Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:17 PM GMT

PDB ID	:	3T4A
Title	:	Structure of a truncated form of Staphylococcal Complement Inhibitor B bound to human C3c at 3.4 Angstrom resolution
Authors	:	Garcia, B.L.; Geisbrecht, B.V.; Summers, B.J.
Deposited on	:	2011-07-25
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

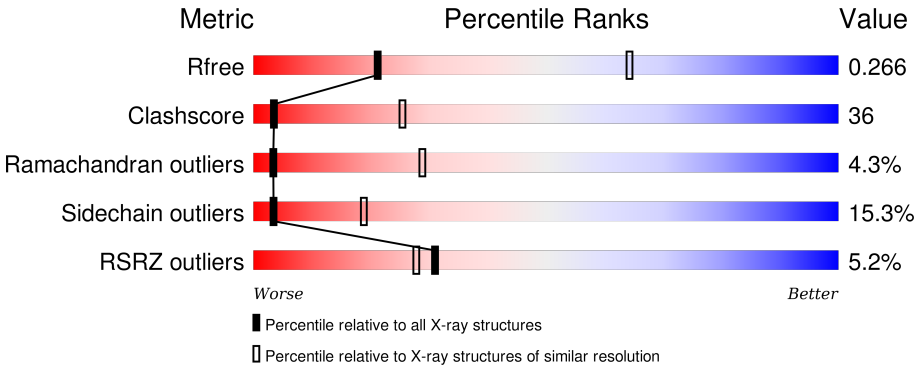
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	645	2% 53% 36% 10%
1	D	645	% 53% 36% 9%
2	B	206	49% 33% 7% 11%
2	E	206	% 52% 30% 6% 11%
3	C	343	21% 21% 50% 13% 14%

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Mol	Chain	Length	Quality of chain
3	F	343	8% 21% 48% 15% 14%
4	G	73	4% 60% 33% 7%
4	H	73	59% 33% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18730 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 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			4931	3141	833	942	15			
1	D	633	Total	C	N	O	S	0	0	0
			4931	3141	833	942	15			

- Molecule 2 is a protein called Complement C3c alpha' chain fragment 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			
2	E	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			

- Molecule 3 is a protein called Complement C3c alpha' chain fragment 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			
3	F	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			

- Molecule 4 is a protein called Fibrinogen-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	68	Total	C	N	O	S	0	0	0
			547	348	94	102	3			
4	H	68	Total	C	N	O	S	0	0	0
			547	348	94	102	3			

There are 10 discrepancies between the modelled and reference sequences:

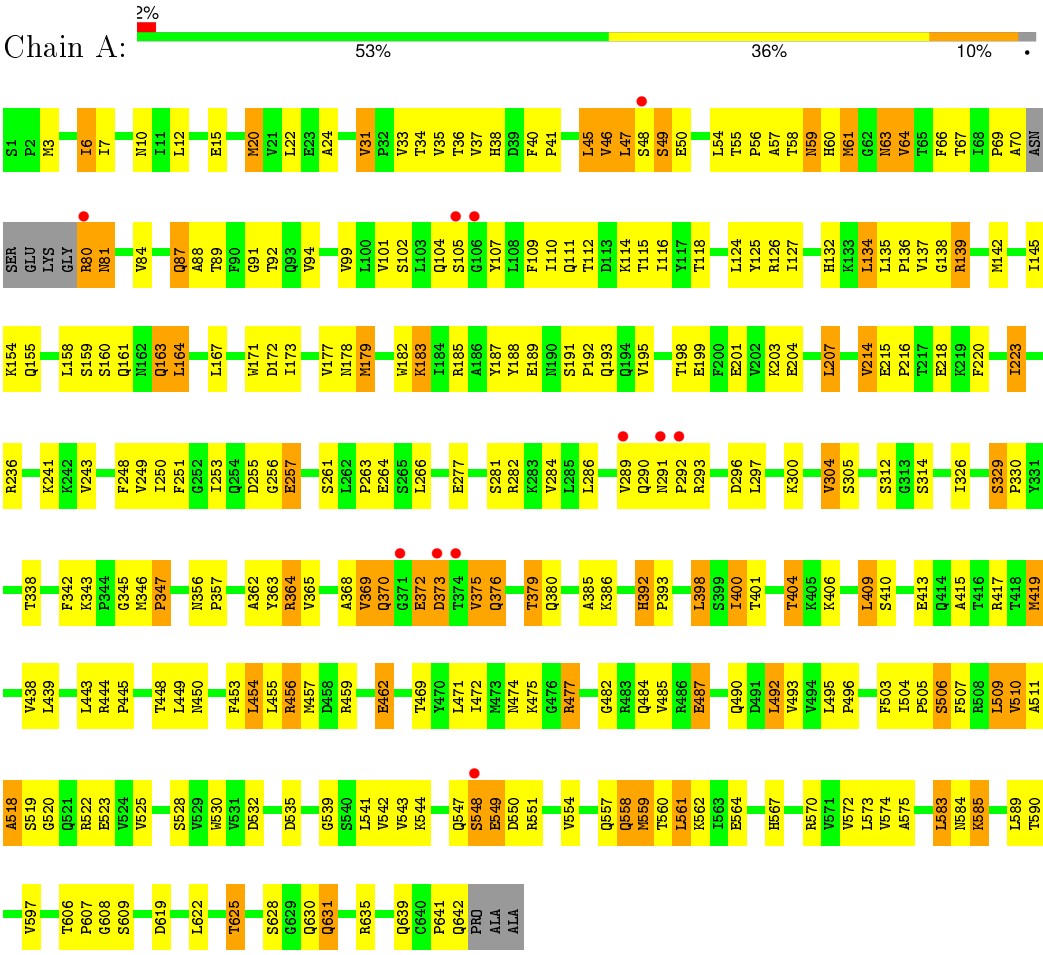
Chain	Residue	Modelled	Actual	Comment	Reference
G	13	GLY	-	EXPRESSION TAG	UNP Q99UU9
G	14	SER	-	EXPRESSION TAG	UNP Q99UU9
G	15	THR	-	EXPRESSION TAG	UNP Q99UU9
G	16	GLY	-	EXPRESSION TAG	UNP Q99UU9
G	17	SER	-	EXPRESSION TAG	UNP Q99UU9
H	13	GLY	-	EXPRESSION TAG	UNP Q99UU9
H	14	SER	-	EXPRESSION TAG	UNP Q99UU9
H	15	THR	-	EXPRESSION TAG	UNP Q99UU9
H	16	GLY	-	EXPRESSION TAG	UNP Q99UU9
H	17	SER	-	EXPRESSION TAG	UNP Q99UU9

3 Residue-property plots (i)

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

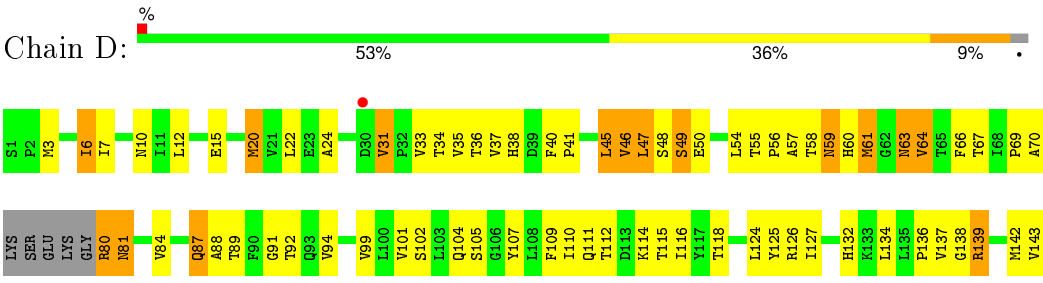
- Molecule 1: Complement C3 beta chain

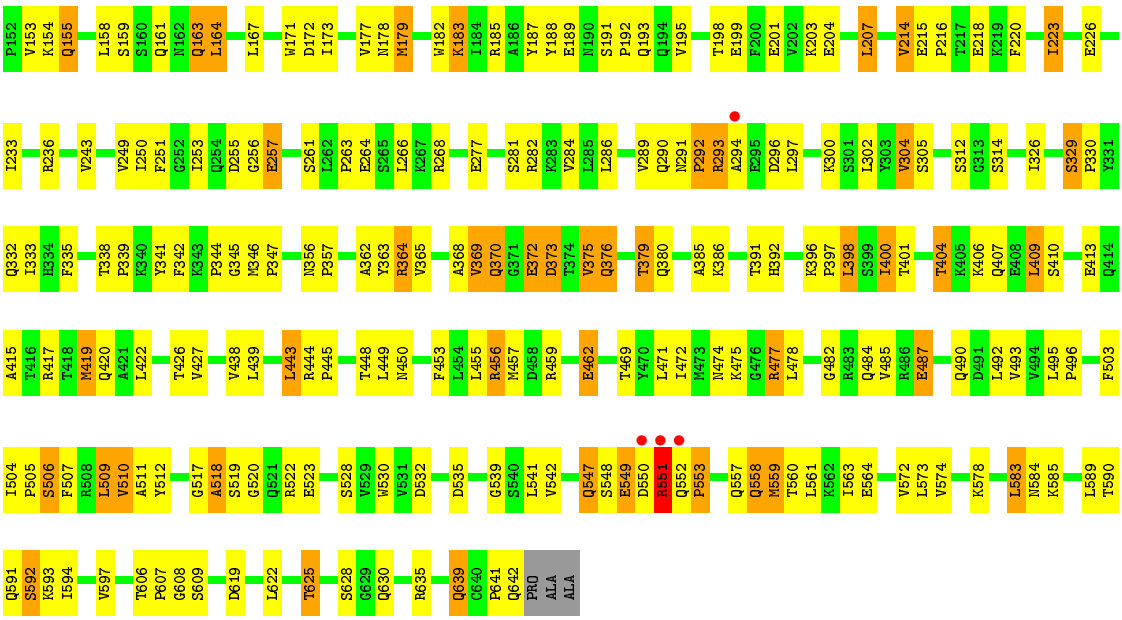
Chain A:



- Molecule 1: Complement C3 beta chain

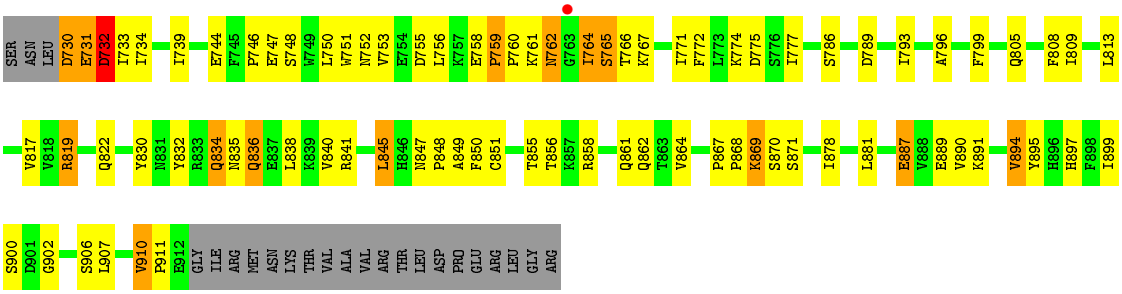
Chain D:





• Molecule 2: Complement C3c alpha' chain fragment 1

Chain B:

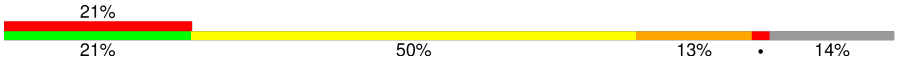


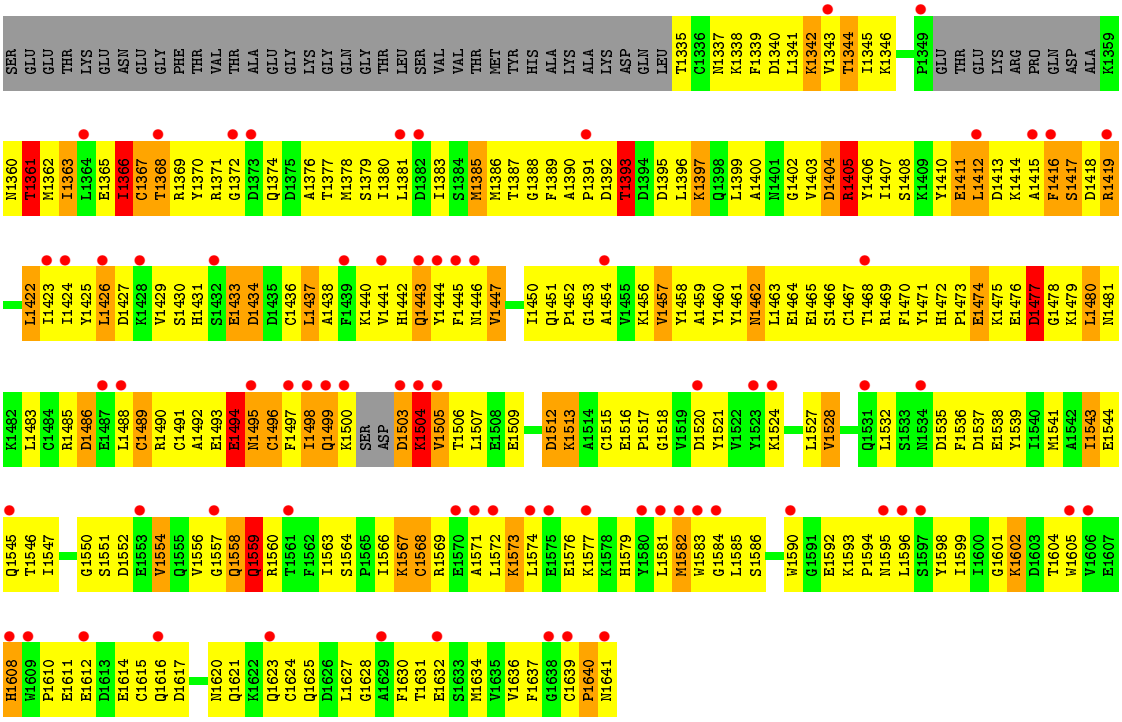
• Molecule 2: Complement C3c alpha' chain fragment 1

Chain E:

• Molecule 3: Complement C3c alpha' chain fragment 2

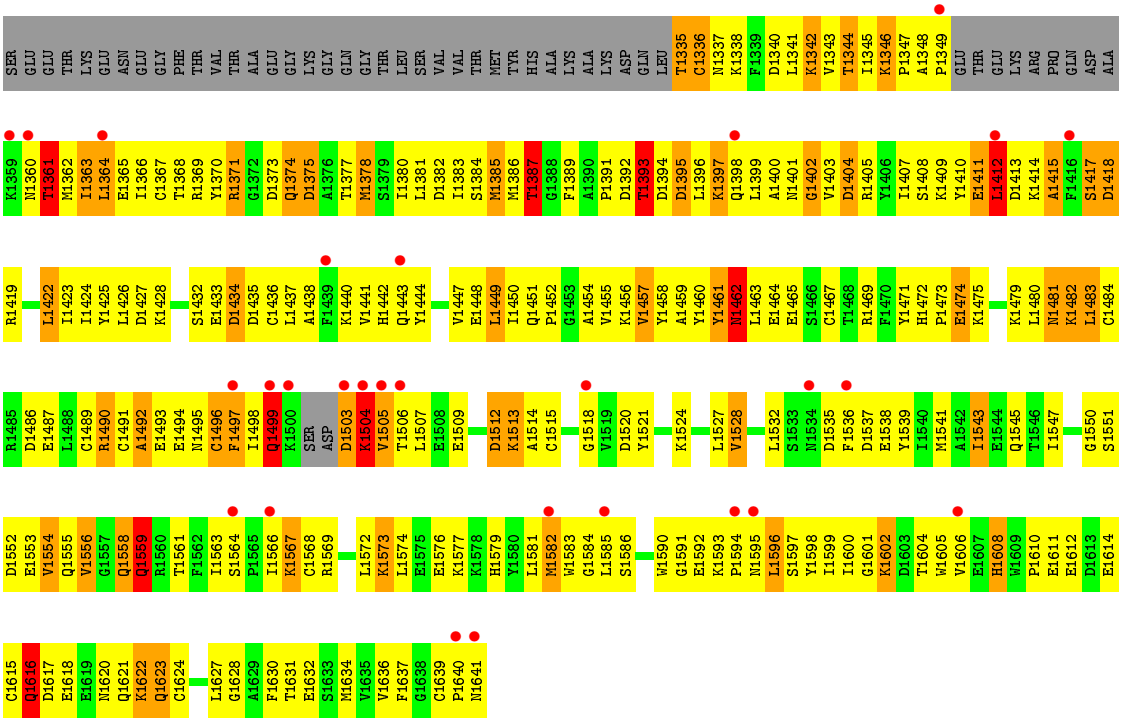
Chain C:





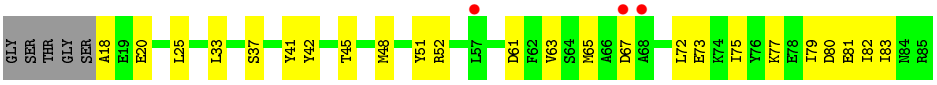
• Molecule 3: Complement C3c alpha' chain fragment 2

Chain F:

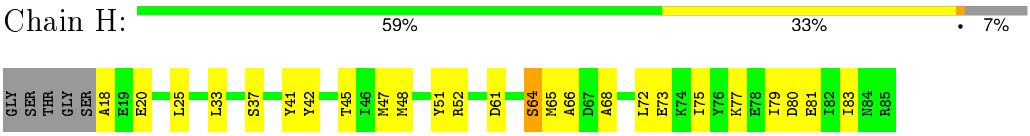


• Molecule 4: Fibrinogen-binding protein

Chain G:



- Molecule 4: Fibrinogen-binding protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.30Å 165.44Å 203.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.71 – 3.40 50.06 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.6 (32.71-3.40) 91.6 (50.06-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.229 , 0.270 0.222 , 0.266	Depositor DCC
R_{free} test set	1920 reflections (4.29%)	DCC
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 46850 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18730	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.52	1/5030 (0.0%)	0.69	0/6837
1	D	0.51	0/5030	0.68	0/6837
2	B	0.50	0/1512	0.65	0/2055
2	E	0.52	0/1512	0.67	0/2055
3	C	0.53	1/2453 (0.0%)	0.72	4/3305 (0.1%)
3	F	0.65	1/2453 (0.0%)	0.78	0/3305
4	G	0.53	0/553	0.65	0/741
4	H	0.52	0/553	0.64	0/741
All	All	0.54	3/19096 (0.0%)	0.70	4/25876 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1623	GLN	C-N	-5.78	1.20	1.34
3	C	1391	PRO	C-N	-5.63	1.21	1.34
1	A	631	GLN	C-N	-5.54	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1419	ARG	CB-CA-C	-5.99	98.41	110.40
3	C	1447	VAL	N-CA-CB	5.88	124.42	111.50
3	C	1405	ARG	N-CA-CB	5.21	119.99	110.60
3	C	1498	ILE	CB-CA-C	5.06	121.72	111.60

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	4931	0	4993	292	0
1	D	4931	0	4993	275	0
2	B	1480	0	1501	98	0
2	E	1480	0	1501	89	0
3	C	2407	0	2316	350	0
3	F	2407	0	2315	287	0
4	G	547	0	568	19	0
4	H	547	0	568	30	0
All	All	18730	0	18755	1362	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 36.

All (1362) 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:C:1389:PHE:CD2	3:C:1443:GLN:HB2	1.46	1.50
3:C:1381:LEU:HD13	3:C:1383:ILE:CG1	1.38	1.47
3:C:1381:LEU:CD1	3:C:1383:ILE:HG13	1.47	1.41
1:A:346:MET:HE3	1:A:456:ARG:CB	1.54	1.36
3:C:1379:SER:C	3:C:1380:ILE:HD12	1.44	1.36
1:A:253:ILE:HD12	1:A:289:VAL:CG1	1.57	1.32
3:F:1494:GLU:CG	3:F:1602:LYS:HD3	1.60	1.31
2:E:758:GLU:OE2	2:E:767:LYS:HB2	1.29	1.28
3:C:1366:ILE:O	3:C:1367:CYS:SG	1.94	1.26
3:C:1376:ALA:HB3	3:C:1429:VAL:CG2	1.69	1.23
3:C:1396:LEU:HB3	3:C:1412:LEU:CD1	1.67	1.22
3:C:1389:PHE:CE2	3:C:1443:GLN:HB2	1.77	1.18
1:A:346:MET:CE	1:A:456:ARG:CB	2.23	1.17
3:C:1389:PHE:CE2	3:C:1443:GLN:CB	2.27	1.17
3:C:1381:LEU:HD13	3:C:1383:ILE:CD1	1.76	1.16
3:C:1389:PHE:CZ	3:C:1443:GLN:HB3	1.79	1.16
3:C:1365:GLU:O	3:C:1366:ILE:HG12	1.47	1.14
1:D:253:ILE:CD1	1:D:302:LEU:CD2	2.24	1.14
3:C:1396:LEU:HB3	3:C:1412:LEU:HD11	1.30	1.13
3:C:1552:ASP:OD1	3:C:1554:VAL:HG12	1.47	1.13
3:C:1390:ALA:HB3	3:C:1416:PHE:CD1	1.84	1.12
3:C:1404:ASP:HA	3:C:1427:ASP:OD1	1.49	1.11
1:A:346:MET:CE	1:A:456:ARG:HB3	1.80	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:HB3	1:A:393:PRO:CD	1.80	1.10
1:A:253:ILE:HD12	1:A:289:VAL:HG11	1.32	1.10
1:D:253:ILE:HD13	1:D:302:LEU:CD2	1.82	1.09
1:A:253:ILE:CD1	1:A:289:VAL:CG1	2.31	1.09
1:A:253:ILE:CD1	1:A:289:VAL:HG11	1.81	1.09
3:C:1389:PHE:CD2	3:C:1443:GLN:CB	2.36	1.07
1:A:392:HIS:HB3	1:A:393:PRO:HD2	1.10	1.06
3:C:1376:ALA:HB3	3:C:1429:VAL:HG22	1.29	1.05
3:C:1404:ASP:HA	3:C:1427:ASP:CG	1.76	1.05
3:F:1494:GLU:HG2	3:F:1602:LYS:HD3	1.07	1.04
3:F:1618:GLU:CA	3:F:1621:GLN:HG3	1.88	1.03
3:F:1494:GLU:HG2	3:F:1602:LYS:CD	1.88	1.03
1:D:547:GLN:O	1:D:547:GLN:HG2	1.54	1.03
1:A:346:MET:CE	1:A:456:ARG:HB2	1.86	1.02
3:F:1618:GLU:HA	3:F:1621:GLN:HG3	1.10	1.02
3:F:1483:LEU:HD21	3:F:1590:TRP:CE2	1.94	1.02
1:A:289:VAL:O	3:F:1594:PRO:HG2	1.59	1.02
1:A:454:LEU:HD22	1:A:492:LEU:HD12	1.37	1.02
1:D:55:THR:HG22	1:D:57:ALA:H	1.25	1.01
1:A:253:ILE:HD12	1:A:289:VAL:HG13	1.43	1.01
3:F:1504:LYS:O	3:F:1505:VAL:HG22	1.61	1.01
1:A:55:THR:HG22	1:A:57:ALA:H	1.25	1.00
3:F:1618:GLU:HA	3:F:1621:GLN:CG	1.90	1.00
3:C:1475:LYS:HE2	3:C:1493:GLU:OE2	1.61	1.00
3:C:1504:LYS:O	3:C:1505:VAL:HG22	1.61	0.99
1:D:253:ILE:CD1	1:D:302:LEU:HD21	1.93	0.99
3:C:1343:VAL:HG22	3:C:1366:ILE:HG23	1.44	0.98
1:A:549:GLU:HG2	1:A:550:ASP:H	1.28	0.98
3:C:1361:THR:HB	3:C:1442:HIS:ND1	1.78	0.98
1:D:3:MET:HE3	1:D:522:ARG:HG2	1.46	0.97
3:C:1367:CYS:HB3	3:C:1434:ASP:OD2	1.65	0.97
3:F:1543:ILE:HD12	3:F:1554:VAL:HG21	1.43	0.96
3:C:1381:LEU:CD1	3:C:1383:ILE:CD1	2.42	0.96
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.45	0.96
3:F:1341:LEU:HD21	3:F:1455:VAL:HG12	1.45	0.96
3:C:1378:MET:HA	3:C:1427:ASP:O	1.64	0.96
3:C:1488:LEU:HD23	3:C:1590:TRP:CH2	2.02	0.95
1:D:63:ASN:O	1:D:64:VAL:HG13	1.68	0.93
1:A:63:ASN:O	1:A:64:VAL:HG13	1.68	0.93
3:F:1483:LEU:HD12	3:F:1484:CYS:N	1.84	0.93
3:C:1340:ASP:O	3:C:1368:THR:HA	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1381:LEU:CD1	3:C:1383:ILE:CG1	2.21	0.92
3:C:1379:SER:O	3:C:1380:ILE:HD12	1.66	0.92
3:C:1389:PHE:CG	3:C:1443:GLN:HB2	2.04	0.92
3:C:1365:GLU:HG2	3:C:1366:ILE:N	1.84	0.92
3:C:1380:ILE:CG2	3:C:1423:ILE:CG2	2.48	0.92
1:A:454:LEU:CD2	1:A:492:LEU:HD12	2.01	0.91
1:A:290:GLN:HG3	1:A:290:GLN:O	1.70	0.91
1:D:372:GLU:HA	1:D:373:ASP:CB	1.99	0.91
1:A:292:PRO:HB3	3:F:1553:GLU:HB3	1.50	0.91
1:A:372:GLU:HA	1:A:373:ASP:CB	1.99	0.91
3:C:1386:MET:HA	3:C:1451:GLN:O	1.70	0.90
3:F:1381:LEU:HD23	3:F:1457:VAL:CG1	2.01	0.90
3:C:1379:SER:C	3:C:1380:ILE:CD1	2.39	0.90
3:F:1407:ILE:HD11	3:F:1424:ILE:HG12	1.53	0.90
3:C:1376:ALA:HB3	3:C:1429:VAL:HG21	1.50	0.90
3:F:1593:LYS:N	3:F:1596:LEU:CD2	2.35	0.89
3:C:1381:LEU:HD12	3:C:1383:ILE:HG13	1.54	0.89
2:E:764:ILE:HG22	2:E:764:ILE:O	1.72	0.89
1:D:541:LEU:HD13	2:E:786:SER:HB3	1.53	0.89
3:C:1381:LEU:HD13	3:C:1383:ILE:HG13	0.93	0.89
1:A:136:PRO:HD2	2:B:789:ASP:HA	1.54	0.89
1:A:372:GLU:CA	1:A:373:ASP:HB2	2.03	0.88
3:F:1494:GLU:HG3	3:F:1602:LYS:HD3	1.54	0.88
1:D:372:GLU:CA	1:D:373:ASP:HB2	2.03	0.88
1:D:372:GLU:N	1:D:373:ASP:HB2	1.88	0.88
1:A:372:GLU:N	1:A:373:ASP:HB2	1.88	0.88
2:E:819:ARG:HG2	2:E:819:ARG:HH11	1.39	0.88
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.56	0.88
1:D:24:ALA:HB3	1:D:60:HIS:HB3	1.56	0.87
3:C:1376:ALA:CB	3:C:1429:VAL:CG2	2.53	0.87
2:E:758:GLU:OE2	2:E:767:LYS:CB	2.20	0.86
1:A:105:SER:HB3	1:A:139:ARG:HE	1.40	0.86
3:C:1404:ASP:HB3	3:C:1427:ASP:HB2	1.55	0.86
2:E:734:ILE:HA	4:H:51:TYR:HE1	1.40	0.86
3:C:1396:LEU:CB	3:C:1412:LEU:HD11	2.06	0.86
1:A:392:HIS:CB	1:A:393:PRO:HD2	2.00	0.86
3:F:1462:ASN:ND2	3:F:1464:GLU:H	1.74	0.85
3:F:1593:LYS:N	3:F:1596:LEU:HD23	1.91	0.85
3:C:1475:LYS:CE	3:C:1493:GLU:OE2	2.24	0.85
3:C:1365:GLU:HG2	3:C:1366:ILE:H	1.40	0.85
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1367:CYS:CB	3:C:1434:ASP:OD2	2.25	0.84
2:B:819:ARG:HG2	2:B:819:ARG:HH11	1.41	0.84
3:F:1592:GLU:CA	3:F:1596:LEU:HD23	2.06	0.84
3:C:1380:ILE:HG21	3:C:1423:ILE:CG2	2.07	0.84
3:F:1592:GLU:C	3:F:1596:LEU:HD23	1.98	0.84
1:D:290:GLN:HG2	1:D:290:GLN:O	1.77	0.84
3:C:1381:LEU:HD12	3:C:1381:LEU:O	1.77	0.84
1:A:549:GLU:HG2	1:A:550:ASP:N	1.93	0.83
1:A:346:MET:HE3	1:A:456:ARG:HB3	0.87	0.83
1:D:69:PRO:HA	1:D:70:ALA:HB3	1.61	0.83
3:C:1389:PHE:CE1	3:C:1443:GLN:HB3	2.13	0.82
3:C:1552:ASP:OD1	3:C:1554:VAL:CG1	2.25	0.82
1:D:105:SER:HB3	1:D:139:ARG:HE	1.41	0.82
1:A:281:SER:OG	1:A:284:VAL:HG23	1.79	0.82
3:C:1389:PHE:HA	3:C:1443:GLN:HA	1.59	0.82
3:F:1462:ASN:HD22	3:F:1462:ASN:C	1.84	0.82
1:D:253:ILE:HD13	1:D:302:LEU:HD22	1.62	0.82
1:D:281:SER:OG	1:D:284:VAL:HG23	1.80	0.81
1:D:10:ASN:HB3	1:D:635:ARG:HD3	1.62	0.81
3:C:1552:ASP:CG	3:C:1554:VAL:HG12	2.00	0.81
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.61	0.81
3:C:1367:CYS:HB3	3:C:1434:ASP:CG	2.01	0.81
1:A:10:ASN:HB3	1:A:635:ARG:HD3	1.62	0.81
3:C:1433:GLU:O	3:C:1434:ASP:HB2	1.81	0.80
1:A:329:SER:HB2	1:A:413:GLU:O	1.81	0.80
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.64	0.80
1:A:628:SER:HB2	1:A:630:GLN:OE1	1.80	0.80
3:C:1443:GLN:HG2	3:C:1443:GLN:O	1.82	0.80
1:D:329:SER:HB2	1:D:413:GLU:O	1.81	0.80
3:C:1343:VAL:HG22	3:C:1366:ILE:CG2	2.12	0.79
1:D:628:SER:HB2	1:D:630:GLN:OE1	1.80	0.79
3:C:1396:LEU:CB	3:C:1412:LEU:CD1	2.57	0.79
1:D:6:ILE:HD13	1:D:22:LEU:HD23	1.64	0.79
1:A:104:GLN:O	1:A:132:HIS:HE1	1.66	0.79
3:C:1495:ASN:HD22	3:C:1496:CYS:N	1.80	0.79
2:B:836:GLN:NE2	2:B:897:HIS:HE1	1.79	0.79
3:C:1454:ALA:HB2	3:C:1470:PHE:CE2	2.16	0.79
1:D:547:GLN:O	1:D:547:GLN:CG	2.30	0.79
3:C:1381:LEU:HD13	3:C:1383:ILE:HD11	1.64	0.78
1:A:207:LEU:HD21	2:B:747:GLU:HG2	1.64	0.78
3:F:1450:ILE:HD11	3:F:1472:HIS:CE1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1380:ILE:HG23	3:C:1423:ILE:HG22	1.63	0.78
3:C:1424:ILE:HG22	3:C:1426:LEU:CD1	2.14	0.78
1:D:104:GLN:O	1:D:132:HIS:HE1	1.66	0.78
1:D:552:GLN:HB3	1:D:553:PRO:HD2	1.63	0.78
3:C:1390:ALA:CB	3:C:1416:PHE:CD1	2.66	0.78
3:F:1590:TRP:O	3:F:1596:LEU:HA	1.83	0.78
4:G:61:ASP:O	4:G:65:MET:HG3	1.82	0.78
3:C:1365:GLU:O	3:C:1366:ILE:CG1	2.30	0.78
3:F:1381:LEU:HD23	3:F:1457:VAL:HG13	1.66	0.78
1:A:45:LEU:HD21	1:A:48:SER:HB3	1.66	0.77
1:D:293:ARG:O	1:D:296:ASP:HB2	1.84	0.77
2:B:734:ILE:HA	4:G:51:TYR:HE1	1.48	0.77
1:D:549:GLU:O	1:D:550:ASP:HB2	1.85	0.77
3:C:1480:LEU:HB3	3:C:1493:GLU:HG3	1.67	0.77
3:F:1397:LYS:H	3:F:1397:LYS:HD3	1.49	0.77
1:A:136:PRO:CD	2:B:789:ASP:HA	2.14	0.77
1:D:45:LEU:HD21	1:D:48:SER:HB3	1.66	0.77
3:F:1344:THR:CG2	3:F:1346:LYS:HE2	2.15	0.77
3:C:1495:ASN:O	3:C:1496:CYS:CB	2.32	0.76
4:H:61:ASP:O	4:H:65:MET:HG3	1.86	0.76
3:C:1543:ILE:HD12	3:C:1554:VAL:HG21	1.67	0.76
3:C:1338:LYS:HD3	3:C:1465:GLU:HB2	1.67	0.76
3:C:1380:ILE:CG2	3:C:1423:ILE:HG22	2.14	0.76
1:A:289:VAL:O	3:F:1594:PRO:CG	2.33	0.75
1:D:606:THR:HG22	1:D:608:GLY:H	1.50	0.75
1:D:400:ILE:H	1:D:400:ILE:HD12	1.50	0.75
1:A:606:THR:HG22	1:A:608:GLY:H	1.50	0.75
3:C:1365:GLU:C	3:C:1366:ILE:CG1	2.54	0.75
3:F:1593:LYS:N	3:F:1596:LEU:HD21	2.01	0.75
3:C:1396:LEU:HB3	3:C:1412:LEU:HD12	1.62	0.75
3:C:1389:PHE:CZ	3:C:1443:GLN:CB	2.54	0.75
3:C:1376:ALA:CB	3:C:1429:VAL:HG22	2.12	0.75
4:G:48:MET:O	4:G:52:ARG:HG3	1.87	0.75
3:C:1481:ASN:ND2	3:C:1567:LYS:HE3	2.00	0.75
3:C:1495:ASN:O	3:C:1496:CYS:HB2	1.83	0.75
3:C:1497:PHE:CE2	3:C:1571:ALA:HB1	2.22	0.75
2:E:836:GLN:NE2	2:E:897:HIS:HE1	1.84	0.75
4:H:48:MET:O	4:H:52:ARG:HG3	1.87	0.75
3:C:1341:LEU:HD13	3:C:1368:THR:HB	1.68	0.75
3:F:1396:LEU:O	3:F:1399:LEU:HB2	1.87	0.75
4:H:18:ALA:N	4:H:65:MET:HE3	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1481:ASN:HD22	3:C:1567:LYS:HE3	1.51	0.75
1:A:400:ILE:H	1:A:400:ILE:HD12	1.50	0.75
3:F:1342:LYS:HB2	3:F:1367:CYS:HB2	1.69	0.74
3:C:1465:GLU:O	3:C:1465:GLU:CG	2.32	0.74
2:E:738:ASN:HB3	4:H:47:MET:SD	2.26	0.74
1:A:253:ILE:CD1	1:A:289:VAL:HG13	2.06	0.74
2:B:836:GLN:H	2:B:868:PRO:HG3	1.52	0.74
3:C:1485:ARG:O	3:C:1486:ASP:HB2	1.86	0.74
1:A:372:GLU:CA	1:A:373:ASP:CB	2.65	0.74
1:A:487:GLU:H	1:A:490:GLN:NE2	1.85	0.74
3:C:1450:ILE:HG22	3:C:1451:GLN:N	2.02	0.74
3:C:1380:ILE:N	3:C:1380:ILE:HD12	2.01	0.74
3:F:1450:ILE:O	3:F:1450:ILE:HD12	1.87	0.74
3:F:1472:HIS:ND1	3:F:1473:PRO:HD2	2.02	0.74
2:E:734:ILE:HG12	4:H:51:TYR:CD1	2.22	0.73
3:C:1345:ILE:HD12	3:C:1363:ILE:O	1.88	0.73
3:F:1344:THR:HG21	3:F:1346:LYS:HE2	1.69	0.73
1:D:487:GLU:H	1:D:490:GLN:NE2	1.85	0.73
1:D:268:ARG:HB2	3:F:1378:MET:CE	2.18	0.73
3:C:1361:THR:CB	3:C:1442:HIS:ND1	2.52	0.73
3:C:1366:ILE:O	3:C:1436:CYS:SG	2.46	0.73
1:D:372:GLU:HA	1:D:373:ASP:HB2	1.66	0.73
3:C:1481:ASN:HB2	3:C:1492:ALA:O	1.87	0.73
2:E:836:GLN:H	2:E:868:PRO:HG3	1.53	0.73
1:D:84:VAL:HG13	1:D:101:VAL:HG21	1.69	0.73
3:C:1426:LEU:HD13	3:C:1426:LEU:N	2.03	0.73
2:E:819:ARG:CG	2:E:819:ARG:HH11	2.01	0.73
3:F:1340:ASP:O	3:F:1368:THR:HA	1.89	0.73
1:D:20:MET:HE1	1:D:35:VAL:HG13	1.71	0.73
1:D:253:ILE:HD12	1:D:302:LEU:HD21	1.70	0.73
1:D:564:GLU:HG2	2:E:766:THR:HG23	1.71	0.72
3:C:1381:LEU:HA	3:C:1456:LYS:O	1.87	0.72
3:C:1443:GLN:CG	3:C:1443:GLN:O	2.38	0.72
1:D:541:LEU:CD1	2:E:786:SER:HB3	2.20	0.72
3:F:1389:PHE:O	3:F:1444:TYR:HE2	1.71	0.72
3:C:1390:ALA:CB	3:C:1416:PHE:HD1	2.02	0.72
3:C:1403:VAL:HG22	3:C:1404:ASP:OD1	1.90	0.72
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.69	0.72
3:C:1592:GLU:OE1	3:C:1592:GLU:HA	1.89	0.72
1:D:253:ILE:HD13	1:D:302:LEU:HD23	1.69	0.72
1:A:253:ILE:HD13	1:A:289:VAL:HG11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1422:LEU:HD23	3:F:1422:LEU:O	1.90	0.72
1:A:641:PRO:O	1:A:642:GLN:HB2	1.90	0.72
1:A:20:MET:HE1	1:A:35:VAL:HG13	1.70	0.72
3:C:1507:LEU:O	3:C:1507:LEU:HD22	1.90	0.71
2:B:819:ARG:HD2	2:B:881:LEU:O	1.90	0.71
1:D:291:ASN:O	1:D:292:PRO:C	2.27	0.71
3:F:1537:ASP:OD2	3:F:1569:ARG:HD2	1.90	0.71
1:A:183:LYS:HZ1	1:A:185:ARG:HD2	1.54	0.71
3:C:1520:ASP:OD1	3:C:1550:GLY:HA3	1.90	0.71
3:C:1337:ASN:O	3:C:1371:ARG:HD3	1.90	0.71
3:F:1520:ASP:OD1	3:F:1550:GLY:HA3	1.90	0.71
3:C:1537:ASP:OD2	3:C:1569:ARG:HD2	1.90	0.71
3:F:1417:SER:OG	3:F:1418:ASP:N	2.19	0.71
2:E:845:LEU:HD21	2:E:891:LYS:HE3	1.72	0.71
4:G:75:ILE:O	4:G:79:ILE:HG13	1.90	0.71
4:H:75:ILE:O	4:H:79:ILE:HG13	1.90	0.71
2:E:756:LEU:HA	2:E:758:GLU:OE1	1.91	0.71
1:A:345:GLY:N	1:A:392:HIS:O	2.24	0.71
1:D:370:GLN:HG2	1:D:401:THR:HB	1.73	0.71
3:C:1497:PHE:HE2	3:C:1571:ALA:HB1	1.56	0.71
3:F:1393:THR:HG23	3:F:1419:ARG:HH12	1.56	0.71
3:C:1365:GLU:C	3:C:1366:ILE:HG12	2.09	0.71
3:C:1543:ILE:HD12	3:C:1554:VAL:CG2	2.20	0.71
3:F:1507:LEU:HD22	3:F:1507:LEU:O	1.90	0.71
3:C:1390:ALA:HB3	3:C:1416:PHE:HD1	1.47	0.71
2:E:820:ASN:ND2	3:F:1489:CYS:HB2	2.06	0.71
3:C:1488:LEU:CD2	3:C:1590:TRP:CH2	2.74	0.71
2:E:819:ARG:HD2	2:E:881:LEU:O	1.91	0.71
1:D:641:PRO:O	1:D:642:GLN:HB2	1.90	0.71
3:C:1379:SER:CA	3:C:1380:ILE:HD12	2.21	0.70
1:D:253:ILE:HD12	1:D:302:LEU:CD2	2.16	0.70
3:F:1592:GLU:HA	3:F:1592:GLU:OE1	1.89	0.70
3:F:1591:GLY:C	3:F:1596:LEU:HB3	2.09	0.70
1:A:370:GLN:HG2	1:A:401:THR:HB	1.73	0.70
1:A:292:PRO:HB3	3:F:1553:GLU:CB	2.21	0.70
2:E:734:ILE:HA	4:H:51:TYR:CE1	2.25	0.70
1:A:48:SER:O	1:A:49:SER:O	2.09	0.70
1:A:567:HIS:CE1	2:B:760:PRO:HD3	2.26	0.70
2:E:734:ILE:HD12	2:E:900:SER:HB3	1.74	0.70
2:B:819:ARG:HH11	2:B:819:ARG:CG	2.04	0.70
3:C:1481:ASN:ND2	3:C:1567:LYS:CE	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LEU:HD21	2:E:747:GLU:HG2	1.73	0.70
1:A:332:GLN:HE21	1:A:357:PRO:HA	1.57	0.70
2:B:910:VAL:HG22	2:B:911:PRO:HD2	1.73	0.69
3:F:1480:LEU:O	3:F:1481:ASN:CG	2.29	0.69
3:F:1592:GLU:HA	3:F:1596:LEU:HD23	1.74	0.69
1:A:290:GLN:O	1:A:290:GLN:CG	2.41	0.69
1:D:372:GLU:CA	1:D:373:ASP:CB	2.65	0.69
3:F:1572:LEU:HD22	3:F:1574:LEU:HD21	1.75	0.69
1:D:253:ILE:CD1	1:D:302:LEU:HD23	2.18	0.69
3:F:1567:LYS:HG3	3:F:1567:LYS:O	1.93	0.69
1:D:69:PRO:HA	1:D:70:ALA:CB	2.22	0.69
3:C:1389:PHE:CD1	3:C:1443:GLN:N	2.60	0.69
3:C:1450:ILE:CG2	3:C:1451:GLN:N	2.56	0.69
1:A:291:ASN:HB3	1:A:292:PRO:HD2	1.74	0.69
1:D:154:LYS:HD2	1:D:171:TRP:CD1	2.27	0.69
2:B:734:ILE:HD12	2:B:900:SER:HB3	1.74	0.69
3:F:1387:THR:HG23	3:F:1451:GLN:H	1.57	0.69
1:D:48:SER:O	1:D:49:SER:O	2.09	0.69
2:B:847:ASN:OD1	2:B:848:PRO:HD2	1.92	0.69
1:A:114:LYS:HE3	1:A:116:ILE:O	1.92	0.69
1:D:332:GLN:HE21	1:D:357:PRO:HA	1.57	0.69
3:F:1462:ASN:HD22	3:F:1464:GLU:H	1.41	0.69
1:A:69:PRO:HA	1:A:70:ALA:CB	2.22	0.68
3:C:1497:PHE:CD1	3:C:1498:ILE:O	2.46	0.68
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.27	0.68
2:E:758:GLU:HG2	2:E:765:SER:HB2	1.76	0.68
3:C:1543:ILE:CD1	3:C:1554:VAL:HG21	2.23	0.68
1:D:114:LYS:HE3	1:D:116:ILE:O	1.92	0.68
3:F:1407:ILE:CD1	3:F:1424:ILE:HG12	2.24	0.68
3:F:1405:ARG:HD3	3:F:1426:LEU:CD2	2.24	0.68
3:C:1567:LYS:O	3:C:1567:LYS:HG3	1.93	0.68
3:C:1344:THR:HG21	3:C:1346:LYS:HE2	1.74	0.68
1:A:104:GLN:O	1:A:132:HIS:CE1	2.46	0.68
1:A:292:PRO:HD2	1:A:296:ASP:OD2	1.93	0.68
3:C:1581:LEU:HD12	3:C:1582:MET:N	2.09	0.68
3:F:1341:LEU:HD21	3:F:1455:VAL:CG1	2.22	0.67
3:F:1581:LEU:HD12	3:F:1582:MET:N	2.09	0.67
3:F:1498:ILE:O	3:F:1499:GLN:O	2.12	0.67
3:C:1365:GLU:CG	3:C:1366:ILE:H	2.08	0.67
2:B:845:LEU:HD21	2:B:891:LYS:HE3	1.76	0.67
2:E:910:VAL:HG22	2:E:911:PRO:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:GLU:HB2	2:B:906:SER:OG	1.94	0.67
3:C:1389:PHE:CG	3:C:1443:GLN:CB	2.70	0.67
1:A:69:PRO:CA	1:A:70:ALA:HB3	2.25	0.67
3:F:1397:LYS:N	3:F:1397:LYS:HD3	2.10	0.67
1:A:126:ARG:NH2	1:A:573:LEU:O	2.28	0.67
1:A:438:VAL:HG23	1:A:450:ASN:O	1.95	0.67
3:C:1572:LEU:HD22	3:C:1574:LEU:HD21	1.75	0.67
2:E:847:ASN:OD1	2:E:848:PRO:HD2	1.95	0.67
2:E:746:PRO:HG3	2:E:774:LYS:HD2	1.75	0.67
3:C:1617:ASP:HB2	3:C:1620:ASN:HB2	1.77	0.67
1:A:236:ARG:HA	1:A:243:VAL:HG23	1.77	0.67
1:D:204:GLU:HG2	2:E:815:TYR:CE2	2.30	0.67
3:C:1426:LEU:CD1	3:C:1426:LEU:N	2.58	0.67
3:F:1341:LEU:HD22	3:F:1457:VAL:HG22	1.75	0.67
3:F:1347:PRO:HA	3:F:1362:MET:HG2	1.76	0.67
2:E:738:ASN:O	4:H:47:MET:CE	2.42	0.67
1:D:126:ARG:NH2	1:D:573:LEU:O	2.28	0.67
1:D:104:GLN:O	1:D:132:HIS:CE1	2.46	0.66
1:D:438:VAL:HG23	1:D:450:ASN:O	1.95	0.66
4:H:18:ALA:N	4:H:65:MET:CE	2.58	0.66
3:F:1404:ASP:HA	3:F:1427:ASP:HB2	1.76	0.66
3:C:1386:MET:SD	3:C:1473:PRO:HD3	2.36	0.66
3:F:1403:VAL:HG22	3:F:1404:ASP:CG	2.15	0.66
1:A:6:ILE:CD1	1:A:22:LEU:HD23	2.26	0.66
1:D:364:ARG:N	1:D:379:THR:HG22	2.10	0.66
3:F:1483:LEU:HD21	3:F:1590:TRP:CD2	2.30	0.66
1:D:69:PRO:CA	1:D:70:ALA:HB3	2.25	0.66
3:F:1411:GLU:O	3:F:1413:ASP:N	2.27	0.66
3:F:1399:LEU:HD23	3:F:1405:ARG:NH1	2.10	0.66
1:D:236:ARG:HA	1:D:243:VAL:HG23	1.77	0.66
2:B:746:PRO:HG3	2:B:774:LYS:HD2	1.78	0.66
1:D:6:ILE:CD1	1:D:22:LEU:HD23	2.26	0.65
1:A:364:ARG:N	1:A:379:THR:HG22	2.10	0.65
3:F:1407:ILE:HD11	3:F:1424:ILE:CG1	2.25	0.65
1:A:530:TRP:CH2	1:A:532:ASP:HB2	2.31	0.65
3:F:1614:GLU:O	3:F:1620:ASN:HB2	1.96	0.65
3:F:1345:ILE:HD12	3:F:1363:ILE:O	1.96	0.65
1:A:400:ILE:HD13	1:A:419:MET:HE3	1.79	0.65
3:C:1390:ALA:O	3:C:1416:PHE:HE1	1.79	0.65
1:A:547:GLN:OE1	1:A:559:MET:HA	1.96	0.65
3:C:1365:GLU:CG	3:C:1366:ILE:N	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:836:GLN:HE21	2:B:897:HIS:HE1	1.42	0.65
3:C:1381:LEU:CD1	3:C:1383:ILE:HD11	2.20	0.65
1:D:22:LEU:HD22	1:D:33:VAL:HG11	1.79	0.65
3:C:1495:ASN:HD22	3:C:1496:CYS:H	1.45	0.65
3:C:1462:ASN:HD21	3:C:1464:GLU:HB2	1.60	0.65
2:B:756:LEU:HA	2:B:758:GLU:OE1	1.96	0.64
2:B:856:THR:H	3:C:1602:LYS:HZ2	1.44	0.64
1:A:372:GLU:HA	1:A:373:ASP:HB2	1.66	0.64
1:A:455:LEU:HD11	1:A:457:MET:HG2	1.78	0.64
1:D:183:LYS:HZ1	1:D:185:ARG:HD2	1.61	0.64
1:A:22:LEU:HD22	1:A:33:VAL:HG11	1.79	0.64
1:D:400:ILE:HD13	1:D:419:MET:HE3	1.78	0.64
1:D:455:LEU:HD11	1:D:457:MET:HG2	1.78	0.64
1:D:530:TRP:CH2	1:D:532:ASP:HB2	2.31	0.64
1:D:116:ILE:HG13	1:D:201:GLU:HB3	1.79	0.64
3:F:1335:THR:O	3:F:1336:CYS:HB2	1.97	0.64
1:D:370:GLN:OE1	1:D:370:GLN:HA	1.98	0.64
3:F:1415:ALA:C	3:F:1417:SER:H	1.99	0.64
4:G:77:LYS:O	4:G:81:GLU:HG3	1.98	0.64
3:F:1616:GLN:OE1	3:F:1616:GLN:N	2.30	0.64
3:C:1389:PHE:CD1	3:C:1441:VAL:HG23	2.33	0.64
3:C:1424:ILE:HG22	3:C:1426:LEU:HD11	1.79	0.64
1:D:6:ILE:HG12	1:D:20:MET:HE3	1.80	0.64
1:A:183:LYS:NZ	1:A:185:ARG:HD2	2.12	0.64
1:D:183:LYS:NZ	1:D:185:ARG:HD2	2.12	0.64
1:A:116:ILE:HG13	1:A:201:GLU:HB3	1.79	0.64
3:F:1593:LYS:CA	3:F:1596:LEU:HD21	2.28	0.64
1:A:6:ILE:HG22	1:A:625:THR:HB	1.80	0.64
3:F:1561:THR:O	3:F:1597:SER:HB3	1.98	0.63
2:E:860:HIS:HE1	3:F:1451:GLN:HE21	1.44	0.63
3:C:1361:THR:CG2	3:C:1442:HIS:ND1	2.61	0.63
3:F:1483:LEU:HD21	3:F:1590:TRP:NE1	2.13	0.63
1:A:370:GLN:HA	1:A:370:GLN:OE1	1.98	0.63
3:C:1546:THR:HG23	3:C:1556:VAL:HG22	1.80	0.63
3:F:1608:HIS:O	3:F:1610:PRO:HD3	1.99	0.63
4:H:77:LYS:O	4:H:81:GLU:HG3	1.98	0.63
3:C:1415:ALA:H	3:C:1419:ARG:NH2	1.96	0.63
2:E:820:ASN:HD21	3:F:1489:CYS:HB2	1.64	0.63
2:E:836:GLN:HE21	2:E:897:HIS:HE1	1.47	0.63
1:D:31:VAL:HG13	1:D:54:LEU:HB2	1.81	0.63
1:A:6:ILE:HG12	1:A:20:MET:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:898:PHE:HB2	4:H:52:ARG:HG2	1.80	0.63
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.81	0.62
3:C:1389:PHE:CE2	3:C:1443:GLN:HB3	2.04	0.62
3:F:1456:LYS:HA	3:F:1467:CYS:O	2.00	0.62
3:C:1481:ASN:HD22	3:C:1567:LYS:CE	2.11	0.62
3:C:1404:ASP:CA	3:C:1427:ASP:CG	2.62	0.62
1:D:590:THR:HB	1:D:593:LYS:HG3	1.82	0.62
1:D:6:ILE:HG22	1:D:625:THR:HB	1.80	0.62
3:F:1346:LYS:O	3:F:1362:MET:HB3	1.99	0.62
3:C:1344:THR:CG2	3:C:1346:LYS:HE2	2.30	0.62
2:E:761:LYS:O	2:E:762:ASN:CB	2.47	0.62
1:D:36:THR:HG21	1:D:38:HIS:CE1	2.35	0.62
3:F:1483:LEU:HD11	3:F:1590:TRP:NE1	2.15	0.62
3:F:1342:LYS:HE2	3:F:1434:ASP:OD2	1.98	0.62
1:A:36:THR:HG21	1:A:38:HIS:CE1	2.35	0.62
3:C:1390:ALA:HB3	3:C:1416:PHE:CE1	2.35	0.62
3:C:1608:HIS:O	3:C:1610:PRO:HD3	1.99	0.62
2:B:836:GLN:NE2	2:B:897:HIS:CE1	2.67	0.62
2:E:887:GLU:HB2	2:E:906:SER:OG	2.00	0.62
3:C:1387:THR:HG23	3:C:1451:GLN:HB3	1.80	0.62
1:D:268:ARG:HB2	3:F:1378:MET:HE2	1.81	0.62
3:C:1475:LYS:NZ	3:C:1493:GLU:OE2	2.32	0.61
4:H:61:ASP:HB3	4:H:64:SER:OG	1.99	0.61
3:C:1337:ASN:HB2	3:C:1338:LYS:HD2	1.82	0.61
1:D:541:LEU:HD13	2:E:786:SER:CB	2.29	0.61
2:B:734:ILE:HA	4:G:51:TYR:CE1	2.34	0.61
2:E:894:VAL:CG1	2:E:899:ILE:HB	2.30	0.61
3:F:1614:GLU:HB3	3:F:1620:ASN:ND2	2.16	0.61
1:A:590:THR:HB	1:A:593:LYS:HG3	1.82	0.61
3:F:1521:TYR:CZ	3:F:1584:GLY:N	2.68	0.61
3:C:1464:GLU:N	3:C:1464:GLU:OE1	2.30	0.61
1:D:590:THR:HG22	1:D:592:SER:H	1.65	0.61
3:F:1371:ARG:HG2	3:F:1371:ARG:NH1	2.14	0.61
1:D:297:LEU:HA	1:D:300:LYS:HD2	1.82	0.61
3:C:1389:PHE:CA	3:C:1443:GLN:HA	2.31	0.61
3:C:1379:SER:O	3:C:1380:ILE:CD1	2.44	0.61
3:F:1483:LEU:HD11	3:F:1590:TRP:HE1	1.65	0.61
3:F:1456:LYS:HE2	3:F:1458:TYR:CD2	2.36	0.61
3:F:1462:ASN:ND2	3:F:1464:GLU:N	2.48	0.61
3:C:1544:GLU:C	3:C:1556:VAL:CG1	2.69	0.61
1:D:606:THR:HG22	1:D:608:GLY:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:THR:HG22	1:A:608:GLY:N	2.16	0.61
3:C:1453:GLY:HA3	3:C:1471:TYR:CZ	2.36	0.61
3:F:1480:LEU:O	3:F:1481:ASN:ND2	2.34	0.61
3:C:1361:THR:HA	3:C:1441:VAL:O	2.01	0.60
3:C:1521:TYR:CZ	3:C:1584:GLY:N	2.68	0.60
3:C:1406:TYR:CE1	3:C:1408:SER:HA	2.36	0.60
1:A:297:LEU:HA	1:A:300:LYS:HD2	1.82	0.60
3:C:1366:ILE:C	3:C:1367:CYS:SG	2.76	0.60
2:E:819:ARG:NH1	2:E:819:ARG:HG2	2.13	0.60
1:D:142:MET:HG3	1:D:187:TYR:CE1	2.36	0.60
2:E:845:LEU:HD22	2:E:889:GLU:HG2	1.83	0.60
1:A:346:MET:HE2	1:A:456:ARG:HB2	1.82	0.60
3:C:1339:PHE:CZ	3:C:1370:TYR:CD1	2.89	0.60
3:F:1405:ARG:HD3	3:F:1426:LEU:HD23	1.83	0.60
1:D:268:ARG:HB2	3:F:1378:MET:HE1	1.82	0.60
3:C:1361:THR:HB	3:C:1442:HIS:CE1	2.37	0.60
1:A:36:THR:CG2	1:A:38:HIS:CE1	2.85	0.60
3:C:1408:SER:C	3:C:1410:TYR:H	2.04	0.60
3:C:1416:PHE:O	3:C:1417:SER:C	2.39	0.60
1:A:606:THR:HB	1:A:619:ASP:HB3	1.84	0.60
1:A:590:THR:HG22	1:A:592:SER:H	1.65	0.60
3:F:1495:ASN:O	3:F:1496:CYS:C	2.39	0.60
1:D:36:THR:CG2	1:D:38:HIS:CE1	2.85	0.60
3:F:1504:LYS:O	3:F:1505:VAL:CG2	2.45	0.60
3:F:1404:ASP:HB3	3:F:1427:ASP:HB2	1.83	0.60
2:E:872:LEU:HD11	3:F:1418:ASP:HB3	1.83	0.60
1:A:142:MET:HG3	1:A:187:TYR:CE1	2.36	0.60
3:C:1388:GLY:O	3:C:1443:GLN:HA	2.01	0.59
3:C:1543:ILE:O	3:C:1557:GLY:N	2.35	0.59
3:F:1490:ARG:HD2	3:F:1590:TRP:CZ3	2.37	0.59
2:E:764:ILE:O	2:E:764:ILE:CG2	2.44	0.59
3:C:1544:GLU:O	3:C:1556:VAL:CG1	2.50	0.59
3:C:1368:THR:HG21	3:C:1457:VAL:HG11	1.84	0.59
1:A:241:LYS:HG3	2:B:832:TYR:CZ	2.37	0.59
4:H:45:THR:HG21	4:H:75:ILE:HD13	1.84	0.59
3:C:1444:TYR:O	3:C:1445:PHE:HB3	2.02	0.59
3:C:1386:MET:HB3	3:C:1450:ILE:HG21	1.84	0.59
1:D:606:THR:HB	1:D:619:ASP:HB3	1.84	0.59
2:B:834:GLN:HE21	2:B:834:GLN:HA	1.68	0.59
3:C:1472:HIS:HB3	3:C:1475:LYS:HB2	1.84	0.59
3:F:1380:ILE:O	3:F:1457:VAL:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:LEU:N	1:D:471:LEU:HD12	2.17	0.59
3:C:1458:TYR:HB3	3:C:1466:SER:HB3	1.84	0.59
3:C:1450:ILE:CG2	3:C:1451:GLN:H	2.16	0.59
3:C:1504:LYS:O	3:C:1505:VAL:CG2	2.45	0.59
1:D:290:GLN:CG	1:D:290:GLN:O	2.49	0.59
3:F:1345:ILE:O	3:F:1345:ILE:HG23	2.01	0.59
3:C:1433:GLU:O	3:C:1434:ASP:CB	2.51	0.59
2:B:894:VAL:CG1	2:B:899:ILE:HB	2.32	0.59
2:E:860:HIS:CE1	3:F:1451:GLN:HE21	2.21	0.59
1:D:550:ASP:O	1:D:551:ARG:C	2.39	0.59
1:D:257:GLU:OE2	1:D:257:GLU:N	2.36	0.59
3:F:1482:LYS:HG2	3:F:1482:LYS:O	2.02	0.58
3:F:1380:ILE:O	3:F:1457:VAL:HA	2.02	0.58
3:F:1407:ILE:HG22	3:F:1412:LEU:HD22	1.85	0.58
3:C:1454:ALA:HB2	3:C:1470:PHE:CD2	2.38	0.58
3:F:1389:PHE:O	3:F:1444:TYR:CE2	2.55	0.58
1:D:143:VAL:O	1:D:155:GLN:HB2	2.03	0.58
3:F:1456:LYS:HE2	3:F:1458:TYR:HD2	1.67	0.58
4:G:45:THR:HG21	4:G:75:ILE:HD13	1.84	0.58
1:D:282:ARG:HH12	1:D:286:LEU:HD12	1.68	0.58
1:D:346:MET:HG2	1:D:347:PRO:HD2	1.86	0.58
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.68	0.58
1:A:471:LEU:HD12	1:A:471:LEU:N	2.17	0.58
1:D:6:ILE:HD11	1:D:20:MET:CG	2.34	0.58
3:C:1397:LYS:HA	3:C:1400:ALA:HB3	1.84	0.58
1:A:472:ILE:HD13	1:A:509:LEU:HD22	1.85	0.58
3:F:1383:ILE:HG12	3:F:1455:VAL:HG22	1.85	0.58
1:D:291:ASN:HB3	1:D:292:PRO:HD2	1.86	0.58
2:B:845:LEU:HD22	2:B:889:GLU:HG2	1.85	0.58
4:H:18:ALA:HB3	4:H:20:GLU:HG2	1.86	0.58
3:C:1338:LYS:CD	3:C:1465:GLU:HB2	2.34	0.58
3:C:1407:ILE:HD11	3:C:1424:ILE:HG12	1.85	0.58
3:C:1380:ILE:CG2	3:C:1423:ILE:HG23	2.32	0.58
3:F:1404:ASP:CA	3:F:1427:ASP:HB2	2.33	0.58
2:E:738:ASN:O	4:H:47:MET:HE1	2.03	0.58
3:F:1590:TRP:O	3:F:1596:LEU:CA	2.50	0.58
1:D:472:ILE:HD13	1:D:509:LEU:HD22	1.85	0.58
1:D:477:ARG:HH11	1:D:477:ARG:HG3	1.68	0.58
3:F:1506:THR:OG1	3:F:1509:GLU:HG3	2.04	0.57
1:D:204:GLU:OE1	2:E:815:TYR:HE2	1.87	0.57
1:A:257:GLU:N	1:A:257:GLU:OE2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:836:GLN:H	2:B:868:PRO:CG	2.16	0.57
3:C:1499:GLN:CD	3:C:1499:GLN:O	2.42	0.57
1:D:404:THR:CG2	1:D:415:ALA:H	2.17	0.57
1:D:67:THR:O	1:D:69:PRO:HD3	2.05	0.57
3:F:1450:ILE:C	3:F:1450:ILE:HD12	2.24	0.57
3:C:1506:THR:OG1	3:C:1509:GLU:HG3	2.04	0.57
1:A:346:MET:O	1:A:347:PRO:O	2.22	0.57
1:A:6:ILE:HD11	1:A:20:MET:CG	2.34	0.57
1:A:474:ASN:HB3	1:A:477:ARG:HH12	1.70	0.57
1:A:330:PRO:HG2	1:A:409:LEU:HD21	1.86	0.57
3:F:1365:GLU:HG3	3:F:1438:ALA:HB2	1.85	0.57
3:F:1381:LEU:HG	3:F:1426:LEU:HD11	1.87	0.57
3:F:1497:PHE:HB3	3:F:1600:ILE:CG2	2.34	0.57
1:A:404:THR:CG2	1:A:415:ALA:H	2.17	0.57
4:G:18:ALA:HB3	4:G:20:GLU:HG2	1.86	0.57
3:F:1623:GLN:O	3:F:1627:LEU:HG	2.04	0.57
1:A:67:THR:O	1:A:69:PRO:HD3	2.05	0.57
3:F:1371:ARG:HG2	3:F:1371:ARG:HH11	1.70	0.57
3:C:1488:LEU:HG	3:C:1489:CYS:H	1.68	0.57
3:C:1406:TYR:CZ	3:C:1408:SER:HA	2.39	0.57
1:A:282:ARG:HH12	1:A:286:LEU:HD12	1.68	0.57
3:C:1380:ILE:O	3:C:1457:VAL:HA	2.05	0.57
1:D:330:PRO:HG2	1:D:409:LEU:HD21	1.86	0.57
1:D:438:VAL:HG22	1:D:449:LEU:HD11	1.86	0.57
2:E:761:LYS:O	2:E:762:ASN:HB2	2.05	0.57
3:C:1472:HIS:CE1	3:C:1474:GLU:HG2	2.40	0.56
3:F:1411:GLU:C	3:F:1413:ASP:H	2.06	0.56
1:A:158:LEU:HD21	1:A:167:LEU:HD22	1.87	0.56
1:D:251:PHE:CE1	1:D:304:VAL:HG13	2.40	0.56
1:D:158:LEU:HD21	1:D:167:LEU:HD22	1.87	0.56
3:C:1563:ILE:HG12	3:C:1598:TYR:O	2.05	0.56
3:F:1563:ILE:HG12	3:F:1598:TYR:O	2.05	0.56
2:E:836:GLN:H	2:E:868:PRO:CG	2.17	0.56
1:A:567:HIS:HA	2:B:765:SER:HB2	1.86	0.56
3:C:1443:GLN:HE21	3:C:1450:ILE:HD11	1.70	0.56
2:E:868:PRO:O	2:E:869:LYS:C	2.44	0.56
3:F:1384:SER:OG	3:F:1454:ALA:HB3	2.05	0.56
3:C:1630:PHE:O	3:C:1634:MET:HG2	2.05	0.56
3:C:1623:GLN:O	3:C:1627:LEU:HG	2.04	0.56
3:C:1376:ALA:CB	3:C:1429:VAL:HG21	2.26	0.56
3:C:1465:GLU:HG2	3:C:1465:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:PHE:CD1	1:D:419:MET:HG2	2.41	0.56
3:C:1445:PHE:CD2	3:C:1445:PHE:O	2.59	0.56
3:C:1437:LEU:HD12	3:C:1437:LEU:C	2.24	0.56
3:C:1476:GLU:O	3:C:1478:GLY:N	2.39	0.56
1:A:456:ARG:HB2	1:A:456:ARG:HH11	1.70	0.56
1:A:45:LEU:HD21	1:A:48:SER:CB	2.35	0.56
3:F:1408:SER:O	3:F:1410:TYR:N	2.38	0.56
3:C:1416:PHE:HZ	3:C:1442:HIS:HB2	1.70	0.56
3:F:1460:TYR:CG	3:F:1461:TYR:N	2.73	0.56
1:D:15:GLU:HG2	1:D:70:ALA:HB2	1.87	0.56
1:D:344:PRO:HA	1:D:391:THR:HG21	1.86	0.56
3:F:1630:PHE:O	3:F:1634:MET:HG2	2.05	0.56
1:A:87:GLN:O	1:A:87:GLN:HG2	2.05	0.56
1:A:248:PHE:CD1	3:C:1378:MET:HE1	2.41	0.56
2:B:822:GLN:NE2	3:C:1470:PHE:CD1	2.72	0.56
1:A:136:PRO:CG	2:B:789:ASP:HA	2.36	0.56
1:A:15:GLU:HG2	1:A:70:ALA:HB2	1.87	0.56
3:F:1497:PHE:N	3:F:1497:PHE:CD2	2.73	0.56
3:F:1371:ARG:CG	3:F:1371:ARG:HH11	2.17	0.56
1:D:474:ASN:HB3	1:D:477:ARG:HH12	1.70	0.56
1:D:456:ARG:HB2	1:D:456:ARG:HH11	1.70	0.56
2:E:756:LEU:CA	2:E:758:GLU:OE1	2.53	0.55
3:C:1404:ASP:O	3:C:1405:ARG:HG2	2.06	0.55
1:A:214:VAL:HB	1:A:233:ILE:CD1	2.36	0.55
3:C:1499:GLN:O	3:C:1500:LYS:C	2.45	0.55
1:A:541:LEU:HD13	2:B:786:SER:HB3	1.88	0.55
1:A:251:PHE:CE1	1:A:304:VAL:HG13	2.40	0.55
3:F:1389:PHE:HA	3:F:1442:HIS:O	2.06	0.55
1:D:45:LEU:HD21	1:D:48:SER:CB	2.35	0.55
3:C:1465:GLU:O	3:C:1465:GLU:HG3	2.04	0.55
1:A:438:VAL:HG22	1:A:449:LEU:HD11	1.86	0.55
1:D:142:MET:HG3	1:D:187:TYR:CZ	2.41	0.55
1:A:142:MET:HG3	1:A:187:TYR:CZ	2.41	0.55
3:F:1636:VAL:HG12	3:F:1637:PHE:CD2	2.42	0.55
4:H:65:MET:O	4:H:68:ALA:N	2.40	0.55
4:G:79:ILE:O	4:G:83:ILE:HG12	2.07	0.55
1:D:87:GLN:O	1:D:87:GLN:HG2	2.05	0.55
3:F:1381:LEU:CD2	3:F:1457:VAL:CG1	2.81	0.55
4:H:79:ILE:O	4:H:83:ILE:HG12	2.07	0.55
3:C:1397:LYS:HD3	3:C:1397:LYS:H	1.72	0.55
3:F:1462:ASN:ND2	3:F:1462:ASN:C	2.56	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1377:THR:O	3:C:1378:MET:C	2.43	0.55
1:D:552:GLN:HB3	1:D:553:PRO:CD	2.32	0.55
1:A:335:PHE:CD1	1:A:419:MET:HG2	2.41	0.55
1:D:151:ILE:O	1:D:153:VAL:HG13	2.07	0.55
1:D:214:VAL:HB	1:D:233:ILE:CD1	2.36	0.55
3:C:1636:VAL:HG12	3:C:1637:PHE:CD2	2.42	0.55
3:C:1342:LYS:O	3:C:1366:ILE:HA	2.07	0.55
1:D:253:ILE:CD1	1:D:302:LEU:HD22	2.27	0.55
1:D:589:LEU:HD12	1:D:590:THR:H	1.72	0.55
3:C:1408:SER:C	3:C:1410:TYR:N	2.59	0.54
3:F:1513:LYS:C	3:F:1515:CYS:H	2.10	0.54
1:A:548:SER:O	1:A:549:GLU:HB3	2.07	0.54
2:B:851:CYS:HB2	2:B:881:LEU:HD21	1.88	0.54
3:F:1364:LEU:HD21	3:F:1471:TYR:CZ	2.43	0.54
3:F:1472:HIS:CD2	3:F:1475:LYS:HD2	2.42	0.54
3:C:1566:ILE:C	3:C:1568:CYS:H	2.10	0.54
3:C:1460:TYR:CG	3:C:1461:TYR:N	2.74	0.54
3:C:1340:ASP:O	3:C:1368:THR:CA	2.51	0.54
3:C:1380:ILE:HG13	3:C:1425:TYR:CD1	2.41	0.54
3:C:1380:ILE:HG22	3:C:1381:LEU:N	2.22	0.54
1:A:549:GLU:CG	1:A:550:ASP:H	2.10	0.54
3:C:1498:ILE:HG21	3:C:1605:TRP:CE3	2.42	0.54
3:F:1566:ILE:HG13	3:F:1569:ARG:HD3	1.90	0.54
3:F:1419:ARG:HG2	3:F:1419:ARG:O	2.06	0.54
2:B:756:LEU:HD23	2:B:758:GLU:OE1	2.07	0.54
2:E:731:GLU:O	2:E:732:ASP:HB2	2.07	0.54
2:E:838:LEU:HD22	2:E:894:VAL:HG21	1.90	0.54
1:A:151:ILE:O	1:A:153:VAL:HG13	2.07	0.54
1:A:312:SER:HB2	1:A:314:SER:OG	2.08	0.54
3:C:1380:ILE:CD1	3:C:1380:ILE:N	2.67	0.54
1:A:550:ASP:OD2	1:A:551:ARG:N	2.29	0.54
4:H:61:ASP:CG	4:H:64:SER:OG	2.46	0.54
3:F:1566:ILE:C	3:F:1568:CYS:H	2.10	0.54
3:C:1380:ILE:HG21	3:C:1423:ILE:HG21	1.84	0.54
1:A:589:LEU:HD12	1:A:590:THR:H	1.72	0.54
1:D:517:GLY:O	1:D:518:ALA:C	2.46	0.54
3:C:1390:ALA:CB	3:C:1416:PHE:HA	2.37	0.54
3:C:1381:LEU:HD11	3:C:1383:ILE:CD1	2.32	0.54
1:A:454:LEU:CD2	1:A:492:LEU:CD1	2.81	0.54
3:C:1566:ILE:HG13	3:C:1569:ARG:HD3	1.90	0.54
3:C:1414:LYS:O	3:C:1415:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1503:ASP:C	3:F:1504:LYS:HD3	2.28	0.54
3:F:1512:ASP:O	3:F:1513:LYS:C	2.47	0.54
3:F:1337:ASN:HB2	3:F:1338:LYS:HD2	1.89	0.54
2:E:756:LEU:C	2:E:758:GLU:OE1	2.47	0.53
1:A:20:MET:HE1	1:A:35:VAL:CG1	2.38	0.53
1:D:453:PHE:HB2	1:D:493:VAL:CG2	2.38	0.53
3:C:1512:ASP:O	3:C:1513:LYS:C	2.47	0.53
1:A:392:HIS:CB	1:A:393:PRO:CD	2.59	0.53
2:B:819:ARG:HG2	2:B:819:ARG:NH1	2.14	0.53
2:B:838:LEU:HD22	2:B:894:VAL:HG21	1.90	0.53
1:A:3:MET:CE	1:A:522:ARG:HG2	2.31	0.53
3:F:1462:ASN:ND2	3:F:1465:GLU:H	2.06	0.53
4:H:61:ASP:OD2	4:H:64:SER:OG	2.27	0.53
2:E:834:GLN:HE21	2:E:834:GLN:HA	1.73	0.53
1:D:312:SER:HB2	1:D:314:SER:OG	2.08	0.53
1:A:558:GLN:HB3	2:B:772:PHE:CE1	2.43	0.53
3:C:1503:ASP:C	3:C:1504:LYS:HD3	2.28	0.53
4:H:65:MET:O	4:H:66:ALA:C	2.46	0.53
3:F:1480:LEU:O	3:F:1481:ASN:CB	2.57	0.53
2:E:767:LYS:HG2	2:E:768:LEU:N	2.23	0.53
3:C:1381:LEU:HD21	3:C:1424:ILE:HB	1.91	0.53
3:C:1411:GLU:OE2	3:C:1422:LEU:HA	2.09	0.53
3:F:1494:GLU:HG2	3:F:1602:LYS:CE	2.39	0.53
3:F:1341:LEU:HD12	3:F:1342:LYS:N	2.24	0.53
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.39	0.53
1:D:578:LYS:HE3	2:E:800:GLU:OE2	2.09	0.53
1:A:290:GLN:HG2	3:F:1594:PRO:HG2	1.91	0.53
1:D:286:LEU:HD11	1:D:294:ALA:HB2	1.91	0.53
3:C:1393:THR:HG23	3:C:1419:ARG:HH22	1.74	0.52
3:F:1385:MET:CE	3:F:1385:MET:HA	2.39	0.52
3:C:1554:VAL:HB	3:C:1560:ARG:CZ	2.39	0.52
3:F:1380:ILE:HG13	3:F:1425:TYR:HD2	1.74	0.52
1:A:289:VAL:HG23	1:A:290:GLN:H	1.74	0.52
3:C:1552:ASP:CG	3:C:1554:VAL:CG1	2.75	0.52
3:F:1407:ILE:HD11	3:F:1424:ILE:CD1	2.39	0.52
3:F:1392:ASP:O	3:F:1393:THR:C	2.47	0.52
1:A:250:ILE:HB	1:A:266:LEU:HD13	1.91	0.52
1:D:250:ILE:HB	1:D:266:LEU:HD13	1.91	0.52
3:F:1497:PHE:HB3	3:F:1600:ILE:HG22	1.92	0.52
3:F:1383:ILE:HB	3:F:1422:LEU:HD23	1.90	0.52
1:D:6:ILE:CG1	1:D:20:MET:HE3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:734:ILE:HG12	4:G:51:TYR:CD1	2.44	0.52
3:F:1364:LEU:HD11	3:F:1471:TYR:CE2	2.45	0.52
1:D:253:ILE:HD11	1:D:302:LEU:HD21	1.88	0.52
1:A:164:LEU:HD12	1:A:164:LEU:O	2.10	0.52
1:A:575:ALA:O	2:B:748:SER:HA	2.10	0.52
1:A:80:ARG:O	1:A:81:ASN:HB2	2.10	0.52
3:C:1389:PHE:CD1	3:C:1443:GLN:CB	2.92	0.52
2:B:855:THR:HG23	2:B:858:ARG:HH12	1.74	0.52
3:F:1618:GLU:C	3:F:1621:GLN:HG3	2.30	0.52
1:D:372:GLU:HA	1:D:373:ASP:HB3	1.88	0.52
2:E:836:GLN:NE2	2:E:897:HIS:CE1	2.71	0.52
3:F:1481:ASN:O	3:F:1492:ALA:HB3	2.10	0.52
3:F:1521:TYR:OH	3:F:1584:GLY:HA3	2.10	0.52
1:D:282:ARG:HG2	1:D:282:ARG:HH11	1.75	0.52
1:A:517:GLY:O	1:A:518:ALA:C	2.46	0.52
1:A:372:GLU:HA	1:A:373:ASP:HB3	1.88	0.52
4:H:61:ASP:CB	4:H:64:SER:OG	2.58	0.52
2:E:734:ILE:HG12	4:H:51:TYR:HD1	1.70	0.52
1:D:20:MET:HE1	1:D:35:VAL:CG1	2.39	0.52
2:E:860:HIS:HE1	3:F:1451:GLN:NE2	2.07	0.52
1:A:220:PHE:CD2	1:A:357:PRO:HG2	2.45	0.52
3:C:1389:PHE:CE1	3:C:1443:GLN:CB	2.85	0.51
3:F:1558:GLN:O	3:F:1559:GLN:HB3	2.10	0.51
1:D:551:ARG:HE	1:D:551:ARG:H	1.56	0.51
1:D:220:PHE:CD2	1:D:357:PRO:HG2	2.45	0.51
1:D:590:THR:HG22	1:D:592:SER:N	2.25	0.51
3:C:1521:TYR:OH	3:C:1584:GLY:HA3	2.10	0.51
3:C:1386:MET:HB3	3:C:1450:ILE:CG2	2.41	0.51
3:C:1614:GLU:C	3:C:1616:GLN:H	2.14	0.51
3:C:1544:GLU:O	3:C:1556:VAL:HG11	2.10	0.51
3:C:1490:ARG:HG3	3:C:1491:CYS:N	2.25	0.51
1:D:591:GLN:O	1:D:594:ILE:HB	2.10	0.51
2:E:894:VAL:HG22	2:E:897:HIS:HB2	1.92	0.51
1:A:289:VAL:HG21	1:A:297:LEU:HD21	1.91	0.51
3:F:1563:ILE:HG13	3:F:1599:ILE:HD13	1.92	0.51
3:F:1437:LEU:HG	3:F:1437:LEU:O	2.09	0.51
1:A:6:ILE:CG1	1:A:20:MET:HE3	2.40	0.51
1:A:472:ILE:CD1	1:A:509:LEU:HD22	2.41	0.51
1:D:164:LEU:O	1:D:164:LEU:HD12	2.10	0.51
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.75	0.51
3:C:1558:GLN:O	3:C:1559:GLN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1363:ILE:HG12	3:C:1440:LYS:HG3	1.93	0.51
3:C:1460:TYR:CZ	3:C:1461:TYR:HB3	2.46	0.51
3:F:1380:ILE:HB	3:F:1458:TYR:CE1	2.46	0.51
1:A:590:THR:HG22	1:A:592:SER:N	2.26	0.51
3:F:1552:ASP:C	3:F:1552:ASP:OD1	2.49	0.51
3:C:1563:ILE:HG13	3:C:1599:ILE:HD13	1.92	0.51
1:A:177:VAL:HG22	1:A:178:ASN:N	2.26	0.51
3:F:1443:GLN:O	3:F:1443:GLN:HG2	2.11	0.51
1:D:177:VAL:HG22	1:D:178:ASN:N	2.26	0.51
3:C:1339:PHE:CE1	3:C:1370:TYR:CE1	2.99	0.51
3:F:1343:VAL:HG11	3:F:1471:TYR:HD2	1.76	0.51
1:D:345:GLY:N	1:D:391:THR:HB	2.26	0.51
1:A:474:ASN:HB3	1:A:477:ARG:NH1	2.26	0.51
1:D:474:ASN:OD1	1:D:475:LYS:HG3	2.10	0.51
1:A:346:MET:O	1:A:347:PRO:C	2.49	0.51
3:C:1593:LYS:N	3:C:1596:LEU:HD21	2.26	0.51
1:D:69:PRO:CA	1:D:70:ALA:CB	2.88	0.51
1:A:69:PRO:CA	1:A:70:ALA:CB	2.88	0.51
3:F:1472:HIS:ND1	3:F:1473:PRO:CD	2.73	0.51
1:A:364:ARG:H	1:A:379:THR:HG22	1.75	0.51
1:D:158:LEU:CD2	1:D:167:LEU:HD22	2.41	0.51
3:F:1601:GLY:H	3:F:1604:THR:HB	1.76	0.51
3:C:1537:ASP:CG	3:C:1569:ARG:HD2	2.32	0.50
1:D:472:ILE:CD1	1:D:509:LEU:HD22	2.41	0.50
3:C:1463:LEU:HG	3:C:1463:LEU:O	2.11	0.50
3:C:1380:ILE:HG13	3:C:1425:TYR:HD1	1.75	0.50
3:F:1462:ASN:ND2	3:F:1465:GLU:HG2	2.26	0.50
3:F:1582:MET:HB3	3:F:1605:TRP:O	2.11	0.50
1:D:126:ARG:HG3	2:E:751:TRP:CZ2	2.46	0.50
3:C:1406:TYR:OH	3:C:1408:SER:HA	2.11	0.50
2:B:730:ASP:HB2	2:B:841:ARG:HH21	1.77	0.50
3:C:1476:GLU:O	3:C:1477:ASP:C	2.48	0.50
1:D:223:ILE:HD12	1:D:223:ILE:N	2.26	0.50
1:D:37:VAL:O	1:D:46:VAL:HG23	2.11	0.50
3:F:1537:ASP:CG	3:F:1569:ARG:HD2	2.31	0.50
1:A:591:GLN:O	1:A:594:ILE:HB	2.10	0.50
3:F:1483:LEU:O	3:F:1484:CYS:SG	2.69	0.50
3:F:1498:ILE:O	3:F:1499:GLN:C	2.49	0.50
1:A:474:ASN:OD1	1:A:475:LYS:HG3	2.11	0.50
1:A:158:LEU:CD2	1:A:167:LEU:HD22	2.41	0.50
1:A:564:GLU:HG2	2:B:766:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1493:GLU:OE1	3:C:1493:GLU:O	2.30	0.50
3:F:1459:ALA:O	3:F:1460:TYR:C	2.50	0.50
1:A:223:ILE:N	1:A:223:ILE:HD12	2.26	0.50
3:F:1524:LYS:HB3	3:F:1545:GLN:HG2	1.94	0.50
3:C:1582:MET:HB3	3:C:1605:TRP:O	2.11	0.50
2:B:758:GLU:OE2	2:B:767:LYS:HE2	2.12	0.50
1:A:445:PRO:HG2	1:A:504:ILE:HD11	1.94	0.50
3:C:1499:GLN:OE1	3:C:1499:GLN:O	2.30	0.50
1:D:80:ARG:O	1:D:81:ASN:HB2	2.10	0.50
3:F:1401:ASN:O	3:F:1402:GLY:O	2.29	0.50
3:F:1404:ASP:CB	3:F:1427:ASP:HB2	2.41	0.50
3:F:1414:LYS:O	3:F:1415:ALA:CB	2.59	0.50
3:C:1413:ASP:OD1	3:C:1413:ASP:O	2.30	0.49
3:F:1572:LEU:HD22	3:F:1574:LEU:CD2	2.42	0.49
3:F:1616:GLN:CA	3:F:1616:GLN:OE1	2.61	0.49
3:C:1397:LYS:N	3:C:1397:LYS:CD	2.75	0.49
1:D:474:ASN:HB3	1:D:477:ARG:NH1	2.26	0.49
1:D:445:PRO:HG2	1:D:504:ILE:HD11	1.94	0.49
3:C:1380:ILE:CG2	3:C:1381:LEU:N	2.74	0.49
2:B:733:ILE:HG12	2:B:734:ILE:H	1.77	0.49
1:D:364:ARG:H	1:D:379:THR:HG22	1.75	0.49
1:A:543:VAL:HG12	2:B:799:PHE:CD2	2.47	0.49
3:F:1482:LYS:NZ	3:F:1484:CYS:SG	2.85	0.49
3:F:1555:GLN:O	3:F:1556:VAL:C	2.50	0.49
3:C:1640:PRO:O	3:C:1641:ASN:O	2.30	0.49
1:A:37:VAL:O	1:A:46:VAL:HG23	2.11	0.49
3:C:1370:TYR:O	3:C:1431:HIS:HB2	2.13	0.49
3:C:1505:VAL:O	3:C:1505:VAL:HG23	2.13	0.49
3:F:1407:ILE:CG1	3:F:1424:ILE:HG12	2.42	0.49
1:D:548:SER:O	1:D:549:GLU:O	2.30	0.49
3:F:1344:THR:HG23	3:F:1346:LYS:HE2	1.92	0.49
3:C:1601:GLY:H	3:C:1604:THR:HB	1.76	0.49
3:C:1365:GLU:C	3:C:1366:ILE:HG13	2.33	0.49
1:D:3:MET:CE	1:D:522:ARG:HG2	2.31	0.49
1:A:379:THR:HA	1:A:385:ALA:HB2	1.94	0.49
3:C:1632:GLU:O	3:C:1636:VAL:HG23	2.13	0.49
1:D:110:ILE:HG12	1:D:127:ILE:HG12	1.94	0.49
1:A:110:ILE:HG12	1:A:127:ILE:HG12	1.93	0.49
3:C:1393:THR:O	3:C:1396:LEU:HB2	2.13	0.49
3:C:1554:VAL:HB	3:C:1560:ARG:NH1	2.28	0.49
3:F:1543:ILE:CD1	3:F:1554:VAL:HG21	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1381:LEU:HB2	3:F:1424:ILE:O	2.13	0.49
3:C:1390:ALA:HB1	3:C:1416:PHE:HA	1.94	0.49
3:F:1386:MET:SD	3:F:1473:PRO:HD3	2.53	0.49
3:C:1524:LYS:HB3	3:C:1545:GLN:HG2	1.94	0.49
3:C:1544:GLU:C	3:C:1556:VAL:HG13	2.33	0.49
3:C:1521:TYR:O	3:C:1583:TRP:HB2	2.13	0.49
3:C:1507:LEU:C	3:C:1507:LEU:HD13	2.33	0.49
3:F:1507:LEU:C	3:F:1507:LEU:HD13	2.33	0.49
1:D:379:THR:HA	1:D:385:ALA:HB2	1.94	0.49
1:A:142:MET:CG	1:A:187:TYR:CE1	2.96	0.49
1:D:282:ARG:NH1	1:D:286:LEU:HD12	2.27	0.49
1:D:142:MET:CG	1:D:187:TYR:CE1	2.96	0.49
3:C:1381:LEU:HD12	3:C:1381:LEU:C	2.32	0.48
3:C:1572:LEU:HD22	3:C:1574:LEU:CD2	2.42	0.48
2:E:847:ASN:ND2	2:E:849:ALA:HB3	2.28	0.48
3:C:1545:GLN:HA	3:C:1556:VAL:CG1	2.42	0.48
1:D:188:TYR:HB2	1:D:191:SER:OG	2.12	0.48
1:A:188:TYR:HB2	1:A:191:SER:OG	2.12	0.48
1:A:291:ASN:OD1	3:F:1594:PRO:HD3	2.13	0.48
3:C:1462:ASN:C	3:C:1462:ASN:HD22	2.17	0.48
3:F:1521:TYR:O	3:F:1583:TRP:HB2	2.13	0.48
1:D:346:MET:H	1:D:391:THR:HB	1.78	0.48
3:F:1365:GLU:CG	3:F:1438:ALA:HB2	2.43	0.48
1:D:396:LYS:HG2	1:D:397:PRO:O	2.14	0.48
2:E:730:ASP:HB2	2:E:841:ARG:NH2	2.27	0.48
3:F:1632:GLU:O	3:F:1636:VAL:HG23	2.12	0.48
1:D:559:MET:HG3	1:D:560:THR:N	2.28	0.48
3:F:1483:LEU:HD12	3:F:1483:LEU:C	2.33	0.48
3:F:1505:VAL:HG23	3:F:1505:VAL:O	2.13	0.48
3:C:1537:ASP:OD2	3:C:1569:ARG:CD	2.61	0.48
1:A:282:ARG:NH1	1:A:286:LEU:HD12	2.27	0.48
3:C:1370:TYR:N	3:C:1430:SER:O	2.35	0.48
3:F:1481:ASN:ND2	3:F:1567:LYS:HE3	2.29	0.48
1:D:236:ARG:CA	1:D:243:VAL:HG23	2.44	0.48
2:B:894:VAL:HG22	2:B:897:HIS:HB2	1.95	0.48
3:F:1537:ASP:OD2	3:F:1569:ARG:CD	2.61	0.48
3:F:1572:LEU:O	3:F:1573:LYS:HG3	2.14	0.48
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.49	0.48
2:E:730:ASP:HB2	2:E:841:ARG:HH21	1.76	0.48
3:C:1467:CYS:SG	3:C:1468:THR:N	2.87	0.48
2:E:819:ARG:CG	2:E:819:ARG:NH1	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:HA	1:D:89:THR:O	2.14	0.48
3:F:1364:LEU:HD21	3:F:1471:TYR:CE2	2.49	0.48
2:E:898:PHE:O	4:H:48:MET:HG3	2.14	0.48
1:A:559:MET:HG3	1:A:560:THR:N	2.28	0.48
3:C:1380:ILE:CG1	3:C:1425:TYR:CD1	2.96	0.48
3:C:1437:LEU:HD12	3:C:1438:ALA:N	2.29	0.48
1:D:109:PHE:CZ	1:D:594:ILE:HG23	2.49	0.48
3:F:1348:ALA:HB1	3:F:1349:PRO:HD2	1.96	0.48
1:A:24:ALA:HB3	1:A:60:HIS:CB	2.38	0.47
3:F:1462:ASN:HD22	3:F:1464:GLU:N	2.10	0.47
1:D:369:VAL:HG12	1:D:370:GLN:H	1.79	0.47
2:E:761:LYS:O	2:E:762:ASN:CG	2.53	0.47
3:F:1371:ARG:CG	3:F:1371:ARG:NH1	2.75	0.47
3:C:1411:GLU:O	3:C:1413:ASP:N	2.47	0.47
3:C:1494:GLU:HG2	3:C:1494:GLU:H	1.47	0.47
1:A:171:TRP:CZ3	1:A:173:ILE:HG12	2.49	0.47
1:D:438:VAL:HG21	1:D:449:LEU:HD21	1.96	0.47
2:E:731:GLU:O	2:E:732:ASP:CB	2.62	0.47
1:A:177:VAL:HG22	1:A:182:TRP:HZ2	1.78	0.47
3:C:1341:LEU:HD22	3:C:1457:VAL:HG22	1.97	0.47
3:C:1572:LEU:O	3:C:1573:LYS:HG3	2.14	0.47
1:A:365:VAL:H	1:A:379:THR:HG22	1.79	0.47
1:D:333:ILE:HD11	1:D:404:THR:HG22	1.97	0.47
2:B:772:PHE:CZ	4:G:82:ILE:HD13	2.50	0.47
1:D:177:VAL:HG22	1:D:182:TRP:HZ2	1.78	0.47
2:B:862:GLN:N	2:B:862:GLN:OE1	2.47	0.47
1:D:335:PHE:CE1	1:D:419:MET:HG2	2.50	0.47
1:D:171:TRP:CZ3	1:D:173:ILE:HG12	2.49	0.47
3:C:1616:GLN:O	3:C:1617:ASP:C	2.53	0.47
3:F:1513:LYS:O	3:F:1515:CYS:N	2.48	0.47
2:B:731:GLU:O	2:B:732:ASP:HB2	2.13	0.47
1:A:369:VAL:HG12	1:A:370:GLN:H	1.79	0.47
1:D:36:THR:HG22	1:D:38:HIS:CE1	2.50	0.47
2:B:730:ASP:HB2	2:B:841:ARG:NH2	2.29	0.47
1:A:398:LEU:O	1:A:420:GLN:HA	2.15	0.47
3:F:1341:LEU:HD22	3:F:1457:VAL:CG2	2.42	0.47
1:A:33:VAL:HA	1:A:89:THR:O	2.14	0.47
1:D:292:PRO:HB2	1:D:296:ASP:OD2	2.13	0.47
3:F:1581:LEU:HD12	3:F:1582:MET:H	1.80	0.47
3:C:1572:LEU:C	3:C:1573:LYS:HG3	2.35	0.47
3:C:1397:LYS:HA	3:C:1400:ALA:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD12	1:A:159:SER:H	1.80	0.47
3:C:1378:MET:CA	3:C:1427:ASP:O	2.52	0.47
1:A:3:MET:HE3	1:A:522:ARG:CG	2.32	0.47
1:A:335:PHE:CE1	1:A:419:MET:HG2	2.50	0.47
3:F:1572:LEU:C	3:F:1573:LYS:HG3	2.35	0.47
3:F:1498:ILE:CG2	3:F:1499:GLN:N	2.78	0.47
1:D:204:GLU:CG	2:E:815:TYR:CE2	2.98	0.47
1:D:158:LEU:HD12	1:D:159:SER:H	1.80	0.47
3:F:1512:ASP:O	3:F:1515:CYS:N	2.47	0.47
1:D:398:LEU:O	1:D:420:GLN:HA	2.15	0.47
2:E:862:GLN:OE1	2:E:862:GLN:N	2.47	0.47
3:C:1472:HIS:CG	3:C:1475:LYS:HD2	2.48	0.47
3:F:1462:ASN:CG	3:F:1465:GLU:HG2	2.34	0.47
1:A:338:THR:HG21	1:A:419:MET:CE	2.45	0.47
3:F:1618:GLU:HA	3:F:1621:GLN:CD	2.33	0.47
1:A:548:SER:O	1:A:549:GLU:CB	2.62	0.47
3:F:1380:ILE:HD13	3:F:1458:TYR:HE1	1.79	0.47
1:D:151:ILE:HD12	1:D:151:ILE:N	2.30	0.47
1:A:363:TYR:O	1:A:364:ARG:HB2	2.14	0.47
3:F:1345:ILE:HA	3:F:1363:ILE:O	2.15	0.47
1:D:344:PRO:HA	1:D:391:THR:CG2	2.45	0.47
1:D:61:MET:HE1	1:D:482:GLY:C	2.34	0.47
3:F:1360:ASN:C	3:F:1361:THR:HG23	2.35	0.47
3:C:1527:LEU:HD11	3:C:1539:TYR:HB3	1.96	0.47
1:D:427:VAL:HG21	1:D:523:GLU:HG3	1.97	0.47
3:C:1497:PHE:HE2	3:C:1571:ALA:CB	2.25	0.47
1:A:438:VAL:HG21	1:A:449:LEU:HD21	1.95	0.47
1:A:404:THR:HG21	1:A:415:ALA:H	1.81	0.47
3:F:1527:LEU:HD11	3:F:1539:TYR:HB3	1.96	0.47
3:C:1380:ILE:CG1	3:C:1425:TYR:HD1	2.28	0.46
1:D:338:THR:HG21	1:D:419:MET:CE	2.45	0.46
3:C:1481:ASN:ND2	3:C:1567:LYS:HE2	2.31	0.46
3:F:1481:ASN:C	3:F:1492:ALA:HB3	2.35	0.46
1:D:363:TYR:O	1:D:364:ARG:HB2	2.14	0.46
1:D:7:ILE:HG21	1:D:471:LEU:CD2	2.45	0.46
1:A:541:LEU:HD23	2:B:796:ALA:HB2	1.97	0.46
2:B:809:ILE:HD13	2:B:890:VAL:HG23	1.96	0.46
2:E:851:CYS:HB2	2:E:881:LEU:HD21	1.97	0.46
1:A:151:ILE:N	1:A:151:ILE:HD12	2.30	0.46
1:D:365:VAL:H	1:D:379:THR:HG22	1.79	0.46
1:A:558:GLN:CB	2:B:772:PHE:CE1	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:GLU:CG	1:D:550:ASP:H	2.28	0.46
1:A:7:ILE:HG21	1:A:471:LEU:CD2	2.45	0.46
1:D:404:THR:HG21	1:D:415:ALA:H	1.80	0.46
3:C:1541:MET:O	3:C:1559:GLN:HA	2.16	0.46
1:A:292:PRO:HG2	1:A:296:ASP:OD2	2.15	0.46
3:F:1404:ASP:O	3:F:1405:ARG:HG2	2.16	0.46
1:D:54:LEU:HB3	1:D:60:HIS:HA	1.98	0.46
2:B:758:GLU:OE2	2:B:767:LYS:CE	2.63	0.46
1:A:236:ARG:CA	1:A:243:VAL:HG23	2.44	0.46
1:A:543:VAL:O	2:B:799:PHE:CG	2.68	0.46
3:C:1385:MET:HA	3:C:1385:MET:HE3	1.97	0.46
1:A:134:LEU:HD13	2:B:793:ILE:HG22	1.96	0.46
3:C:1411:GLU:C	3:C:1413:ASP:N	2.69	0.46
3:C:1396:LEU:CB	3:C:1412:LEU:HD12	2.36	0.46
3:C:1397:LYS:H	3:C:1397:LYS:CD	2.28	0.46
1:A:214:VAL:HB	1:A:233:ILE:HD13	1.98	0.46
1:A:250:ILE:HG13	1:A:266:LEU:HB2	1.97	0.46
1:A:469:THR:O	1:A:511:ALA:HA	2.16	0.46
3:F:1641:ASN:N	3:F:1641:ASN:HD22	2.13	0.46
3:F:1541:MET:O	3:F:1559:GLN:HA	2.16	0.46
1:A:135:LEU:HD22	2:B:789:ASP:O	2.16	0.46
2:B:739:ILE:CG2	2:B:891:LYS:HD3	2.46	0.46
1:D:255:ASP:HA	1:D:256:GLY:HA2	1.63	0.46
3:F:1447:VAL:HG22	3:F:1448:GLU:N	2.31	0.46
3:C:1416:PHE:CZ	3:C:1442:HIS:HB2	2.51	0.46
2:B:739:ILE:HD11	2:B:900:SER:HB2	1.97	0.46
3:C:1485:ARG:CD	3:C:1536:PHE:CE2	2.99	0.46
1:D:214:VAL:HB	1:D:233:ILE:HD13	1.98	0.46
1:D:469:THR:O	1:D:511:ALA:HA	2.16	0.46
3:F:1386:MET:O	3:F:1387:THR:C	2.55	0.46
2:B:762:ASN:C	2:B:764:ILE:H	2.20	0.46
3:F:1413:ASP:O	3:F:1413:ASP:OD2	2.34	0.46
1:D:572:VAL:HG12	2:E:753:VAL:HG22	1.96	0.46
3:C:1590:TRP:O	3:C:1596:LEU:HA	2.16	0.45
3:F:1461:TYR:CD1	3:F:1462:ASN:HB2	2.51	0.45
3:C:1494:GLU:HB2	3:C:1495:ASN:H	1.53	0.45
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.30	0.45
1:A:541:LEU:HB3	2:B:796:ALA:HB2	1.98	0.45
1:D:250:ILE:HG13	1:D:266:LEU:HB2	1.97	0.45
1:A:177:VAL:CG2	1:A:182:TRP:HZ2	2.30	0.45
1:A:292:PRO:CD	1:A:296:ASP:OD2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1343:VAL:CG2	3:C:1366:ILE:HG23	2.31	0.45
3:F:1452:PRO:HG3	3:F:1472:HIS:HD2	1.81	0.45
1:A:333:ILE:HD11	1:A:404:THR:HG22	1.97	0.45
1:A:427:VAL:HG21	1:A:523:GLU:HG3	1.97	0.45
1:A:61:MET:HE1	1:A:482:GLY:C	2.36	0.45
1:D:24:ALA:HB3	1:D:60:HIS:CB	2.38	0.45
1:D:549:GLU:CG	1:D:550:ASP:N	2.79	0.45
1:A:338:THR:HG21	1:A:419:MET:HE1	1.98	0.45
2:B:761:LYS:O	2:B:762:ASN:CB	2.64	0.45
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.60	0.45
1:D:216:PRO:HB2	1:D:218:GLU:O	2.16	0.45
1:A:216:PRO:HB2	1:A:218:GLU:O	2.16	0.45
1:D:443:LEU:HD23	1:D:443:LEU:HA	1.81	0.45
1:D:289:VAL:HG23	1:D:290:GLN:N	2.32	0.45
3:C:1495:ASN:ND2	3:C:1496:CYS:H	2.10	0.45
3:F:1386:MET:HG3	3:F:1471:TYR:HE1	1.81	0.45
3:F:1463:LEU:HD23	3:F:1463:LEU:O	2.17	0.45
1:A:54:LEU:HB3	1:A:60:HIS:HA	1.98	0.45
1:A:59:ASN:O	1:A:60:HIS:HB2	2.17	0.45
3:F:1460:TYR:CZ	3:F:1461:TYR:HB3	2.51	0.45
1:D:409:LEU:HB3	1:D:410:SER:H	1.63	0.45
2:B:868:PRO:O	2:B:869:LYS:C	2.55	0.45
1:A:36:THR:HG22	1:A:38:HIS:CE1	2.50	0.45
1:D:477:ARG:CG	1:D:477:ARG:HH11	2.30	0.45
3:F:1528:VAL:HG23	3:F:1541:MET:HA	1.98	0.45
3:F:1482:LYS:HG2	3:F:1484:CYS:SG	2.56	0.45
3:F:1381:LEU:HD23	3:F:1457:VAL:HG12	1.92	0.45
3:F:1403:VAL:HG13	3:F:1403:VAL:O	2.17	0.45
1:D:56:PRO:HD3	1:D:60:HIS:HE1	1.82	0.45
1:D:503:PHE:HD1	1:D:507:PHE:CD1	2.35	0.45
1:D:136:PRO:HD2	2:E:789:ASP:HA	1.99	0.45
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.51	0.45
1:A:362:ALA:O	1:A:379:THR:HG21	2.17	0.45
3:C:1462:ASN:HD22	3:C:1464:GLU:H	1.65	0.45
3:C:1528:VAL:HG23	3:C:1541:MET:HA	1.98	0.45
3:F:1374:GLN:O	3:F:1375:ASP:O	2.35	0.45
4:G:63:VAL:O	4:G:67:ASP:HB2	2.16	0.45
1:A:567:HIS:ND1	2:B:760:PRO:HB3	2.32	0.45
1:D:179:MET:HG3	1:D:203:LYS:HA	1.99	0.45
3:F:1628:GLY:O	3:F:1632:GLU:HG3	2.17	0.45
1:D:177:VAL:CG2	1:D:182:TRP:HZ2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:HD3	1:A:60:HIS:HE1	1.82	0.45
3:F:1387:THR:CG2	3:F:1451:GLN:HB3	2.46	0.45
2:E:744:GLU:O	2:E:746:PRO:HD2	2.17	0.45
3:C:1453:GLY:HA3	3:C:1471:TYR:CE2	2.51	0.45
1:D:345:GLY:HA2	1:D:391:THR:O	2.16	0.45
1:A:471:LEU:HD22	1:A:622:LEU:HD13	1.99	0.45
1:A:404:THR:HG23	1:A:415:ALA:H	1.82	0.45
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.99	0.45
3:F:1593:LYS:CA	3:F:1596:LEU:CD2	2.92	0.45
1:D:59:ASN:O	1:D:60:HIS:HB2	2.17	0.45
1:A:625:THR:HA	1:A:631:GLN:HB3	1.99	0.45
3:F:1497:PHE:CD1	3:F:1606:VAL:HB	2.52	0.45
3:F:1614:GLU:O	3:F:1620:ASN:CB	2.64	0.45
1:A:484:GLN:OE1	1:A:495:LEU:HB2	2.17	0.45
3:C:1340:ASP:N	3:C:1369:ARG:O	2.50	0.44
1:D:293:ARG:O	1:D:296:ASP:N	2.45	0.44
2:B:847:ASN:ND2	2:B:849:ALA:HB3	2.31	0.44
2:E:855:THR:HG23	2:E:858:ARG:HH12	1.82	0.44
3:F:1615:CYS:O	3:F:1617:ASP:N	2.50	0.44
3:F:1382:ASP:HB3	3:F:1456:LYS:HB3	1.99	0.44
1:D:362:ALA:O	1:D:379:THR:HG21	2.17	0.44
3:F:1408:SER:O	3:F:1411:GLU:N	2.48	0.44
3:C:1408:SER:OG	3:C:1410:TYR:HB3	2.16	0.44
3:C:1628:GLY:O	3:C:1632:GLU:HG3	2.17	0.44
1:D:484:GLN:OE1	1:D:495:LEU:HB2	2.17	0.44
3:C:1404:ASP:HB3	3:C:1427:ASP:CB	2.39	0.44
1:A:454:LEU:HD21	1:A:492:LEU:HD12	1.94	0.44
1:A:6:ILE:HD11	1:A:20:MET:HG3	1.99	0.44
2:E:895:TYR:C	2:E:897:HIS:H	2.19	0.44
3:C:1617:ASP:O	3:C:1621:GLN:HG3	2.18	0.44
1:A:583:LEU:HA	1:A:583:LEU:HD12	1.78	0.44
1:D:6:ILE:HD11	1:D:20:MET:HG3	1.99	0.44
2:B:894:VAL:HG11	2:B:899:ILE:HB	1.99	0.44
2:B:758:GLU:O	2:B:765:SER:OG	2.35	0.44
1:D:183:LYS:HZ2	1:D:185:ARG:CG	2.31	0.44
1:D:471:LEU:HD22	1:D:622:LEU:HD13	1.99	0.44
1:A:286:LEU:HA	1:A:286:LEU:HD23	1.60	0.44
1:A:503:PHE:HD1	1:A:507:PHE:CD1	2.35	0.44
3:F:1483:LEU:O	3:F:1489:CYS:SG	2.76	0.44
1:D:329:SER:HA	1:D:330:PRO:HD3	1.74	0.44
3:C:1621:GLN:O	3:C:1625:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:LEU:C	2:B:752:ASN:HD22	2.20	0.44
3:C:1495:ASN:ND2	3:C:1496:CYS:N	2.59	0.44
1:A:547:GLN:OE1	1:A:559:MET:CA	2.65	0.44
1:D:510:VAL:HB	1:D:528:SER:HB3	2.00	0.44
1:D:193:GLN:H	1:D:193:GLN:NE2	2.15	0.44
3:F:1617:ASP:O	3:F:1621:GLN:HG2	2.18	0.44
2:B:895:TYR:C	2:B:897:HIS:H	2.19	0.44
2:B:764:ILE:HG22	2:B:764:ILE:O	2.18	0.44
2:B:772:PHE:HZ	4:G:82:ILE:HD13	1.83	0.44
2:B:867:PRO:HB2	2:B:870:SER:OG	2.17	0.44
1:A:179:MET:HG3	1:A:203:LYS:HA	1.99	0.44
1:D:375:VAL:HG12	1:D:376:GLN:H	1.83	0.44
1:A:289:VAL:O	1:A:290:GLN:HG2	2.17	0.44
1:A:454:LEU:HD21	1:A:492:LEU:CD1	2.48	0.44
2:B:910:VAL:CG2	2:B:911:PRO:HD2	2.45	0.44
1:D:179:MET:CE	1:D:204:GLU:HG3	2.47	0.44
3:C:1459:ALA:O	3:C:1460:TYR:C	2.56	0.44
1:A:223:ILE:H	1:A:223:ILE:HD12	1.83	0.44
3:C:1451:GLN:HA	3:C:1452:PRO:HD3	1.78	0.43
3:F:1561:THR:O	3:F:1598:TYR:N	2.46	0.43
3:C:1503:ASP:O	3:C:1504:LYS:HB3	2.18	0.43
3:F:1383:ILE:HB	3:F:1422:LEU:CD2	2.48	0.43
3:F:1412:LEU:HD12	3:F:1412:LEU:HA	1.61	0.43
1:D:47:LEU:O	1:D:47:LEU:HD23	2.18	0.43
3:F:1498:ILE:CG2	3:F:1499:GLN:HG2	2.48	0.43
3:C:1615:CYS:C	3:C:1616:GLN:OE1	2.57	0.43
1:D:404:THR:HG23	1:D:415:ALA:H	1.82	0.43
1:A:179:MET:CE	1:A:204:GLU:HG3	2.47	0.43
2:E:830:TYR:CD1	2:E:871:SER:HB3	2.53	0.43
1:D:639:GLN:HB2	1:D:639:GLN:HE21	1.65	0.43
1:A:248:PHE:CD1	3:C:1378:MET:CE	3.01	0.43
3:F:1483:LEU:HD12	3:F:1484:CYS:H	1.76	0.43
3:C:1593:LYS:HA	3:C:1594:PRO:HA	1.87	0.43
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.33	0.43
3:C:1360:ASN:C	3:C:1361:THR:HG23	2.39	0.43
1:A:290:GLN:OE1	3:F:1558:GLN:HG3	2.17	0.43
3:C:1552:ASP:OD1	3:C:1560:ARG:NH1	2.50	0.43
3:F:1591:GLY:HA3	3:F:1596:LEU:HA	2.00	0.43
1:D:3:MET:HE3	1:D:522:ARG:CG	2.33	0.43
3:F:1380:ILE:HG13	3:F:1425:TYR:CD2	2.53	0.43
3:F:1405:ARG:HG2	3:F:1426:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:733:ILE:HG12	2:E:734:ILE:H	1.83	0.43
1:A:6:ILE:HD12	1:A:6:ILE:HA	1.68	0.43
1:A:47:LEU:HD23	1:A:47:LEU:O	2.18	0.43
3:F:1414:LYS:O	3:F:1415:ALA:HB3	2.19	0.43
2:E:739:ILE:CG2	2:E:891:LYS:HD3	2.48	0.43
3:F:1497:PHE:CD1	3:F:1606:VAL:HG21	2.53	0.43
2:B:731:GLU:O	2:B:732:ASP:CB	2.66	0.43
1:A:375:VAL:HG12	1:A:376:GLN:H	1.83	0.43
1:A:193:GLN:NE2	1:A:193:GLN:H	2.15	0.43
3:C:1411:GLU:C	3:C:1413:ASP:H	2.22	0.43
3:C:1426:LEU:H	3:C:1426:LEU:HD13	1.81	0.43
3:F:1483:LEU:HD22	3:F:1599:ILE:HD11	2.00	0.43
1:D:505:PRO:O	1:D:506:SER:HB3	2.17	0.43
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.77	0.43
3:C:1446:ASN:N	3:C:1446:ASN:HD22	2.16	0.43
3:C:1381:LEU:CD2	3:C:1383:ILE:HD11	2.49	0.43
3:C:1366:ILE:HG22	3:C:1367:CYS:H	1.84	0.43
2:B:739:ILE:CD1	2:B:900:SER:HB2	2.48	0.43
2:B:840:VAL:HG22	2:B:894:VAL:HB	2.01	0.43
1:A:409:LEU:HB3	1:A:410:SER:H	1.63	0.43
2:B:750:LEU:HD12	2:B:750:LEU:HA	1.86	0.43
4:G:41:TYR:HD2	4:G:42:TYR:CE2	2.37	0.43
3:C:1372:GLY:O	3:C:1431:HIS:ND1	2.51	0.43
1:A:289:VAL:HG23	1:A:290:GLN:N	2.33	0.43
1:A:63:ASN:C	1:A:64:VAL:HG13	2.37	0.43
1:D:126:ARG:HG3	2:E:751:TRP:HZ2	1.82	0.43
1:A:363:TYR:HA	1:A:379:THR:CG2	2.49	0.43
3:C:1462:ASN:ND2	3:C:1464:GLU:HB2	2.31	0.43
1:D:282:ARG:NH1	1:D:282:ARG:HG2	2.33	0.43
1:A:510:VAL:HB	1:A:528:SER:HB3	2.00	0.43
1:A:505:PRO:O	1:A:506:SER:HB3	2.17	0.43
3:C:1389:PHE:CG	3:C:1443:GLN:CA	3.02	0.43
3:C:1443:GLN:O	3:C:1443:GLN:OE1	2.37	0.43
1:A:329:SER:CB	1:A:413:GLU:O	2.61	0.43
3:F:1397:LYS:HA	3:F:1400:ALA:CB	2.48	0.43
3:C:1506:THR:OG1	3:C:1507:LEU:N	2.52	0.43
2:B:760:PRO:O	2:B:761:LYS:CG	2.67	0.43
1:D:363:TYR:HA	1:D:379:THR:CG2	2.49	0.43
2:B:809:ILE:HD12	2:B:902:GLY:HA2	2.01	0.43
2:B:850:PHE:CD2	2:B:878:ILE:HD12	2.53	0.43
2:E:758:GLU:CD	2:E:767:LYS:HB2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1474:GLU:O	3:F:1475:LYS:C	2.57	0.43
1:A:439:LEU:HD12	1:A:439:LEU:N	2.34	0.43
2:B:834:GLN:NE2	2:B:869:LYS:HD2	2.34	0.43
3:C:1440:LYS:HB2	3:C:1440:LYS:HE2	1.79	0.43
3:F:1408:SER:C	3:F:1410:TYR:N	2.72	0.43
4:H:41:TYR:HD2	4:H:42:TYR:CE2	2.37	0.43
1:A:570:ARG:HA	2:B:755:ASP:HA	2.00	0.43
1:A:343:LYS:HB2	1:A:346:MET:HB3	2.01	0.43
3:C:1396:LEU:HD13	3:C:1412:LEU:HD12	2.00	0.43
3:F:1386:MET:HE1	3:F:1389:PHE:CZ	2.54	0.43
2:E:834:GLN:NE2	2:E:869:LYS:HD2	2.34	0.43
1:A:561:LEU:HD22	2:B:771:ILE:HD13	2.01	0.43
2:B:744:GLU:O	2:B:746:PRO:HD2	2.19	0.42
2:E:841:ARG:HD3	2:E:861:GLN:HB2	2.00	0.42
3:F:1394:ASP:O	3:F:1395:ASP:C	2.57	0.42
1:A:115:THR:HB	1:A:584:ASN:OD1	2.19	0.42
3:C:1576:GLU:O	3:C:1577:LYS:HB2	2.18	0.42
3:C:1381:LEU:HD22	3:C:1383:ILE:HD11	2.01	0.42
1:A:47:LEU:HG	1:A:48:SER:N	2.34	0.42
1:D:291:ASN:HD22	1:D:291:ASN:N	2.16	0.42
1:A:375:VAL:HG12	1:A:376:GLN:N	2.34	0.42
1:D:111:GLN:O	1:D:125:TYR:HA	2.19	0.42
3:C:1403:VAL:HG13	3:C:1403:VAL:O	2.20	0.42
3:F:1381:LEU:HD11	3:F:1437:LEU:HD21	2.00	0.42
4:G:18:ALA:N	4:G:65:MET:HE3	2.34	0.42
2:B:762:ASN:C	2:B:764:ILE:N	2.72	0.42
1:D:183:LYS:HG2	1:D:199:GLU:HG2	2.01	0.42
3:C:1545:GLN:HA	3:C:1556:VAL:HG11	2.00	0.42
1:A:453:PHE:HB2	1:A:493:VAL:HG22	2.00	0.42
1:A:554:VAL:HG22	2:B:805:GLN:HG3	2.01	0.42
3:F:1576:GLU:O	3:F:1577:LYS:HB2	2.18	0.42
4:G:72:LEU:O	4:G:73:GLU:C	2.58	0.42
1:D:459:ARG:HA	1:D:462:GLU:HG2	2.01	0.42
3:F:1380:ILE:HD13	3:F:1458:TYR:CE1	2.54	0.42
1:D:409:LEU:HA	1:D:409:LEU:HD12	1.84	0.42
3:C:1454:ALA:CB	3:C:1470:PHE:CE2	2.95	0.42
3:F:1397:LYS:HA	3:F:1400:ALA:HB3	2.00	0.42
1:D:606:THR:C	1:D:608:GLY:H	2.22	0.42
1:A:606:THR:C	1:A:608:GLY:H	2.22	0.42
2:B:855:THR:HB	3:C:1602:LYS:NZ	2.34	0.42
3:C:1408:SER:O	3:C:1410:TYR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:PHE:HB2	1:D:493:VAL:HG22	2.00	0.42
1:D:115:THR:HB	1:D:584:ASN:OD1	2.19	0.42
1:D:40:PHE:HA	1:D:41:PRO:HA	1.76	0.42
3:C:1500:LYS:HG3	3:C:1500:LYS:H	1.53	0.42
1:A:427:VAL:CG2	1:A:523:GLU:HG3	2.50	0.42
1:D:375:VAL:HG12	1:D:376:GLN:N	2.34	0.42
1:D:583:LEU:HD12	1:D:583:LEU:HA	1.78	0.42
1:D:439:LEU:HD12	1:D:439:LEU:N	2.34	0.42
3:C:1417:SER:OG	3:C:1418:ASP:N	2.52	0.42
3:C:1383:ILE:HB	3:C:1422:LEU:HD23	2.01	0.42
1:A:255:ASP:HA	1:A:256:GLY:HA2	1.63	0.42
3:F:1615:CYS:C	3:F:1617:ASP:N	2.72	0.42
3:F:1483:LEU:HD21	3:F:1590:TRP:CD1	2.55	0.42
3:F:1364:LEU:HD21	3:F:1471:TYR:OH	2.20	0.42
3:C:1581:LEU:HD12	3:C:1582:MET:H	1.80	0.42
3:F:1497:PHE:HD1	3:F:1606:VAL:HB	1.85	0.42
2:E:731:GLU:HG3	2:E:731:GLU:H	1.66	0.42
1:A:557:GLN:HG2	1:A:558:GLN:N	2.35	0.42
3:F:1361:THR:HB	3:F:1441:VAL:O	2.19	0.42
3:C:1611:GLU:HG3	3:C:1612:GLU:H	1.85	0.42
1:A:40:PHE:HA	1:A:41:PRO:HA	1.76	0.42
3:F:1593:LYS:HA	3:F:1596:LEU:HD21	2.00	0.42
3:F:1403:VAL:HG22	3:F:1404:ASP:OD2	2.19	0.42
1:A:138:GLY:O	1:A:139:ARG:HG2	2.20	0.42
1:A:183:LYS:HG2	1:A:199:GLU:HG2	2.01	0.42
1:A:183:LYS:NZ	1:A:185:ARG:CD	2.82	0.42
2:B:841:ARG:HD3	2:B:861:GLN:HB2	2.01	0.42
3:C:1640:PRO:HB2	3:C:1641:ASN:H	1.65	0.42
1:D:50:GLU:HG3	1:D:66:PHE:HB3	2.01	0.42
3:F:1536:PHE:O	3:F:1536:PHE:CD1	2.73	0.42
3:F:1462:ASN:HD21	3:F:1465:GLU:H	1.66	0.42
2:B:836:GLN:O	2:B:836:GLN:HG3	2.19	0.42
3:C:1536:PHE:CD1	3:C:1536:PHE:O	2.73	0.42
1:A:404:THR:HG23	1:A:415:ALA:N	2.35	0.42
3:F:1513:LYS:C	3:F:1515:CYS:N	2.73	0.42
1:D:453:PHE:HB2	1:D:493:VAL:HG23	2.02	0.42
3:F:1486:ASP:HB3	3:F:1487:GLU:H	1.58	0.42
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.77	0.42
1:A:386:LYS:O	1:A:386:LYS:HG2	2.20	0.42
3:C:1389:PHE:CE2	3:C:1443:GLN:CG	2.99	0.42
1:A:255:ASP:OD1	1:A:300:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1558:GLN:O	3:F:1559:GLN:CB	2.68	0.42
1:D:522:ARG:HB3	1:D:630:GLN:HE22	1.85	0.42
3:C:1594:PRO:HD2	3:C:1595:ASN:ND2	2.34	0.42
2:B:760:PRO:O	2:B:761:LYS:HG3	2.19	0.42
3:C:1344:THR:HG22	3:C:1344:THR:O	2.19	0.42
1:D:456:ARG:NH1	1:D:456:ARG:HB2	2.35	0.42
2:E:842:VAL:O	2:E:861:GLN:HA	2.20	0.42
1:D:469:THR:HG21	1:D:512:TYR:HE2	1.85	0.42
1:A:111:GLN:O	1:A:125:TYR:HA	2.19	0.42
4:H:72:LEU:O	4:H:73:GLU:C	2.58	0.42
3:F:1611:GLU:HG3	3:F:1612:GLU:H	1.85	0.42
3:F:1503:ASP:O	3:F:1504:LYS:HB3	2.18	0.42
1:A:64:VAL:CG2	1:A:64:VAL:O	2.68	0.42
1:A:369:VAL:CG1	1:A:400:ILE:HG22	2.50	0.42
1:D:153:VAL:O	1:D:154:LYS:HB2	2.20	0.42
3:C:1462:ASN:ND2	3:C:1464:GLU:OE1	2.53	0.42
1:D:404:THR:HG23	1:D:415:ALA:N	2.35	0.42
1:A:163:GLN:O	1:A:164:LEU:HB3	2.20	0.42
1:D:223:ILE:HD12	1:D:223:ILE:H	1.83	0.42
3:F:1594:PRO:HD2	3:F:1595:ASN:ND2	2.34	0.41
3:F:1381:LEU:CD1	3:F:1437:LEU:HD21	2.49	0.41
1:D:138:GLY:O	1:D:139:ARG:HG2	2.20	0.41
1:D:338:THR:HG23	1:D:339:PRO:HD2	2.02	0.41
2:E:894:VAL:HG11	2:E:899:ILE:HB	2.00	0.41
3:C:1485:ARG:HD3	3:C:1536:PHE:CE2	2.55	0.41
2:E:910:VAL:CG2	2:E:911:PRO:HD2	2.47	0.41
3:C:1639:CYS:O	3:C:1640:PRO:C	2.58	0.41
1:A:50:GLU:HG3	1:A:66:PHE:HB3	2.01	0.41
1:D:557:GLN:HG2	1:D:558:GLN:N	2.35	0.41
3:C:1339:PHE:HA	3:C:1369:ARG:O	2.19	0.41
3:C:1367:CYS:C	3:C:1434:ASP:OD2	2.58	0.41
1:A:56:PRO:HG3	1:A:60:HIS:CE1	2.56	0.41
1:D:369:VAL:CG1	1:D:400:ILE:HG22	2.50	0.41
1:D:356:ASN:HB3	1:D:357:PRO:CD	2.50	0.41
1:D:365:VAL:H	1:D:379:THR:CG2	2.33	0.41
1:D:495:LEU:HD12	1:D:496:PRO:HD2	2.02	0.41
1:A:368:ALA:HB2	1:A:376:GLN:HG2	2.02	0.41
2:E:750:LEU:C	2:E:752:ASN:HD22	2.24	0.41
1:A:459:ARG:HA	1:A:462:GLU:HG2	2.01	0.41
2:B:733:ILE:HB	2:B:895:TYR:CD2	2.55	0.41
1:D:163:GLN:O	1:D:164:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:GLN:CD	1:D:193:GLN:H	2.23	0.41
3:F:1579:HIS:CD2	3:F:1611:GLU:OE2	2.74	0.41
3:F:1369:ARG:CG	3:F:1370:TYR:N	2.82	0.41
3:C:1387:THR:N	3:C:1450:ILE:HG23	2.35	0.41
1:A:248:PHE:HD1	3:C:1378:MET:CE	2.33	0.41
1:D:56:PRO:HG3	1:D:60:HIS:CE1	2.55	0.41
3:F:1497:PHE:CD1	3:F:1606:VAL:CG2	3.03	0.41
3:F:1408:SER:O	3:F:1409:LYS:C	2.58	0.41
4:G:77:LYS:O	4:G:80:ASP:HB2	2.21	0.41
4:H:77:LYS:HE2	4:H:81:GLU:OE2	2.20	0.41
1:D:594:ILE:O	1:D:597:VAL:HB	2.21	0.41
1:D:427:VAL:CG2	1:D:523:GLU:HG3	2.50	0.41
2:B:777:ILE:HD12	2:B:808:PHE:CD1	2.55	0.41
2:B:761:LYS:O	2:B:762:ASN:CG	2.58	0.41
1:A:356:ASN:HB3	1:A:357:PRO:CD	2.50	0.41
1:A:365:VAL:H	1:A:379:THR:CG2	2.33	0.41
1:D:368:ALA:HB2	1:D:376:GLN:HG2	2.02	0.41
1:D:12:LEU:HG	1:D:99:VAL:HG11	2.02	0.41
1:D:189:GLU:O	1:D:192:PRO:HD3	2.21	0.41
1:D:47:LEU:HG	1:D:48:SER:N	2.33	0.41
3:C:1485:ARG:HD2	3:C:1536:PHE:CZ	2.56	0.41
3:C:1558:GLN:O	3:C:1559:GLN:CB	2.68	0.41
3:C:1518:GLY:HA3	3:C:1585:LEU:HD22	2.02	0.41
3:C:1376:ALA:H	3:C:1429:VAL:CG2	2.34	0.41
3:C:1396:LEU:O	3:C:1399:LEU:HB2	2.21	0.41
1:A:522:ARG:HB3	1:A:630:GLN:HE22	1.85	0.41
1:D:64:VAL:O	1:D:64:VAL:CG2	2.68	0.41
1:D:45:LEU:HD11	1:D:48:SER:HB3	2.01	0.41
1:A:453:PHE:HB2	1:A:493:VAL:HG23	2.02	0.41
1:A:12:LEU:HG	1:A:99:VAL:HG11	2.02	0.41
1:D:444:ARG:HG3	1:D:444:ARG:HH11	1.86	0.41
1:A:45:LEU:HD11	1:A:48:SER:HB3	2.01	0.41
2:E:840:VAL:HG22	2:E:894:VAL:HB	2.03	0.41
1:A:594:ILE:O	1:A:597:VAL:HB	2.21	0.41
2:E:750:LEU:HD11	2:E:769:MET:CE	2.51	0.41
3:C:1341:LEU:CD1	3:C:1368:THR:HB	2.44	0.41
3:F:1591:GLY:CA	3:F:1596:LEU:HB3	2.51	0.41
3:C:1472:HIS:HE1	3:C:1474:GLU:HG2	1.86	0.41
3:F:1460:TYR:O	3:F:1462:ASN:N	2.52	0.41
3:F:1397:LYS:N	3:F:1397:LYS:CD	2.80	0.41
3:C:1363:ILE:O	3:C:1363:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1506:THR:OG1	3:F:1507:LEU:N	2.52	0.41
1:A:153:VAL:O	1:A:154:LYS:HB2	2.20	0.41
3:F:1335:THR:O	3:F:1336:CYS:CB	2.65	0.41
1:D:517:GLY:O	1:D:518:ALA:O	2.38	0.41
1:D:177:VAL:HG22	1:D:178:ASN:H	1.85	0.41
1:A:342:PHE:CE2	1:A:398:LEU:HB2	2.56	0.41
1:A:469:THR:HG21	1:A:512:TYR:HE2	1.85	0.41
1:A:495:LEU:HD12	1:A:496:PRO:HD2	2.02	0.41
3:C:1579:HIS:CD2	3:C:1611:GLU:OE2	2.74	0.41
1:A:189:GLU:O	1:A:192:PRO:HD3	2.21	0.41
3:F:1518:GLY:HA3	3:F:1585:LEU:HD22	2.03	0.41
1:A:444:ARG:HG3	1:A:444:ARG:HH11	1.86	0.41
1:A:585:LYS:HB3	1:A:585:LYS:HE3	1.91	0.41
1:D:253:ILE:HD12	1:D:302:LEU:HD23	1.95	0.41
1:D:107:TYR:CE2	1:D:132:HIS:HA	2.56	0.41
3:F:1368:THR:HG22	3:F:1435:ASP:O	2.21	0.41
3:F:1497:PHE:CG	3:F:1498:ILE:N	2.87	0.41
1:D:204:GLU:OE1	2:E:815:TYR:CE2	2.72	0.41
4:H:77:LYS:O	4:H:80:ASP:HB2	2.21	0.41
1:D:255:ASP:OD1	1:D:300:LYS:HE3	2.20	0.41
1:D:312:SER:HB2	2:E:873:SER:OG	2.21	0.41
1:A:160:SER:C	1:A:163:GLN:HB2	2.42	0.41
4:G:41:TYR:HD2	4:G:42:TYR:CD2	2.38	0.41
1:A:513:TYR:CZ	1:A:525:VAL:HG11	2.56	0.41
3:C:1483:LEU:HD12	3:C:1483:LEU:HA	1.89	0.41
3:C:1380:ILE:HG23	3:C:1423:ILE:CG2	2.29	0.40
3:C:1472:HIS:HE1	3:C:1474:GLU:CG	2.33	0.40
1:D:63:ASN:C	1:D:64:VAL:HG13	2.37	0.40
4:G:77:LYS:HE2	4:G:81:GLU:OE2	2.20	0.40
4:H:41:TYR:HD2	4:H:42:TYR:CD2	2.38	0.40
3:C:1360:ASN:HD22	3:C:1362:MET:CE	2.34	0.40
3:F:1591:GLY:O	3:F:1596:LEU:HB3	2.22	0.40
1:A:35:VAL:HG22	1:A:88:ALA:CB	2.51	0.40
1:D:407:GLN:C	1:D:409:LEU:H	2.24	0.40
1:D:35:VAL:HG22	1:D:88:ALA:CB	2.51	0.40
1:D:6:ILE:HD12	1:D:6:ILE:HA	1.68	0.40
1:A:107:TYR:CE2	1:A:132:HIS:HA	2.56	0.40
1:D:151:ILE:HG22	1:D:153:VAL:HG12	2.03	0.40
2:B:855:THR:HB	3:C:1602:LYS:HZ2	1.87	0.40
1:A:346:MET:HE1	1:A:456:ARG:CB	2.40	0.40
3:F:1504:LYS:HD3	3:F:1504:LYS:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:895:TYR:O	2:B:897:HIS:N	2.44	0.40
1:D:48:SER:C	1:D:49:SER:O	2.60	0.40
4:H:18:ALA:N	4:H:65:MET:HE1	2.34	0.40
1:D:338:THR:HG21	1:D:419:MET:HE1	2.02	0.40
3:F:1566:ILE:C	3:F:1568:CYS:N	2.75	0.40
3:C:1512:ASP:O	3:C:1515:CYS:N	2.52	0.40
1:A:517:GLY:O	1:A:518:ALA:O	2.38	0.40
1:A:177:VAL:HG22	1:A:178:ASN:H	1.85	0.40
1:A:193:GLN:CD	1:A:193:GLN:H	2.24	0.40
1:A:544:LYS:HG3	1:A:562:LYS:HB3	2.02	0.40
3:C:1516:GLU:HB3	3:C:1517:PRO:CD	2.51	0.40
2:E:778:THR:OG1	2:E:779:THR:N	2.54	0.40
1:D:341:TYR:HA	1:D:422:LEU:O	2.21	0.40
3:C:1472:HIS:CD2	3:C:1475:LYS:HD2	2.57	0.40
1:D:563:ILE:O	2:E:766:THR:HA	2.22	0.40
2:B:758:GLU:O	2:B:759:PRO:C	2.60	0.40
1:D:346:MET:CG	1:D:347:PRO:HD2	2.51	0.40
1:A:226:GLU:HA	1:A:282:ARG:HD2	2.03	0.40
1:D:342:PHE:CE2	1:D:398:LEU:HB2	2.56	0.40
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.56	0.40
1:D:386:LYS:HG2	1:D:386:LYS:O	2.20	0.40
3:C:1411:GLU:CD	3:C:1422:LEU:HA	2.42	0.40
3:F:1450:ILE:CD1	3:F:1472:HIS:CE1	2.96	0.40
1:A:530:TRP:CZ3	1:A:532:ASP:HB2	2.56	0.40
1:D:183:LYS:NZ	1:D:185:ARG:CD	2.82	0.40
1:D:471:LEU:HB3	1:D:478:LEU:HD21	2.04	0.40
3:F:1622:LYS:HD2	3:F:1622:LYS:HA	1.55	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	629/645 (98%)	553 (88%)	57 (9%)	19 (3%)	5 39
1	D	629/645 (98%)	548 (87%)	62 (10%)	19 (3%)	5 39
2	B	181/206 (88%)	157 (87%)	18 (10%)	6 (3%)	5 37
2	E	181/206 (88%)	157 (87%)	19 (10%)	5 (3%)	6 41
3	C	290/343 (84%)	226 (78%)	42 (14%)	22 (8%)	1 13
3	F	290/343 (84%)	213 (73%)	48 (17%)	29 (10%)	1 7
4	G	66/73 (90%)	56 (85%)	10 (15%)	0	100 100
4	H	66/73 (90%)	55 (83%)	11 (17%)	0	100 100
All	All	2332/2534 (92%)	1965 (84%)	267 (11%)	100 (4%)	3 29

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	347	PRO
1	A	392	HIS
1	A	518	ALA
1	A	549	GLU
2	B	836	GLN
3	C	1361	THR
3	C	1417	SER
3	C	1434	ASP
3	C	1477	ASP
3	C	1496	CYS
3	C	1640	PRO
1	D	49	SER
1	D	292	PRO
1	D	518	ALA
1	D	549	GLU
2	E	836	GLN
3	F	1375	ASP
3	F	1402	GLY
3	F	1412	LEU
3	F	1415	ALA
3	F	1481	ASN
3	F	1496	CYS
3	F	1499	GLN
3	F	1556	VAL
1	A	59	ASN
1	A	574	VAL

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Mol	Chain	Res	Type
2	B	762	ASN
3	C	1366	ILE
3	C	1367	CYS
3	C	1402	GLY
3	C	1486	ASP
3	C	1504	LYS
3	C	1512	ASP
3	C	1528	VAL
1	D	59	ASN
1	D	551	ARG
1	D	574	VAL
3	F	1361	THR
3	F	1461	TYR
3	F	1492	ALA
3	F	1504	LYS
3	F	1512	ASP
3	F	1528	VAL
1	A	63	ASN
1	A	64	VAL
1	A	372	GLU
1	A	548	SER
2	B	835	ASN
2	B	869	LYS
3	C	1392	ASP
3	C	1412	LEU
3	C	1494	GLU
3	C	1513	LYS
3	C	1602	LYS
1	D	63	ASN
1	D	64	VAL
1	D	372	GLU
2	E	762	ASN
2	E	835	ASN
2	E	869	LYS
3	F	1336	CYS
3	F	1449	LEU
3	F	1462	ASN
3	F	1513	LYS
3	F	1602	LYS
3	F	1616	GLN
1	A	375	VAL
1	A	376	GLN

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Mol	Chain	Res	Type
2	B	732	ASP
3	C	1505	VAL
3	C	1559	GLN
1	D	375	VAL
1	D	376	GLN
2	E	732	ASP
3	F	1387	THR
3	F	1493	GLU
3	F	1505	VAL
3	F	1514	ALA
3	F	1559	GLN
3	F	1640	PRO
1	A	81	ASN
1	A	506	SER
1	A	607	PRO
2	B	759	PRO
1	D	81	ASN
1	D	506	SER
1	D	607	PRO
3	F	1393	THR
1	A	539	GLY
3	C	1393	THR
1	D	539	GLY
1	D	553	PRO
3	C	1547	ILE
3	F	1547	ILE
1	A	91	GLY
1	A	520	GLY
1	D	520	GLY
3	F	1391	PRO
1	D	91	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	558/567 (98%)	476 (85%)	82 (15%)	4 20
1	D	558/567 (98%)	474 (85%)	84 (15%)	3 19
2	B	171/191 (90%)	155 (91%)	16 (9%)	11 42
2	E	171/191 (90%)	154 (90%)	17 (10%)	10 39
3	C	270/309 (87%)	218 (81%)	52 (19%)	2 8
3	F	270/309 (87%)	204 (76%)	66 (24%)	1 4
4	G	57/60 (95%)	54 (95%)	3 (5%)	28 67
4	H	57/60 (95%)	53 (93%)	4 (7%)	19 58
All	All	2112/2254 (94%)	1788 (85%)	324 (15%)	3 19

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	20	MET
1	A	31	VAL
1	A	34	THR
1	A	45	LEU
1	A	46	VAL
1	A	47	LEU
1	A	58	THR
1	A	61	MET
1	A	80	ARG
1	A	87	GLN
1	A	92	THR
1	A	94	VAL
1	A	102	SER
1	A	112	THR
1	A	118	THR
1	A	134	LEU
1	A	137	VAL
1	A	139	ARG
1	A	145	ILE
1	A	155	GLN
1	A	161	GLN
1	A	163	GLN
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	172	ASP
1	A	179	MET
1	A	183	LYS
1	A	195	VAL
1	A	198	THR
1	A	207	LEU
1	A	214	VAL
1	A	215	GLU
1	A	223	ILE
1	A	226	GLU
1	A	249	VAL
1	A	257	GLU
1	A	261	SER
1	A	263	PRO
1	A	264	GLU
1	A	277	GLU
1	A	293	ARG
1	A	304	VAL
1	A	305	SER
1	A	326	ILE
1	A	329	SER
1	A	364	ARG
1	A	369	VAL
1	A	370	GLN
1	A	373	ASP
1	A	379	THR
1	A	380	GLN
1	A	398	LEU
1	A	400	ILE
1	A	404	THR
1	A	406	LYS
1	A	409	LEU
1	A	417	ARG
1	A	419	MET
1	A	426	THR
1	A	443	LEU
1	A	448	THR
1	A	454	LEU
1	A	456	ARG
1	A	462	GLU
1	A	477	ARG
1	A	485	VAL

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Mol	Chain	Res	Type
1	A	487	GLU
1	A	492	LEU
1	A	509	LEU
1	A	510	VAL
1	A	519	SER
1	A	535	ASP
1	A	542	VAL
1	A	558	GLN
1	A	559	MET
1	A	561	LEU
1	A	583	LEU
1	A	585	LYS
1	A	592	SER
1	A	609	SER
1	A	625	THR
1	A	639	GLN
2	B	730	ASP
2	B	731	GLU
2	B	732	ASP
2	B	764	ILE
2	B	765	SER
2	B	775	ASP
2	B	813	LEU
2	B	817	VAL
2	B	819	ARG
2	B	834	GLN
2	B	845	LEU
2	B	864	VAL
2	B	887	GLU
2	B	894	VAL
2	B	907	LEU
2	B	910	VAL
3	C	1335	THR
3	C	1342	LYS
3	C	1344	THR
3	C	1361	THR
3	C	1363	ILE
3	C	1366	ILE
3	C	1368	THR
3	C	1374	GLN
3	C	1385	MET
3	C	1393	THR

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Mol	Chain	Res	Type
3	C	1395	ASP
3	C	1397	LYS
3	C	1404	ASP
3	C	1405	ARG
3	C	1411	GLU
3	C	1416	PHE
3	C	1422	LEU
3	C	1426	LEU
3	C	1433	GLU
3	C	1437	LEU
3	C	1443	GLN
3	C	1447	VAL
3	C	1457	VAL
3	C	1462	ASN
3	C	1469	ARG
3	C	1474	GLU
3	C	1477	ASP
3	C	1479	LYS
3	C	1480	LEU
3	C	1489	CYS
3	C	1494	GLU
3	C	1495	ASN
3	C	1499	GLN
3	C	1503	ASP
3	C	1504	LYS
3	C	1532	LEU
3	C	1535	ASP
3	C	1538	GLU
3	C	1543	ILE
3	C	1551	SER
3	C	1554	VAL
3	C	1558	GLN
3	C	1559	GLN
3	C	1564	SER
3	C	1567	LYS
3	C	1568	CYS
3	C	1573	LYS
3	C	1582	MET
3	C	1586	SER
3	C	1608	HIS
3	C	1624	CYS
3	C	1631	THR

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Mol	Chain	Res	Type
1	D	6	ILE
1	D	20	MET
1	D	31	VAL
1	D	34	THR
1	D	45	LEU
1	D	46	VAL
1	D	47	LEU
1	D	58	THR
1	D	61	MET
1	D	80	ARG
1	D	87	GLN
1	D	92	THR
1	D	94	VAL
1	D	102	SER
1	D	112	THR
1	D	118	THR
1	D	134	LEU
1	D	137	VAL
1	D	139	ARG
1	D	145	ILE
1	D	155	GLN
1	D	161	GLN
1	D	163	GLN
1	D	164	LEU
1	D	172	ASP
1	D	179	MET
1	D	183	LYS
1	D	195	VAL
1	D	198	THR
1	D	207	LEU
1	D	214	VAL
1	D	215	GLU
1	D	223	ILE
1	D	226	GLU
1	D	249	VAL
1	D	257	GLU
1	D	261	SER
1	D	263	PRO
1	D	264	GLU
1	D	277	GLU
1	D	293	ARG
1	D	304	VAL

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Mol	Chain	Res	Type
1	D	305	SER
1	D	326	ILE
1	D	329	SER
1	D	364	ARG
1	D	369	VAL
1	D	370	GLN
1	D	373	ASP
1	D	379	THR
1	D	380	GLN
1	D	392	HIS
1	D	398	LEU
1	D	400	ILE
1	D	404	THR
1	D	406	LYS
1	D	409	LEU
1	D	417	ARG
1	D	419	MET
1	D	426	THR
1	D	443	LEU
1	D	448	THR
1	D	456	ARG
1	D	462	GLU
1	D	477	ARG
1	D	485	VAL
1	D	487	GLU
1	D	492	LEU
1	D	509	LEU
1	D	510	VAL
1	D	519	SER
1	D	535	ASP
1	D	542	VAL
1	D	547	GLN
1	D	551	ARG
1	D	558	GLN
1	D	559	MET
1	D	561	LEU
1	D	583	LEU
1	D	585	LYS
1	D	592	SER
1	D	609	SER
1	D	625	THR
1	D	639	GLN

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Mol	Chain	Res	Type
2	E	730	ASP
2	E	731	GLU
2	E	732	ASP
2	E	757	LYS
2	E	764	ILE
2	E	775	ASP
2	E	813	LEU
2	E	817	VAL
2	E	819	ARG
2	E	834	GLN
2	E	845	LEU
2	E	851	CYS
2	E	864	VAL
2	E	887	GLU
2	E	894	VAL
2	E	907	LEU
2	E	910	VAL
3	F	1335	THR
3	F	1342	LYS
3	F	1344	THR
3	F	1346	LYS
3	F	1361	THR
3	F	1363	ILE
3	F	1364	LEU
3	F	1366	ILE
3	F	1371	ARG
3	F	1373	ASP
3	F	1374	GLN
3	F	1377	THR
3	F	1378	MET
3	F	1385	MET
3	F	1387	THR
3	F	1393	THR
3	F	1395	ASP
3	F	1397	LYS
3	F	1398	GLN
3	F	1404	ASP
3	F	1411	GLU
3	F	1412	LEU
3	F	1417	SER
3	F	1418	ASP
3	F	1422	LEU

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Mol	Chain	Res	Type
3	F	1423	ILE
3	F	1428	LYS
3	F	1432	SER
3	F	1433	GLU
3	F	1434	ASP
3	F	1436	CYS
3	F	1440	LYS
3	F	1449	LEU
3	F	1457	VAL
3	F	1462	ASN
3	F	1469	ARG
3	F	1474	GLU
3	F	1479	LYS
3	F	1482	LYS
3	F	1483	LEU
3	F	1490	ARG
3	F	1491	CYS
3	F	1497	PHE
3	F	1499	GLN
3	F	1503	ASP
3	F	1504	LYS
3	F	1532	LEU
3	F	1535	ASP
3	F	1538	GLU
3	F	1543	ILE
3	F	1551	SER
3	F	1554	VAL
3	F	1558	GLN
3	F	1559	GLN
3	F	1564	SER
3	F	1567	LYS
3	F	1573	LYS
3	F	1582	MET
3	F	1586	SER
3	F	1596	LEU
3	F	1608	HIS
3	F	1616	GLN
3	F	1622	LYS
3	F	1624	CYS
3	F	1631	THR
3	F	1639	CYS
4	G	25	LEU

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Mol	Chain	Res	Type
4	G	33	LEU
4	G	37	SER
4	H	25	LEU
4	H	33	LEU
4	H	37	SER
4	H	64	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	38	HIS
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	132	HIS
1	A	193	GLN
1	A	318	GLN
1	A	332	GLN
1	A	395	GLN
1	A	429	ASN
1	A	490	GLN
1	A	634	GLN
1	A	639	GLN
2	B	738	ASN
2	B	752	ASN
2	B	770	ASN
2	B	834	GLN
2	B	836	GLN
2	B	897	HIS
3	C	1360	ASN
3	C	1443	GLN
3	C	1446	ASN
3	C	1462	ASN
3	C	1481	ASN
3	C	1495	ASN
3	C	1579	HIS
3	C	1595	ASN
1	D	10	ASN
1	D	38	HIS
1	D	60	HIS
1	D	87	GLN

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Mol	Chain	Res	Type
1	D	104	GLN
1	D	132	HIS
1	D	155	GLN
1	D	181	GLN
1	D	193	GLN
1	D	290	GLN
1	D	291	ASN
1	D	318	GLN
1	D	332	GLN
1	D	395	GLN
1	D	429	ASN
1	D	490	GLN
1	D	634	GLN
1	D	639	GLN
2	E	738	ASN
2	E	752	ASN
2	E	762	ASN
2	E	770	ASN
2	E	820	ASN
2	E	834	GLN
2	E	836	GLN
2	E	860	HIS
2	E	897	HIS
3	F	1337	ASN
3	F	1401	ASN
3	F	1462	ASN
3	F	1499	GLN
3	F	1559	GLN
3	F	1579	HIS
3	F	1595	ASN
3	F	1641	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	633/645 (98%)	0.08	11 (1%) 73 67	25, 50, 86, 148	0
1	D	633/645 (98%)	0.03	5 (0%) 87 83	21, 53, 85, 141	0
2	B	183/206 (88%)	-0.14	1 (0%) 91 89	27, 54, 93, 121	0
2	E	183/206 (88%)	-0.20	3 (1%) 74 69	26, 48, 76, 126	0
3	C	296/343 (86%)	1.38	72 (24%) 1 1	24, 116, 155, 187	0
3	F	296/343 (86%)	0.77	28 (9%) 10 10	26, 90, 126, 147	0
4	G	68/73 (93%)	0.08	3 (4%) 38 34	35, 59, 106, 115	0
4	H	68/73 (93%)	-0.18	0 100 100	36, 47, 67, 79	0
All	All	2360/2534 (93%)	0.27	123 (5%) 31 28	21, 59, 127, 187	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1500	LYS	7.5
3	F	1641	ASN	7.1
3	C	1503	ASP	6.5
3	C	1415	ALA	5.7
3	C	1499	GLN	4.9
3	C	1606	VAL	4.8
3	C	1412	LEU	4.6
3	C	1497	PHE	4.4
3	C	1445	PHE	4.2
3	F	1594	PRO	4.1
3	C	1349	PRO	4.0
3	F	1500	LYS	4.0
3	F	1503	ASP	3.7
3	C	1605	TRP	3.7
2	E	763	GLY	3.7
1	A	292	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	1583	TRP	3.5
3	C	1608	HIS	3.5
3	C	1534	ASN	3.5
3	C	1364	LEU	3.5
1	A	291	ASN	3.5
1	A	373	ASP	3.4
3	F	1536	PHE	3.4
3	F	1359	LYS	3.3
3	C	1416	PHE	3.3
3	C	1368	THR	3.3
1	D	551	ARG	3.3
3	C	1498	ILE	3.3
3	F	1506	THR	3.2
3	C	1487	GLU	3.2
3	C	1609	TRP	3.2
3	C	1641	ASN	3.1
3	F	1499	GLN	3.1
3	C	1545	GLN	3.1
3	F	1504	LYS	3.1
3	C	1553	GLU	3.1
3	C	1582	MET	3.0
3	C	1439	PHE	3.0
3	C	1581	LEU	3.0
3	C	1441	VAL	3.0
3	C	1446	ASN	3.0
3	C	1574	LEU	3.0
3	C	1520	ASP	2.9
3	F	1416	PHE	2.9
3	C	1570	GLU	2.9
4	G	67	ASP	2.9
3	C	1419	ARG	2.9
3	C	1571	ALA	2.8
3	C	1372	GLY	2.8
1	D	294	ALA	2.8
3	F	1505	VAL	2.8
3	C	1561	THR	2.8
3	C	1426	LEU	2.7
3	F	1566	ILE	2.7
3	C	1639	CYS	2.7
3	F	1606	VAL	2.7
3	F	1412	LEU	2.7
2	E	765	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	1349	PRO	2.6
2	E	762	ASN	2.6
3	C	1381	LEU	2.6
3	C	1623	GLN	2.6
3	F	1534	ASN	2.6
3	C	1382	ASP	2.6
3	F	1595	ASN	2.6
1	A	374	THR	2.6
3	C	1443	GLN	2.5
3	C	1454	ALA	2.5
3	F	1585	LEU	2.5
3	F	1582	MET	2.5
3	F	1640	PRO	2.4
3	C	1584	GLY	2.4
1	A	289	VAL	2.4
3	C	1629	ALA	2.4
3	C	1505	VAL	2.4
3	C	1495	ASN	2.4
3	C	1523	TYR	2.4
3	C	1343	VAL	2.4
1	A	548	SER	2.4
3	C	1373	ASP	2.4
1	A	105	SER	2.4
1	D	552	GLN	2.4
3	C	1432	SER	2.3
3	F	1564	SER	2.3
3	C	1444	TYR	2.3
3	C	1612	GLU	2.3
1	A	48	SER	2.3
3	C	1424	ILE	2.3
3	C	1632	GLU	2.3
3	C	1531	GLN	2.3
3	C	1638	GLY	2.2
3	C	1504	LYS	2.2
3	C	1597	SER	2.2
2	B	763	GLY	2.2
1	D	30	ASP	2.2
1	A	80	ARG	2.2
1	A	371	GLY	2.2
3	F	1518	GLY	2.2
3	C	1423	ILE	2.2
3	C	1590	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	1360	ASN	2.2
3	C	1596	LEU	2.2
3	F	1364	LEU	2.2
3	F	1398	GLN	2.1
3	C	1468	THR	2.1
3	C	1557	GLY	2.1
3	C	1488	LEU	2.1
3	C	1575	GLU	2.1
3	F	1497	PHE	2.1
1	A	106	GLY	2.1
3	C	1580	TYR	2.1
3	C	1572	LEU	2.0
3	C	1595	ASN	2.0
3	C	1428	LYS	2.0
3	C	1577	LYS	2.0
4	G	68	ALA	2.0
3	C	1616	GLN	2.0
3	C	1524	LYS	2.0
3	F	1443	GLN	2.0
4	G	57	LEU	2.0
1	D	550	ASP	2.0
3	C	1391	PRO	2.0
3	F	1439	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.