:MET:CE	2.63	0.46
3:F:1618:GLU:O	3:F:1619:GLU:C	2.54	0.46
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
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
2:B:756:LEU:HA	2:B:758:GLU:OE1	2.14	0.46
2:B:894:VAL:CG2	2:B:899:ILE:HB	2.45	0.46
3:C:1530:VAL:HG12	3:C:1532:LEU:CD1	2.45	0.46
3:C:1534:ASN:O	3:C:1566:ILE:CD1	2.64	0.46
1:A: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
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
1:D:7:ILE:HA	1:D:623:THR:O	2.14	0.46
1:A:105:SER:O	1:A:132:HIS:CD2	2.68	0.46
3:C:1392:ASP:HB2	3:C:1442:HIS:NE2	2.30	0.46
2:E:733:ILE:CG1	2:E:734:ILE:N	2.75	0.46
4:M:7:SER:O	4:M:8:ASN:C	2.54	0.46
1:D:185:ARG:HA	1:D:196:PHE:O	2.16	0.46
1:D:357:PRO:O	1:D:358:ASP:C	2.53	0.46
3:C:1386:MET:O	3:C:1387:THR:C	2.53	0.46
3:C:1389:PHE:HD1	3:C:1441:VAL:CG2	2.26	0.46
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: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
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
2:E:744:GLU:C	2:E:746:PRO:HD3	2.37	0.46
4:M:49:GLN:O	4:M:50:LYS:C	2.53	0.46
3:F:1389:PHE:N	3:F:1389:PHE:HD2	2.14	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:292:PRO:O	1:A:293:ARG:C	2.53	0.46
1:A:339:PRO:O	1:A:340:LYS:HD3	2.16	0.46
1:A:375:VAL:CG2	1:A:387:LEU:HD22	2.46	0.46
2:B:833:ARG:HH22	2:B:899:ILE:CD1	2.24	0.46
3:C:1537:ASP:OD2	3:C:1569:ARG:HD3	2.16	0.46
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:7:SER:O	4:P:8:ASN:C	2.54	0.46
4:P:23:LEU:HD11	4:P:51:ALA:HB1	1.97	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:D:97:LYS:NZ	1:D:632:THR:O	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
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:164:LEU:O	2:B:787:MET:HG2	2.15	0.45
3:C:1403:VAL:C	3:C:1405:ARG:H	2.18	0.45
3:C:1562:PHE:CE2	3:C:1582:MET:HE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:1409:LYS:HA	3:F:1412:LEU:HB2	1.99	0.45
1:D:339:PRO:O	1:D:340:LYS:HD3	2.16	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
2:E:894:VAL:CG2	2:E:899:ILE:HB	2.45	0.45
4:P:29:ASN:O	4:P:30:GLU:C	2.54	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:C:1618:GLU:HA	3:C:1621:GLN:CD	2.37	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
2:B:733:ILE:HB	2:B:895:TYR:CD2	2.51	0.45
3:C:1506:THR:O	3:C:1508:GLU:N	2.49	0.45
4:M:29:ASN:O	4:M:30:GLU:C	2.55	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
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
3:C:1546:THR:C	3:C:1548:LYS:N	2.70	0.45
4:M:64:SER:O	4:M:65:GLU:C	2.55	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:744:GLU:C	2:B:746:PRO:HD3	2.37	0.45
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.45
3:C:1337:ASN:C	3:C:1337:ASN:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1341:LEU:HD23	3:C:1469:ARG:H	1.82	0.45
3:C:1506:THR:CB	3:C:1509:GLU:HG2	2.46	0.45
2:E:786:SER:HB3	1:D:541:LEU:CD2	2.39	0.45
2:E:789:ASP:HA	1:D:136:PRO:CG	2.47	0.45
2:E:844:LEU:HD12	2:E:845:LEU:N	2.32	0.45
3:F:1337:ASN:OD1	3:F:1337:ASN:C	2.54	0.45
3:F:1510:ARG:HG3	3:F:1583:TRP:HH2	1.81	0.45
1:A: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
3:F:1582:MET:HE2	3:F:1582:MET:HB2	1.62	0.45
1:D:434:LEU:HB2	1:D:513:TYR:HE2	1.81	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
3:C:1581:LEU:HD23	3:C:1627:LEU:HD21	1.99	0.44
3:F:1524:LYS:C	3:F:1525:THR:CG2	2.85	0.44
3:F:1526:ARG:NH2	3:F:1544:GLU:OE1	2.48	0.44
1: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:271:ILE:O	1:D:271:ILE:HG22	2.16	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: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:F:1612:GLU:C	3:F:1614:GLU:H	2.20	0.44
1:D:634:GLN:HE22	1:D:635:ARG:C	2.19	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
4:P:26:LEU:O	4:P:29:ASN:N	2.50	0.44
3:F:1409:LYS:O	3:F:1410:TYR:C	2.56	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:A:210:PHE:HB3	1:A:237:PHE:HA	1.99	0.44
1:A:410:SER:OG	1:A:413:GLU:HG3	2.18	0.44
2:B:817:VAL:HG22	2:B:907:LEU:HD12	1.99	0.44
3:C:1460:TYR:CG	3:C:1461:TYR:N	2.86	0.44
2:E:817:VAL:HG22	2:E:907:LEU:HD12	1.99	0.44
4:M:66:ALA:O	4:M:67:LYS:C	2.53	0.44
1:D:404:THR:HG1	1:D:415:ALA:H	1.66	0.44
1:D:541:LEU:HD12	1:D:541:LEU:HA	1.77	0.44
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
3:F:1406:TYR:C	3:F:1406:TYR:CD2	2.88	0.44
1:D:83:PHE:HD1	1:D:99:VAL:C	2.21	0.44
1:A:380:GLN:O	1:A:382:ASP:N	2.51	0.44
1:A:465:ILE:HD11	1:A:515:LEU:HD13	2.00	0.44
2:B:835:ASN:O	2:B:836:GLN:HB3	2.17	0.44
2:B:844:LEU:HD12	2:B:845:LEU:N	2.32	0.44
3:C:1409:LYS:O	3:C:1410:TYR:C	2.56	0.44
3:C:1551:SER:C	3:C:1593:LYS:HZ3	2.18	0.44
2:E:835:ASN:O	2:E:836:GLN:HB3	2.17	0.44
4:P:64:SER:O	4:P:65:GLU:C	2.55	0.44
4:P:73:ILE:O	4:P:77:ILE:HG13	2.18	0.44
1: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
2:B:863:THR:HB	4:P:7:SER:HB2	1.99	0.44
3:C:1641:ASN:HD22	3:C:1641:ASN:N	2.15	0.44
2:E:730:ASP:CG	2:E:730:ASP:O	2.56	0.44
2:E:819:ARG:NH1	2:E:883:THR:HG23	2.32	0.44
3:F:1416:PHE:CD2	3:F:1417:SER:N	2.85	0.44
1:D:20:MET:HG2	1:D:64:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ASN:HB2	1:D:148:PRO:CD	2.48	0.44
2:B:730:ASP:CG	2:B:730:ASP:O	2.55	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:D:530:TRP:CD1	1:D:530:TRP:C	2.91	0.43
1:A:124:LEU:HD12	2:B:751:TRP:CG	2.53	0.43
2:B:840:VAL:HG13	2:B:893:ALA:O	2.18	0.43
3:C:1444:TYR:CD1	3:C:1444:TYR:C	2.92	0.43
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: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
1:A:615:GLY:O	1:A:616:VAL:C	2.56	0.43
3:F:1482:LYS:HB2	3:F:1489:CYS:SG	2.58	0.43
3:F:1509:GLU:CA	3:F:1512:ASP:HB3	2.48	0.43
3:F:1558:GLN:HG2	3:F:1559:GLN:H	1.83	0.43
1:A:20:MET:HG2	1:A:64:VAL:CG2	2.47	0.43
1:A:83:PHE:CD1	1:A:100:LEU:HA	2.54	0.43
1:A:84:VAL:HG22	1:A:85:THR:H	1.84	0.43
2:B:778:THR:OG1	2:B:779:THR:N	2.52	0.43
2:E:751:TRP:CG	1:D:124:LEU:HD12	2.53	0.43
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
3:F:1516:GLU:O	3:F:1517:PRO:C	2.55	0.43
1:D:36:THR:HA	1:D:47:LEU:O	2.17	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
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
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
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
1:D:38:HIS:HE1	1:D:45:LEU:CD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:ILE:HB	1:D:635:ARG:HH12	1.84	0.43
1:A:83:PHE:HD1	1:A:99:VAL:C	2.21	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: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
3:F:1503:ASP:C	3:F:1505:VAL:N	2.71	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:603:ILE:HB	1:A:635:ARG:HH12	1.84	0.43
3:C:1575:GLU:H	3:C:1580:TYR:HH	1.62	0.43
4:P:15:LEU:HD22	4:P:60:PHE:CE1	2.53	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
1:D:477:ARG:HH11	1:D:477:ARG:CG	2.31	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:1544:GLU:C	3:C:1545:GLN:HG3	2.36	0.43
3:F:1503:ASP:O	3:F:1504:LYS:C	2.58	0.43
1:D:454:LEU:HA	1:D:491:ASP:O	2.19	0.43
1:D:458:ASP:O	1:D:460:ALA:N	2.52	0.43
1:D:583:LEU:HA	1:D:583:LEU:HD23	1.76	0.43
2:B:865:THR:OG1	4:P:11:GLN:HG2	2.19	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:1444:TYR:C	3:F:1444:TYR:CD1	2.92	0.43
1:A:138:GLY:HA2	1:A:160:SER:HG	1.79	0.42
1:A:219:LYS:HD2	1:A:358:ASP:OD2	2.19	0.42
1:A:458:ASP:O	1:A:460:ALA:N	2.52	0.42
2:B:778:THR:HG23	2:B:779:THR:N	2.34	0.42
3:C:1607:GLU:O	3:C:1608:HIS:O	2.37	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1378:MET:HE2	1:D:248:PHE:HD1	1.83	0.42
3:F:1631:THR:C	3:F:1633:SER:N	2.72	0.42
3:F:1634:MET:O	3:F:1635:VAL:C	2.58	0.42
5:D:646:NAG:O3	5:D:646:NAG:H62	2.19	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: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
2:B:877:VAL:HG13	3:C:1451:GLN:CD	2.39	0.42
3:C:1602:LYS:C	3:C:1604:THR:H	2.22	0.42
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
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
1:A:530:TRP:CD1	1:A:530:TRP:C	2.91	0.42
2:B:729:LEU:HD13	2:B:737:GLU:OE2	2.20	0.42
3:C:1531:GLN:C	3:C:1532:LEU:HD13	2.40	0.42
2:E:749:TRP:CE3	2:E:750:LEU:HB2	2.54	0.42
3:F:1378:MET:HA	3:F:1426:LEU:O	2.19	0.42
3:F:1460:TYR:HB2	1:D:248:PHE:CD2	2.55	0.42
3:F:1495:ASN:HD21	3:F:1602:LYS:HG3	1.83	0.42
3:F:1615:CYS:C	3:F:1617:ASP:N	2.72	0.42
1:D:20:MET:HG2	1:D:64:VAL:HG11	2.02	0.42
1:A:61:MET:CE	1:A:483:ARG:HG2	2.50	0.42
3:C:1370:TYR:O	3:C:1431:HIS:HA	2.19	0.42
3:C:1416:PHE:C	3:C:1416:PHE:HD2	2.20	0.42
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
1:D:289:VAL:O	1:D:290:GLN:HG2	1.97	0.42
3:C:1378:MET:HA	3:C:1426:LEU:O	2.19	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:1416:PHE:C	3:F:1416:PHE:HD2	2.20	0.42
3:F:1496:CYS:O	3:F:1497:PHE:CB	2.50	0.42
3:F:1524:LYS:CD	3:F:1525:THR:N	2.75	0.42
3:F:1569:ARG:C	3:F:1570:GLU:CD	2.78	0.42
1:A:453:PHE:CB	1:A:493:VAL:HG23	2.41	0.42
2:B:833:ARG:HD2	2:B:834:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:852:SER:C	2:B:854:ALA:N	2.73	0.42
3:C:1513:LYS:O	3:C:1516:GLU:CG	2.57	0.42
3:C:1520:ASP:O	3:C:1521:TYR:HB3	2.20	0.42
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:1572:LEU:C	3:F:1574:LEU:HD21	2.32	0.42
3:F:1631:THR:O	3:F:1633:SER:N	2.53	0.42
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: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
3:C:1587:SER:C	3:C:1589:PHE:H	2.23	0.42
2:E:778:THR:OG1	2:E:779:THR:N	2.52	0.42
2:E:852:SER:C	2:E:854:ALA:N	2.73	0.42
3:F:1624:CYS:O	3:F:1625:GLN:C	2.58	0.42
1: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:1409:LYS:C	3:F:1411:GLU:H	2.23	0.42
3:F:1497:PHE:CE1	3:F:1498:ILE:HD11	2.54	0.42
3:F:1543:ILE:C	3:F:1545:GLN:N	2.73	0.42
1:D:291:ASN:N	1:D:292:PRO:HD3	2.34	0.42
1:D:294:ALA:O	1:D:295:GLU:C	2.58	0.42
1:D:455:LEU:CD1	1:D:457:MET:HG2	2.49	0.42
1:D:509:LEU:HB3	1:D:529:VAL:CG1	2.50	0.42
1:D:613:TYR:CD2	1:D:614:ALA:N	2.88	0.42
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
2:E:863:THR:HB	4:M:7:SER:CB	2.50	0.42
4:P:15:LEU:HD12	4:P:15:LEU:HA	1.82	0.42
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:O	1:A:298:VAL:HG12	2.18	0.41
1:A:634:GLN:HE22	1:A:635:ARG:C	2.19	0.41
4:M:26:LEU:O	4:M:29:ASN:HB2	2.19	0.41
1:D:47:LEU:HD23	1:D:47:LEU:C	2.41	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:509:LEU:HB3	1:A:529:VAL:CG1	2.50	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
4:M:29:ASN:O	4:M:31:LEU:N	2.53	0.41
3:F:1600:ILE:C	3:F:1604:THR:HG21	2.41	0.41
3:F:1601:GLY:N	3:F:1604:THR:HG22	2.34	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:D:615:GLY:O	1:D:616:VAL:C	2.56	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
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
1:A:294:ALA:O	1:A:295:GLU:C	2.58	0.41
3:C:1472:HIS:CE1	3:C:1473:PRO:HD2	2.55	0.41
2:E:789:ASP:O	1:D:135:LEU:HD22	2.19	0.41
4:P:13:GLU:O	4:P:13:GLU:HG2	2.20	0.41
3:F:1390:ALA:HA	3:F:1391:PRO:HD3	1.92	0.41
3:F:1509:GLU:O	3:F:1512:ASP:N	2.53	0.41
3:F:1524:LYS:C	3:F:1525:THR:HG22	2.39	0.41
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:A:344:PRO:HG3	1:A:423:PRO:HB3	2.03	0.41
1:A:346:MET:O	1:A:391:THR:CG2	2.57	0.41
1:A:556:GLY:HA2	2:B:773:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:TYR:CD2	1:A:614:ALA:N	2.88	0.41
3:C:1611:GLU:HG2	3:C:1612:GLU:N	2.36	0.41
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
3:F:1527:LEU:HD12	3:F:1575:GLU:C	2.40	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:47:LEU:HD23	1:A:47:LEU:C	2.41	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:1633:SER:O	3:F:1634:MET:C	2.56	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: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
2:B:804:MET:HG2	2:B:805:GLN:N	2.35	0.41
2:B:818:VAL:HA	2:B:910:VAL:O	2.21	0.41
3:C:1514:ALA:C	3:C:1516:GLU:H	2.23	0.41
1:D: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1605:TRP:C	3:F:1606:VAL:HG23	2.42	0.41
1:D:380:GLN:C	1:D:382:ASP:H	2.25	0.41
1:D:508:ARG:CZ	1:D:604:GLY:HA3	2.51	0.41
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
3:C:1508:GLU:O	3:C:1509:GLU:C	2.58	0.40
4:P:61:LYS:HB3	4:P:62:LYS:H	1.78	0.40
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
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: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:1556:VAL:C	3:C:1558:GLN:H	2.25	0.40
3:F:1622:LYS:HG3	3:F:1623:GLN:H	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1410:TYR:C	3:C:1410:TYR:CD2	2.95	0.40
3:C:1509:GLU:HA	3:C:1512:ASP:OD2	2.21	0.40
2:E:818:VAL:HA	2:E:910:VAL:O	2.20	0.40
3:F:1615:CYS:O	3:F:1616:GLN:C	2.60	0.40
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
1:A:380:GLN:C	1:A:382:ASP:H	2.25	0.40
3:C:1526:ARG:CG	3:C:1542:ALA:CB	2.84	0.40
3:C:1568:CYS:O	3:C:1570:GLU:N	2.53	0.40
3:C:1574:LEU:HA	3:C:1580:TYR:CE1	2.56	0.40
2:E:793:ILE:CG1	2:E:794:CYS:N	2.85	0.40
3:F:1498:ILE:HG12	3:F:1498:ILE:H	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	637/645 (99%)	557 (87%)	69 (11%)	11 (2%)	7 36
1	D	637/645 (99%)	557 (87%)	69 (11%)	11 (2%)	7 36
2	B	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	12 45
2	E	182/206 (88%)	162 (89%)	18 (10%)	2 (1%)	12 45
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 2
4	M	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	P	82/88 (93%)	60 (73%)	19 (23%)	3 (4%)	2 22
All	All	2378/2564 (93%)	1970 (83%)	298 (12%)	110 (5%)	2 18

All (110) Ramachandran outliers are listed below:

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

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

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	563/567 (99%)	529 (94%)	34 (6%)	16 43
1	D	563/567 (99%)	529 (94%)	34 (6%)	16 43
2	B	172/191 (90%)	142 (83%)	30 (17%)	1 9
2	E	172/191 (90%)	142 (83%)	30 (17%)	1 9
3	C	266/309 (86%)	210 (79%)	56 (21%)	1 5
3	F	268/309 (87%)	202 (75%)	66 (25%)	0 3
4	M	76/79 (96%)	67 (88%)	9 (12%)	4 21
4	P	76/79 (96%)	66 (87%)	10 (13%)	3 18
All	All	2156/2292 (94%)	1887 (88%)	269 (12%)	3 19

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA

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(^{o})	Ideal(^{o})
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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	641/645 (99%)	0.48	39 (6%) 28 21	18, 53, 106, 172	0
1	D	641/645 (99%)	0.46	23 (3%) 46 31	18, 53, 106, 172	0
2	B	184/206 (89%)	0.14	2 (1%) 77 59	19, 50, 80, 114	0
2	E	184/206 (89%)	0.27	3 (1%) 70 51	25, 57, 87, 120	0
3	C	293/343 (85%)	0.76	34 (11%) 11 9	35, 87, 198, 230	0
3	F	295/343 (86%)	1.18	57 (19%) 4 3	31, 93, 143, 194	0
4	M	84/88 (95%)	-0.01	0 100 100	48, 68, 105, 175	0
4	P	84/88 (95%)	-0.03	0 100 100	43, 65, 101, 184	0
All	All	2406/2564 (93%)	0.52	158 (6%) 26 19	18, 63, 125, 230	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1557	GLY	6.7
1	A	78	LYS	6.3
3	C	1610	PRO	5.2
1	A	48	SER	5.2
3	F	1391	PRO	5.1
3	F	1441	VAL	4.9
1	A	41	PRO	4.9
1	A	64	VAL	4.9
3	F	1559	GLN	4.8
3	F	1412	LEU	4.8
3	F	1387	THR	4.8
3	F	1417	SER	4.7
3	F	1420	ASN	4.5
3	C	1627	LEU	4.4
3	C	1631	THR	4.3
3	F	1612	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	1612	GLU	4.1
3	C	1632	GLU	4.1
3	F	1626	ASP	4.1
3	F	1396	LEU	4.1
1	D	48	SER	4.1
3	F	1594	PRO	4.1
3	C	1624	CYS	3.9
3	C	1628	GLY	3.9
1	A	439	LEU	3.9
3	C	1616	GLN	3.8
3	C	1545	GLN	3.8
3	C	1635	VAL	3.7
1	A	99	VAL	3.7
3	C	1594	PRO	3.7
3	C	1637	PHE	3.7
3	F	1498	ILE	3.6
3	C	1609	TRP	3.6
3	F	1483	LEU	3.6
3	F	1449	LEU	3.6
1	D	518	ALA	3.5
3	F	1442	HIS	3.5
1	A	54	LEU	3.5
3	F	1556	VAL	3.5
3	C	1526	ARG	3.4
1	A	79	GLY	3.4
3	F	1390	ALA	3.3
1	A	49	SER	3.3
1	D	19	THR	3.3
3	F	1348	ALA	3.3
1	A	437	SER	3.3
3	C	1544	GLU	3.3
3	F	1508	GLU	3.2
1	A	461	HIS	3.2
3	F	1361	THR	3.2
3	F	1411	GLU	3.2
1	D	78	LYS	3.2
3	F	1640	PRO	3.2
3	C	1547	ILE	3.1
1	A	80	ARG	3.1
1	D	98	VAL	3.1
3	F	1450	ILE	3.1
1	A	46	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	1613	ASP	3.0
1	A	102	SER	3.0
3	C	1623	GLN	3.0
3	F	1533	SER	2.9
3	F	1358	ALA	2.9
3	F	1419	ARG	2.9
3	C	1358	ALA	2.9
1	A	82	LYS	2.9
3	F	1496	CYS	2.9
1	A	103	LEU	2.9
3	C	1559	GLN	2.9
1	A	637	GLU	2.9
1	A	452	ASN	2.9
2	E	911	PRO	2.8
3	C	1556	VAL	2.8
1	D	491	ASP	2.8
3	F	1360	ASN	2.8
3	F	1363	ILE	2.8
1	D	530	TRP	2.8
3	F	1535	ASP	2.8
3	F	1506	THR	2.8
3	F	1596	LEU	2.8
3	F	1514	ALA	2.8
1	D	105	SER	2.8
1	D	437	SER	2.8
1	A	451	VAL	2.7
1	A	36	THR	2.7
3	C	1507	LEU	2.7
1	D	494	VAL	2.7
3	C	1555	GLN	2.7
1	D	439	LEU	2.6
1	D	528	SER	2.6
1	A	95	VAL	2.6
3	F	1492	ALA	2.6
3	F	1414	LYS	2.6
3	F	1470	PHE	2.6
1	A	349	ASP	2.6
3	F	1416	PHE	2.6
3	C	1625	GLN	2.6
1	A	521	GLN	2.5
3	C	1615	CYS	2.5
3	F	1347	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	1460	TYR	2.5
3	F	1488	LEU	2.5
1	D	645	ALA	2.5
1	A	97	LYS	2.4
2	E	729	LEU	2.4
3	C	1638	GLY	2.4
1	A	445	PRO	2.4
3	C	1618	GLU	2.4
3	F	1505	VAL	2.4
3	F	1389	PHE	2.4
3	F	1445	PHE	2.4
3	F	1537	ASP	2.4
2	B	729	LEU	2.4
3	F	1386	MET	2.4
3	F	1489	CYS	2.4
1	D	103	LEU	2.4
3	F	1443	GLN	2.4
3	C	1636	VAL	2.3
1	D	512	TYR	2.3
1	A	636	ALA	2.3
1	D	644	ALA	2.3
3	C	1607	GLU	2.3
3	C	1621	GLN	2.3
3	F	1447	VAL	2.3
3	F	1362	MET	2.3
1	A	40	PHE	2.2
1	A	548	SER	2.2
1	D	52	THR	2.2
3	C	1630	PHE	2.2
3	F	1444	TYR	2.2
3	C	1620	ASN	2.2
1	A	73	GLU	2.2
1	D	610	GLY	2.2
1	A	27	ALA	2.2
1	D	36	THR	2.2
3	F	1388	GLY	2.2
1	D	435	HIS	2.2
1	A	16	SER	2.2
3	F	1418	ASP	2.2
3	F	1613	ASP	2.1
3	F	1504	LYS	2.1
3	F	1349	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	804	MET	2.1
1	A	618	SER	2.1
1	A	52	THR	2.1
1	A	623	THR	2.1
1	D	473	MET	2.1
3	F	1637	PHE	2.1
1	A	35	VAL	2.1
1	D	634	GLN	2.1
1	A	105	SER	2.1
1	D	132	HIS	2.0
1	A	12	LEU	2.0
1	A	375	VAL	2.0
1	A	87	GLN	2.0
3	C	1558	GLN	2.0
2	E	804	MET	2.0
3	F	1384	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^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.