W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:11 AM GMT

PDB ID	:	3DPN
Title	:	Crystal Structure of cpaf s499a mutant
Authors	:	Chai, J.; Huang, Z.
Deposited on	:	2008-07-09
Resolution	:	3.30 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 (i)) 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 3.30 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	Percentile Ranks	Value
Rfree		0.306
Clashscore		46
Ramachandran outliers		8.2%
Sidechain outliers		10.6%
RSRZ outliers		6.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
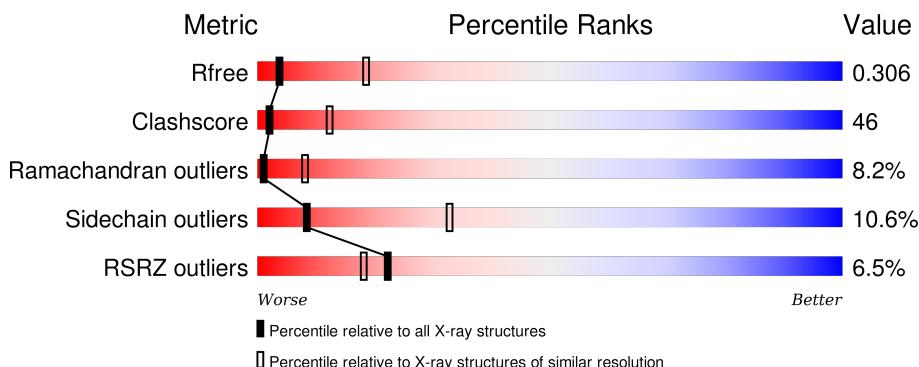
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	583	9% / 36% 45% 9% · 8%
1	B	583	3% / 36% 45% 9% · 8%
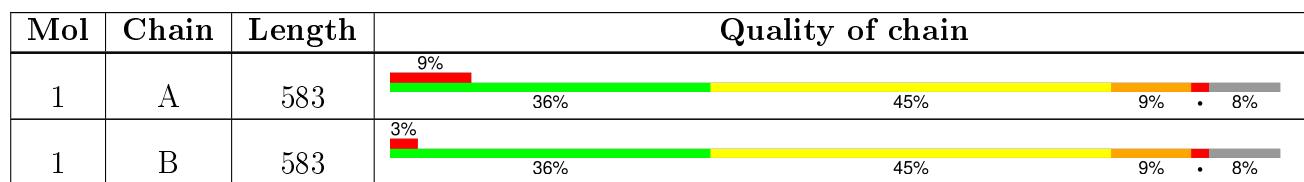
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8476 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 Protein CT_858.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4238	2719	709	796	14			
1	B	537	Total	C	N	O	S	0	0	0
			4238	2719	709	796	14			

There are 14 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	499	ALA	SER	ENGINEERED	UNP O84866
A	610	HIS	-	EXPRESSION TAG	UNP O84866
A	611	HIS	-	EXPRESSION TAG	UNP O84866
A	612	HIS	-	EXPRESSION TAG	UNP O84866
A	613	HIS	-	EXPRESSION TAG	UNP O84866
A	614	HIS	-	EXPRESSION TAG	UNP O84866
A	615	HIS	-	EXPRESSION TAG	UNP O84866
B	499	ALA	SER	ENGINEERED	UNP O84866
B	610	HIS	-	EXPRESSION TAG	UNP O84866
B	611	HIS	-	EXPRESSION TAG	UNP O84866
B	612	HIS	-	EXPRESSION TAG	UNP O84866
B	613	HIS	-	EXPRESSION TAG	UNP O84866
B	614	HIS	-	EXPRESSION TAG	UNP O84866
B	615	HIS	-	EXPRESSION TAG	UNP O84866

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Protein CT_858
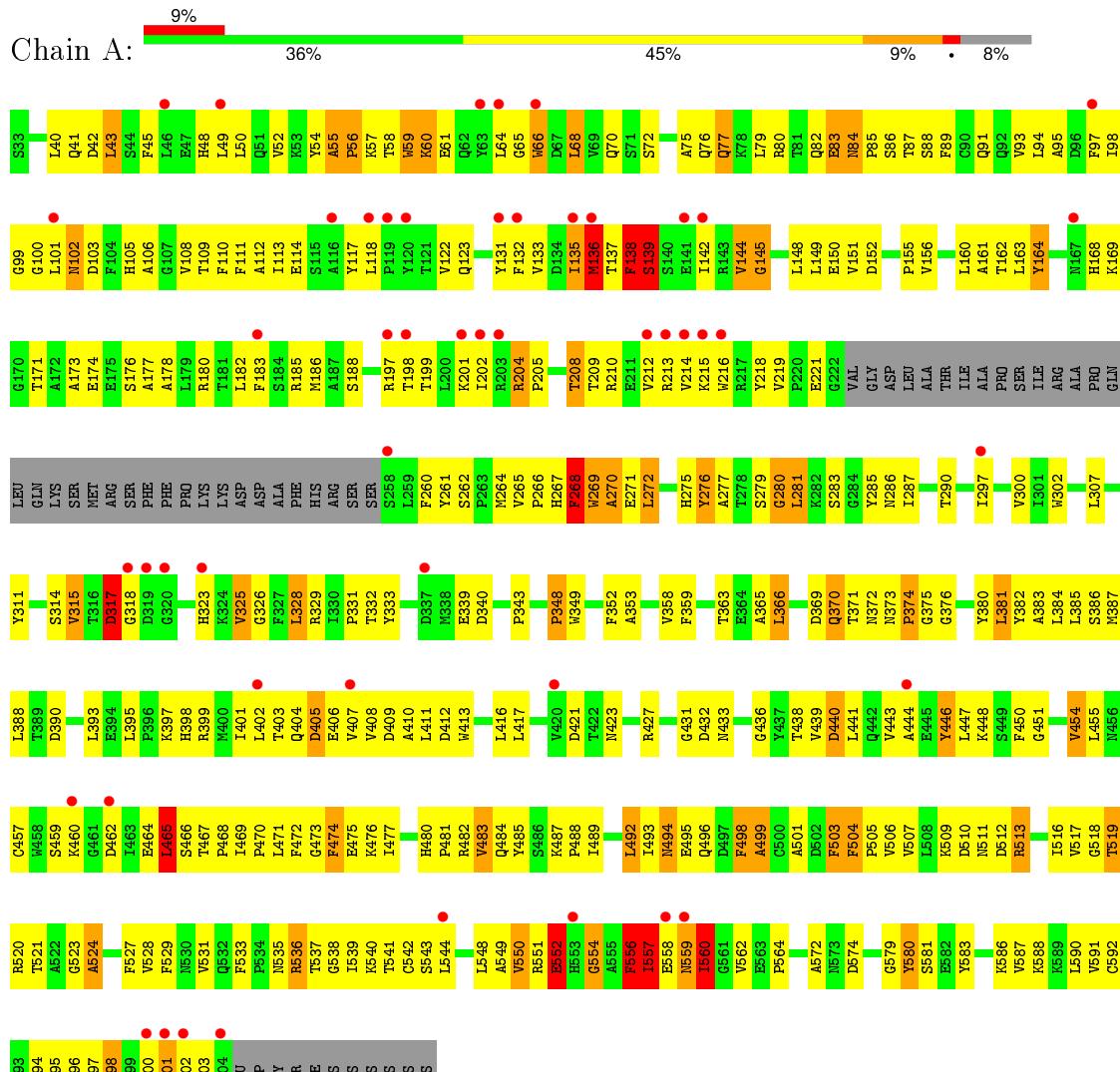
- Molecule 1: Protein CT_858
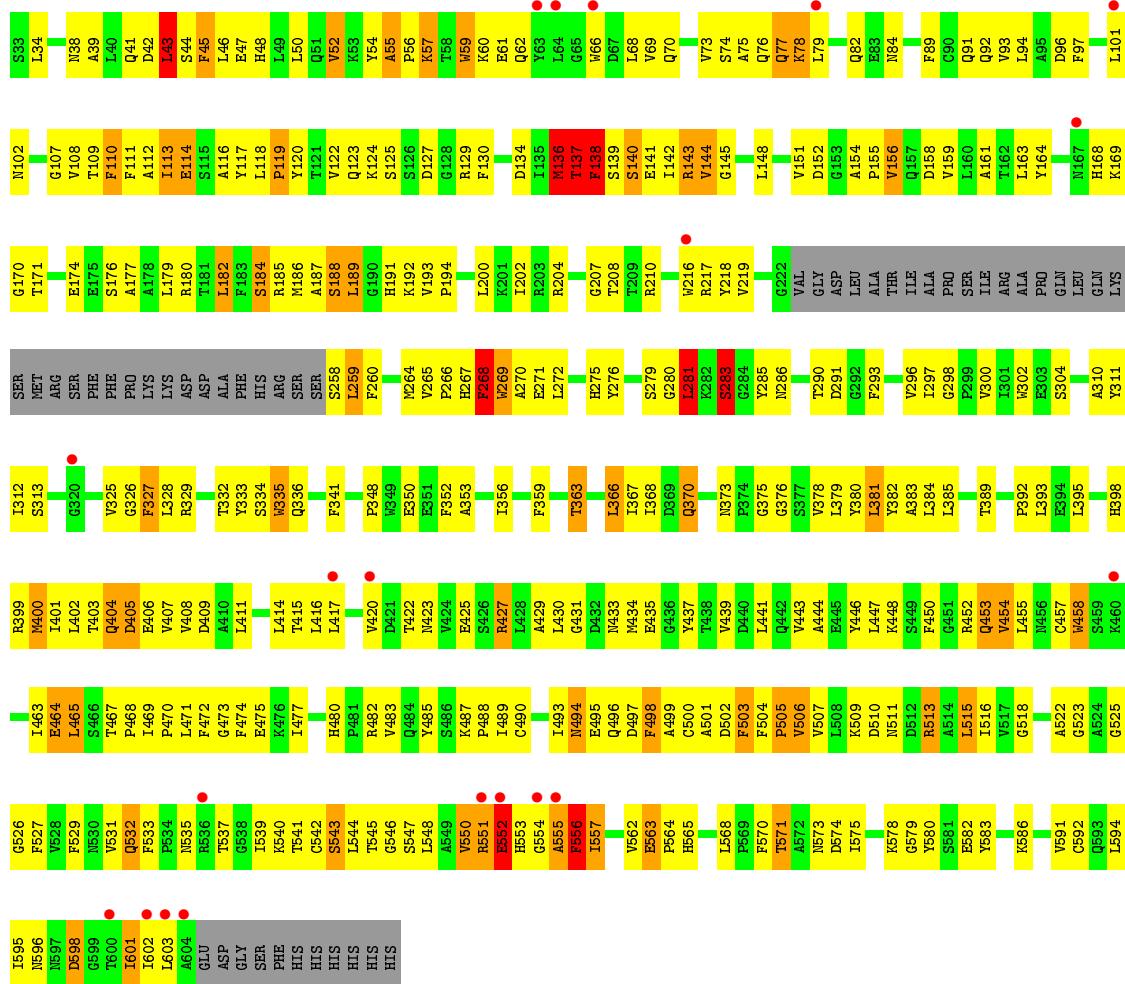
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	192.67Å 192.67Å 338.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 49.90 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.30) 98.7 (49.90-3.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [1]	2.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.305 0.261 , 0.306	Depositor DCC
R_{free} test set	1800 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	100.6	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 132.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	3 of 39050 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8476	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.47	0/4344	0.76	4/5905 (0.1%)
1	B	0.48	0/4344	0.79	6/5905 (0.1%)
All	All	0.47	0/8688	0.78	10/11810 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	PHE	N-CA-C	11.85	143.00	111.00
1	B	556	PHE	N-CA-C	7.79	132.03	111.00
1	A	554	GLY	N-CA-C	6.73	129.92	113.10
1	B	281	LEU	N-CA-C	-6.38	93.78	111.00
1	B	137	THR	C-N-CA	-5.65	107.58	121.70
1	A	560	ILE	CB-CA-C	-5.50	100.59	111.60
1	B	136	MET	N-CA-C	5.49	125.81	111.00
1	B	598	ASP	N-CA-C	5.26	125.20	111.00
1	A	557	ILE	N-CA-C	5.19	125.02	111.00
1	A	135	ILE	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	PHE	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4238	0	4157	386	0
1	B	4238	0	4157	384	0
All	All	8476	0	8314	768	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 (768) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:VAL:HG12	1:A:554:GLY:HA2	1.29	1.12
1:B:54:TYR:CZ	1:B:56:PRO:HG2	1.90	1.05
1:A:557:ILE:HG22	1:A:558:GLU:N	1.71	1.04
1:B:47:GLU:HG3	1:B:68:LEU:HD11	1.39	1.04
1:A:398:HIS:HD2	1:A:471:LEU:HD21	1.22	1.01
1:A:54:TYR:CZ	1:A:56:PRO:HG2	1.97	1.00
1:A:408:VAL:HA	1:A:411:LEU:HD12	1.43	0.99
1:A:398:HIS:CD2	1:A:471:LEU:HD21	1.99	0.96
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.48	0.95
1:A:523:GLY:HA2	1:A:560:ILE:HG22	1.47	0.95
1:A:359:PHE:O	1:A:363:THR:HG22	1.65	0.94
1:A:427:ARG:HA	1:A:439:VAL:HG11	1.50	0.92
1:B:516:ILE:H	1:B:565:HIS:CD2	1.90	0.90
1:A:601:ILE:HG22	1:A:602:ILE:HG13	1.54	0.89
1:B:119:PRO:HG3	1:B:137:THR:HB	1.53	0.87
1:B:118:LEU:HG	1:B:216:TRP:CE3	2.10	0.87
1:A:457:CYS:SG	1:A:467:THR:HG22	2.14	0.87
1:A:557:ILE:HG22	1:A:558:GLU:H	1.37	0.87
1:B:136:MET:HE3	1:B:283:SER:HB3	1.56	0.86
1:A:427:ARG:HG2	1:A:439:VAL:HB	1.57	0.86
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.11	0.86
1:A:144:VAL:HG12	1:A:145:GLY:H	1.39	0.86
1:A:180:ARG:HD2	1:A:496:GLN:HE21	1.41	0.85
1:B:515:LEU:HD23	1:B:565:HIS:HD2	1.40	0.84
1:B:119:PRO:HB2	1:B:137:THR:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ARG:HB3	1:B:555:ALA:HB3	1.58	0.84
1:B:367:ILE:HD11	1:B:591:VAL:HG21	1.61	0.83
1:B:366:LEU:HD13	1:B:368:ILE:HD11	1.61	0.82
1:A:451:GLY:O	1:A:454:VAL:HG23	1.80	0.82
1:A:431:GLY:O	1:A:439:VAL:HG21	1.80	0.81
1:A:523:GLY:CA	1:A:560:ILE:HG22	2.10	0.81
1:B:515:LEU:HD23	1:B:565:HIS:CD2	2.17	0.80
1:B:395:LEU:HD11	1:B:477:ILE:HG13	1.64	0.80
1:B:161:ALA:HA	1:B:164:TYR:CD2	2.17	0.79
1:B:457:CYS:SG	1:B:467:THR:HG22	2.22	0.79
1:B:554:GLY:O	1:B:556:PHE:N	2.15	0.79
1:A:468:PRO:HB3	1:A:550:VAL:HG21	1.65	0.79
1:A:177:ALA:HA	1:A:180:ARG:HD3	1.62	0.79
1:A:556:PHE:O	1:A:557:ILE:HG12	1.83	0.78
1:A:402:LEU:CD2	1:A:454:VAL:HG12	2.14	0.78
1:A:135:ILE:HD11	1:A:142:ILE:HG22	1.65	0.78
1:B:571:THR:HG23	1:B:574:ASP:OD2	1.84	0.78
1:A:176:SER:OG	1:A:495:GLU:HG3	1.83	0.78
1:A:506:VAL:HG13	1:A:507:VAL:N	1.99	0.77
1:A:455:LEU:HD23	1:A:455:LEU:N	1.99	0.76
1:B:592:CYS:HA	1:B:595:ILE:HD12	1.66	0.76
1:B:66:TRP:CH2	1:B:68:LEU:HB2	2.21	0.76
1:B:177:ALA:HA	1:B:180:ARG:HD3	1.67	0.75
1:B:264:MET:CE	1:B:526:GLY:H	1.97	0.75
1:B:264:MET:HE3	1:B:526:GLY:H	1.50	0.75
1:A:43:LEU:HD11	1:A:75:ALA:CB	2.17	0.75
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.66	0.75
1:A:180:ARG:HH11	1:A:180:ARG:HB2	1.52	0.74
1:B:452:ARG:O	1:B:454:VAL:N	2.19	0.74
1:B:326:GLY:O	1:B:366:LEU:HD23	1.88	0.73
1:B:367:ILE:HD11	1:B:591:VAL:CG2	2.18	0.73
1:B:112:ALA:O	1:B:188:SER:HB3	1.88	0.73
1:A:133:VAL:HB	1:A:285:TYR:CE1	2.23	0.73
1:B:350:GLU:O	1:B:353:ALA:HB3	1.87	0.73
1:B:184:SER:O	1:B:185:ARG:HD3	1.89	0.73
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.23	0.72
1:B:389:THR:HG21	1:B:393:LEU:HD11	1.70	0.72
1:A:144:VAL:HG12	1:A:145:GLY:N	2.04	0.72
1:A:43:LEU:HD11	1:A:75:ALA:HB1	1.71	0.72
1:B:543:SER:C	1:B:544:LEU:HD23	2.10	0.72
1:B:379:LEU:O	1:B:382:TYR:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:VAL:CG1	1:A:554:GLY:HA2	2.15	0.71
1:B:55:ALA:HB2	1:B:546:GLY:O	1.90	0.71
1:B:557:ILE:O	1:B:557:ILE:HG22	1.90	0.71
1:B:144:VAL:HG12	1:B:145:GLY:N	2.06	0.71
1:A:506:VAL:HB	1:A:562:VAL:HG21	1.73	0.70
1:A:267:HIS:CG	1:A:268:PHE:H	2.08	0.70
1:B:119:PRO:CG	1:B:137:THR:HB	2.21	0.70
1:B:537:THR:HG22	1:B:537:THR:O	1.90	0.70
1:A:529:PHE:O	1:A:543:SER:HA	1.90	0.70
1:B:258:SER:O	1:B:260:PHE:N	2.21	0.70
1:A:559:ASN:O	1:A:560:ILE:HB	1.91	0.70
1:A:516:ILE:HD12	1:A:516:ILE:H	1.56	0.70
1:B:136:MET:HE3	1:B:283:SER:H	1.56	0.70
1:A:446:TYR:O	1:A:473:GLY:HA3	1.92	0.69
1:B:54:TYR:CZ	1:B:56:PRO:CG	2.74	0.69
1:A:402:LEU:N	1:A:402:LEU:HD12	2.08	0.69
1:B:502:ASP:OD2	1:B:562:VAL:HG23	1.93	0.69
1:A:111:PHE:CE1	1:A:540:LYS:HA	2.27	0.69
1:A:352:PHE:HD2	1:A:387:MET:CE	2.06	0.69
1:B:171:THR:OG1	1:B:174:GLU:HG3	1.92	0.68
1:A:54:TYR:CZ	1:A:101:LEU:HD13	2.29	0.68
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.24	0.68
1:B:433:ASN:HA	1:B:439:VAL:HG23	1.75	0.68
1:A:54:TYR:CE1	1:A:56:PRO:HG2	2.29	0.68
1:A:402:LEU:HD23	1:A:454:VAL:HG12	1.74	0.68
1:A:557:ILE:CG2	1:A:558:GLU:H	1.97	0.68
1:A:556:PHE:C	1:A:557:ILE:HG12	2.13	0.67
1:B:537:THR:O	1:B:537:THR:CG2	2.42	0.67
1:A:352:PHE:CD2	1:A:387:MET:CE	2.76	0.67
1:A:557:ILE:CG2	1:A:558:GLU:N	2.42	0.67
1:A:180:ARG:NH1	1:A:180:ARG:CB	2.57	0.67
1:B:398:HIS:HB3	1:B:547:SER:HB2	1.76	0.67
1:A:276:TYR:CE1	1:A:286:ASN:HB3	2.30	0.67
1:B:516:ILE:H	1:B:565:HIS:HD2	1.42	0.67
1:B:552:GLU:OE2	1:B:555:ALA:HB2	1.95	0.67
1:A:383:ALA:O	1:A:386:SER:HB3	1.94	0.67
1:A:587:VAL:O	1:A:591:VAL:HG23	1.95	0.67
1:A:516:ILE:N	1:A:516:ILE:HD12	2.09	0.67
1:B:471:LEU:HD22	1:B:527:PHE:CE1	2.30	0.67
1:A:118:LEU:HD12	1:A:183:PHE:CD2	2.31	0.66
1:A:559:ASN:O	1:A:560:ILE:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:THR:OG1	1:B:468:PRO:HD2	1.96	0.66
1:A:506:VAL:CG1	1:A:507:VAL:N	2.58	0.66
1:A:518:GLY:O	1:A:564:PRO:HG3	1.95	0.66
1:A:177:ALA:O	1:A:180:ARG:HB2	1.95	0.66
1:B:464:GLU:O	1:B:465:LEU:HB2	1.95	0.66
1:B:136:MET:HE2	1:B:281:LEU:HA	1.77	0.66
1:A:536:ARG:HB3	1:A:536:ARG:HH11	1.61	0.66
1:A:535:ASN:ND2	1:A:539:ILE:HB	2.11	0.66
1:B:543:SER:O	1:B:544:LEU:HD23	1.96	0.65
1:B:168:HIS:CE1	1:B:170:GLY:HA2	2.31	0.65
1:B:108:VAL:HG12	1:B:109:THR:N	2.11	0.65
1:B:414:LEU:C	1:B:416:LEU:H	1.99	0.65
1:B:489:ILE:HD12	1:B:513:ARG:HH11	1.62	0.65
1:A:40:LEU:CD2	1:A:76:GLN:HG2	2.27	0.65
1:B:143:ARG:HH21	1:B:204:ARG:NH1	1.95	0.65
1:B:136:MET:CE	1:B:283:SER:HB3	2.27	0.65
1:B:591:VAL:O	1:B:594:LEU:HB2	1.97	0.65
1:B:502:ASP:O	1:B:506:VAL:HG12	1.96	0.65
1:A:328:LEU:HD11	1:A:352:PHE:HE1	1.62	0.65
1:A:352:PHE:CD2	1:A:387:MET:HE2	2.32	0.65
1:B:359:PHE:O	1:B:363:THR:HB	1.96	0.65
1:B:368:ILE:HD13	1:B:489:ILE:HG23	1.78	0.65
1:B:192:LYS:O	1:B:194:PRO:HD3	1.97	0.65
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.31	0.64
1:B:143:ARG:NH2	1:B:204:ARG:HD2	2.12	0.64
1:B:601:ILE:HG22	1:B:602:ILE:HG13	1.79	0.64
1:B:161:ALA:HA	1:B:164:TYR:HD2	1.60	0.64
1:A:602:ILE:HG22	1:A:603:LEU:N	2.11	0.64
1:B:179:LEU:HD23	1:B:182:LEU:HD12	1.79	0.64
1:B:186:MET:H	1:B:191:HIS:CD2	2.16	0.64
1:A:122:VAL:HG12	1:A:123:GLN:N	2.13	0.64
1:A:440:ASP:O	1:A:443:VAL:N	2.29	0.64
1:A:494:ASN:N	1:A:494:ASN:HD22	1.93	0.64
1:A:401:ILE:C	1:A:402:LEU:HD12	2.18	0.64
1:B:169:LYS:HA	1:B:169:LYS:HE2	1.80	0.64
1:A:180:ARG:CZ	1:A:268:PHE:CZ	2.81	0.64
1:B:180:ARG:HB2	1:B:180:ARG:NH1	2.12	0.64
1:A:369:ASP:HA	1:A:492:LEU:HB2	1.80	0.64
1:A:592:CYS:HA	1:A:595:ILE:HG12	1.80	0.63
1:A:180:ARG:CB	1:A:180:ARG:HH11	2.11	0.63
1:A:103:ASP:OD1	1:A:105:HIS:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.81	0.63
1:A:393:LEU:HB3	1:A:511:ASN:ND2	2.11	0.63
1:A:489:ILE:HG13	1:A:513:ARG:NH2	2.14	0.63
1:A:114:GLU:HB2	1:A:221:GLU:HB2	1.80	0.63
1:B:74:SER:O	1:B:77:GLN:HB2	1.98	0.63
1:B:400:MET:HB2	1:B:402:LEU:HD21	1.80	0.63
1:A:297:ILE:HG23	1:A:311:TYR:OH	1.99	0.63
1:A:79:LEU:HD21	1:A:93:VAL:HG11	1.80	0.62
1:B:180:ARG:HD2	1:B:496:GLN:NE2	2.14	0.62
1:A:105:HIS:HD2	1:A:528:VAL:HG12	1.64	0.62
1:B:143:ARG:HE	1:B:204:ARG:NH1	1.96	0.62
1:A:48:HIS:CE1	1:A:52:VAL:HG21	2.33	0.62
1:B:125:SER:HA	1:B:575:ILE:CD1	2.30	0.62
1:A:328:LEU:HD22	1:A:329:ARG:N	2.14	0.62
1:B:108:VAL:HG12	1:B:109:THR:H	1.65	0.62
1:A:315:VAL:CG1	1:A:588:LYS:HD2	2.29	0.62
1:A:520:ARG:HD3	1:A:559:ASN:OD1	1.99	0.62
1:A:59:TRP:CH2	1:A:557:ILE:HB	2.35	0.62
1:B:552:GLU:OE2	1:B:555:ALA:CB	2.48	0.62
1:A:387:MET:HG2	1:A:480:HIS:HD2	1.64	0.62
1:B:381:LEU:C	1:B:381:LEU:HD13	2.19	0.62
1:B:341:PHE:CE1	1:B:348:PRO:HD3	2.35	0.62
1:A:204:ARG:HB3	1:A:205:PRO:HD2	1.81	0.62
1:A:326:GLY:O	1:A:366:LEU:HD23	1.99	0.62
1:B:54:TYR:CE1	1:B:56:PRO:HG2	2.35	0.61
1:A:59:TRP:CZ2	1:A:557:ILE:HB	2.35	0.61
1:B:591:VAL:O	1:B:595:ILE:HG13	2.00	0.61
1:A:506:VAL:CG1	1:A:507:VAL:H	2.13	0.61
1:B:471:LEU:HD22	1:B:527:PHE:HE1	1.65	0.61
1:B:352:PHE:CE2	1:B:356:ILE:HD11	2.35	0.61
1:B:398:HIS:HA	1:B:548:LEU:O	2.00	0.61
1:A:592:CYS:HA	1:A:595:ILE:CG1	2.29	0.61
1:B:122:VAL:HG12	1:B:123:GLN:N	2.15	0.61
1:A:106:ALA:HA	1:A:543:SER:O	1.99	0.61
1:A:137:THR:HG22	1:A:137:THR:O	2.01	0.61
1:B:498:PHE:CD1	1:B:498:PHE:N	2.69	0.61
1:A:409:ASP:HA	1:A:412:ASP:OD2	2.01	0.61
1:A:267:HIS:CG	1:A:268:PHE:N	2.69	0.61
1:A:583:TYR:O	1:A:587:VAL:HG23	2.00	0.61
1:A:122:VAL:HG13	1:A:131:TYR:O	2.00	0.61
1:A:365:ALA:HB2	1:A:595:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HB2	1:B:208:THR:HG23	1.82	0.61
1:A:173:ALA:HA	1:A:495:GLU:HB2	1.83	0.61
1:A:332:THR:HA	1:A:374:PRO:HD2	1.83	0.61
1:B:138:PHE:HD2	1:B:140:SER:HB2	1.65	0.60
1:A:464:GLU:O	1:A:465:LEU:HB2	2.01	0.60
1:A:446:TYR:C	1:A:473:GLY:HA3	2.20	0.60
1:A:493:ILE:HG13	1:A:519:THR:O	2.01	0.60
1:B:55:ALA:HB3	1:B:56:PRO:CD	2.30	0.60
1:B:136:MET:HE2	1:B:281:LEU:CA	2.31	0.60
1:A:66:TRP:CH2	1:A:68:LEU:HB2	2.37	0.60
1:B:89:PHE:O	1:B:93:VAL:HG23	2.01	0.60
1:A:365:ALA:HB2	1:A:595:ILE:CD1	2.31	0.60
1:A:160:LEU:HD21	1:A:182:LEU:HD12	1.83	0.60
1:A:399:ARG:HH11	1:A:399:ARG:HG3	1.67	0.60
1:B:116:ALA:HB3	1:B:185:ARG:HB2	1.83	0.60
1:A:556:PHE:C	1:A:556:PHE:CD2	2.75	0.59
1:A:180:ARG:HB3	1:A:180:ARG:NH1	2.15	0.59
1:A:591:VAL:HA	1:A:594:LEU:HD12	1.84	0.59
1:B:542:CYS:SG	1:B:544:LEU:HD21	2.42	0.59
1:B:264:MET:HG2	1:B:526:GLY:O	2.02	0.59
1:A:60:LYS:HD2	1:A:64:LEU:HD12	1.82	0.59
1:B:535:ASN:ND2	1:B:539:ILE:HB	2.18	0.59
1:B:158:ASP:O	1:B:161:ALA:HB3	2.03	0.59
1:B:494:ASN:ND2	1:B:496:GLN:H	1.99	0.59
1:B:136:MET:CE	1:B:281:LEU:HD23	2.31	0.59
1:A:59:TRP:CE2	1:A:557:ILE:HG13	2.38	0.59
1:A:590:LEU:HD23	1:A:600:THR:HG21	1.83	0.59
1:B:45:PHE:O	1:B:48:HIS:HB3	2.02	0.59
1:B:497:ASP:O	1:B:522:ALA:HB3	2.03	0.59
1:A:397:LYS:O	1:A:550:VAL:HG23	2.02	0.59
1:B:601:ILE:N	1:B:601:ILE:HD12	2.18	0.59
1:A:269:TRP:O	1:A:272:LEU:N	2.35	0.59
1:B:503:PHE:HA	1:B:506:VAL:CG1	2.33	0.58
1:B:111:PHE:CD2	1:B:540:LYS:HB2	2.37	0.58
1:A:182:LEU:HD23	1:A:182:LEU:C	2.24	0.58
1:A:297:ILE:HD11	1:A:325:VAL:CG1	2.33	0.58
1:A:551:ARG:HD2	1:A:552:GLU:HG3	1.84	0.58
1:A:556:PHE:O	1:A:557:ILE:CG1	2.50	0.58
1:A:602:ILE:CG2	1:A:603:LEU:N	2.67	0.58
1:A:506:VAL:HG22	1:A:510:ASP:OD2	2.04	0.58
1:B:417:LEU:HD13	1:B:444:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PHE:CE2	1:B:540:LYS:HB2	2.39	0.58
1:B:136:MET:SD	1:B:281:LEU:HD23	2.43	0.58
1:B:571:THR:O	1:B:575:ILE:HG13	2.03	0.58
1:A:50:LEU:HD12	1:A:68:LEU:HD12	1.85	0.58
1:B:502:ASP:O	1:B:505:PRO:HG2	2.04	0.58
1:A:517:VAL:HG12	1:A:518:GLY:N	2.19	0.58
1:A:474:PHE:CD1	1:A:474:PHE:N	2.72	0.58
1:B:202:ILE:HG12	1:B:210:ARG:O	2.04	0.58
1:B:110:PHE:CD1	1:B:110:PHE:N	2.71	0.58
1:B:151:VAL:O	1:B:152:ASP:HB2	2.03	0.58
1:A:72:SER:O	1:A:75:ALA:HB3	2.04	0.57
1:A:59:TRP:O	1:A:61:GLU:N	2.37	0.57
1:A:411:LEU:HD13	1:B:411:LEU:HD11	1.85	0.57
1:B:50:LEU:O	1:B:54:TYR:HB3	2.04	0.57
1:A:180:ARG:NH1	1:A:268:PHE:CZ	2.72	0.57
1:B:119:PRO:CB	1:B:137:THR:HB	2.35	0.57
1:A:118:LEU:HD12	1:A:183:PHE:HD2	1.68	0.57
1:A:135:ILE:O	1:A:136:MET:O	2.22	0.57
1:B:94:LEU:O	1:B:97:PHE:HB3	2.04	0.57
1:A:509:LYS:HB2	1:A:516:ILE:CD1	2.34	0.57
1:A:474:PHE:HD1	1:A:474:PHE:N	2.02	0.57
1:B:407:VAL:O	1:B:411:LEU:HG	2.05	0.57
1:A:541:THR:HG22	1:A:542:CYS:N	2.20	0.57
1:A:352:PHE:HD2	1:A:387:MET:HE1	1.69	0.57
1:A:405:ASP:HA	1:A:408:VAL:HG23	1.86	0.56
1:A:591:VAL:O	1:A:594:LEU:HB2	2.05	0.56
1:B:38:ASN:O	1:B:39:ALA:C	2.43	0.56
1:A:307:LEU:CD2	1:A:348:PRO:HB3	2.35	0.56
1:B:311:TYR:OH	1:B:327:PHE:CD1	2.56	0.56
1:B:122:VAL:HG11	1:B:130:PHE:HB3	1.87	0.56
1:B:180:ARG:HD2	1:B:496:GLN:HE21	1.70	0.56
1:A:469:ILE:HG23	1:A:470:PRO:HD2	1.88	0.56
1:A:474:PHE:H	1:A:474:PHE:HD1	1.53	0.56
1:B:427:ARG:HA	1:B:431:GLY:O	2.04	0.56
1:A:118:LEU:HG	1:A:216:TRP:CE3	2.41	0.56
1:B:265:VAL:HG13	1:B:266:PRO:HD2	1.87	0.56
1:B:138:PHE:CD2	1:B:140:SER:HB2	2.41	0.56
1:B:467:THR:O	1:B:469:ILE:HG13	2.06	0.56
1:B:56:PRO:O	1:B:57:LYS:C	2.44	0.56
1:B:161:ALA:HA	1:B:164:TYR:CE2	2.40	0.56
1:B:117:TYR:CD2	1:B:217:ARG:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ASP:C	1:A:439:VAL:HG23	2.26	0.55
1:A:471:LEU:HD22	1:A:527:PHE:HE1	1.71	0.55
1:B:144:VAL:HG12	1:B:145:GLY:H	1.71	0.55
1:B:399:ARG:NH2	1:B:465:LEU:HD23	2.20	0.55
1:A:269:TRP:O	1:A:270:ALA:C	2.45	0.55
1:B:176:SER:OG	1:B:495:GLU:HG3	2.05	0.55
1:A:517:VAL:HG12	1:A:518:GLY:H	1.71	0.55
1:A:105:HIS:CD2	1:A:528:VAL:HG12	2.42	0.55
1:A:398:HIS:HD2	1:A:471:LEU:CD2	2.08	0.55
1:B:125:SER:HA	1:B:575:ILE:HD11	1.88	0.55
1:A:387:MET:HG2	1:A:480:HIS:CD2	2.41	0.55
1:B:54:TYR:HD1	1:B:544:LEU:HB3	1.72	0.55
1:A:509:LYS:HB2	1:A:516:ILE:HD13	1.88	0.55
1:B:427:ARG:HG2	1:B:439:VAL:HB	1.89	0.55
1:B:398:HIS:HD2	1:B:471:LEU:HG	1.72	0.55
1:B:573:ASN:HB2	1:B:582:GLU:OE2	2.07	0.55
1:A:89:PHE:O	1:A:93:VAL:HG23	2.06	0.55
1:A:412:ASP:O	1:A:416:LEU:HB2	2.06	0.55
1:B:114:GLU:HA	1:B:219:VAL:O	2.06	0.55
1:A:405:ASP:HA	1:A:408:VAL:CG2	2.37	0.55
1:B:411:LEU:CD2	1:B:455:LEU:HD11	2.36	0.55
1:B:550:VAL:HG21	1:B:554:GLY:HA2	1.89	0.55
1:B:310:ALA:HA	1:B:327:PHE:O	2.07	0.55
1:A:79:LEU:CD2	1:A:93:VAL:HG11	2.36	0.55
1:A:433:ASN:N	1:A:439:VAL:HG23	2.22	0.54
1:B:335:TRP:HB2	1:B:348:PRO:CG	2.35	0.54
1:B:532:GLN:O	1:B:533:PHE:HB3	2.07	0.54
1:B:499:ALA:O	1:B:502:ASP:N	2.32	0.54
1:B:498:PHE:HD1	1:B:498:PHE:N	2.05	0.54
1:B:363:THR:HG21	1:B:485:TYR:CE1	2.43	0.54
1:A:307:LEU:HD21	1:A:348:PRO:HB3	1.90	0.54
1:B:450:PHE:O	1:B:454:VAL:HG23	2.08	0.54
1:B:333:TYR:C	1:B:376:GLY:HA3	2.27	0.54
1:A:387:MET:HB3	1:A:483:VAL:HG22	1.90	0.54
1:B:378:VAL:O	1:B:381:LEU:HB3	2.07	0.54
1:B:116:ALA:HB2	1:B:194:PRO:HD2	1.89	0.54
1:B:107:GLY:HA3	1:B:267:HIS:CD2	2.43	0.54
1:B:541:THR:HG22	1:B:542:CYS:N	2.24	0.53
1:B:50:LEU:HD23	1:B:544:LEU:HD13	1.90	0.53
1:A:557:ILE:HG22	1:A:559:ASN:H	1.73	0.53
1:B:452:ARG:C	1:B:454:VAL:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:THR:HG21	1:B:485:TYR:HE1	1.73	0.53
1:A:317:ASP:N	1:A:317:ASP:OD2	2.40	0.53
1:A:549:ALA:O	1:A:556:PHE:HB3	2.08	0.53
1:A:352:PHE:CD2	1:A:387:MET:HE1	2.43	0.53
1:B:187:ALA:C	1:B:189:LEU:H	2.12	0.53
1:B:297:ILE:CD1	1:B:313:SER:HB2	2.39	0.53
1:B:56:PRO:O	1:B:59:TRP:N	2.42	0.53
1:A:551:ARG:O	1:A:552:GLU:C	2.47	0.53
1:A:110:PHE:HA	1:A:538:GLY:O	2.09	0.53
1:B:77:GLN:O	1:B:79:LEU:N	2.41	0.53
1:A:395:LEU:HD21	1:A:477:ILE:HD11	1.90	0.53
1:A:150:GLU:HG2	1:A:155:PRO:HA	1.90	0.53
1:A:450:PHE:O	1:A:454:VAL:HG22	2.09	0.53
1:B:389:THR:HG21	1:B:393:LEU:CD1	2.39	0.53
1:B:333:TYR:N	1:B:375:GLY:O	2.38	0.53
1:B:204:ARG:HB2	1:B:208:THR:CG2	2.38	0.53
1:A:537:THR:HG22	1:A:537:THR:O	2.08	0.53
1:B:427:ARG:HB2	1:B:427:ARG:NH1	2.24	0.53
1:A:265:VAL:HG13	1:A:266:PRO:HD2	1.90	0.53
1:B:463:ILE:O	1:B:465:LEU:N	2.42	0.53
1:B:443:VAL:O	1:B:446:TYR:HB2	2.08	0.53
1:A:182:LEU:HD22	1:A:183:PHE:CD1	2.44	0.52
1:A:487:LYS:CB	1:A:488:PRO:HD2	2.32	0.52
1:A:416:LEU:HD23	1:A:416:LEU:O	2.09	0.52
1:B:120:TYR:N	1:B:120:TYR:CD1	2.77	0.52
1:B:179:LEU:O	1:B:182:LEU:N	2.37	0.52
1:B:433:ASN:CA	1:B:439:VAL:HG23	2.39	0.52
1:B:414:LEU:O	1:B:416:LEU:N	2.43	0.52
1:B:54:TYR:CD1	1:B:544:LEU:HB3	2.44	0.52
1:A:506:VAL:HG13	1:A:507:VAL:H	1.69	0.52
1:B:494:ASN:HD22	1:B:494:ASN:C	2.12	0.52
1:A:480:HIS:HB3	1:A:483:VAL:O	2.09	0.52
1:A:180:ARG:HB3	1:A:180:ARG:CZ	2.40	0.52
1:A:541:THR:CG2	1:A:542:CYS:N	2.72	0.52
1:B:119:PRO:CB	1:B:137:THR:H	2.16	0.52
1:A:144:VAL:CG1	1:A:145:GLY:H	2.15	0.52
1:B:327:PHE:C	1:B:327:PHE:HD2	2.13	0.52
1:B:379:LEU:O	1:B:382:TYR:HB2	2.09	0.52
1:A:399:ARG:HG3	1:A:399:ARG:NH1	2.25	0.52
1:A:108:VAL:HG12	1:A:109:THR:N	2.24	0.52
1:A:161:ALA:HA	1:A:164:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:O	1:B:159:VAL:N	2.43	0.52
1:B:505:PRO:HG2	1:B:506:VAL:H	1.75	0.52
1:B:265:VAL:CG1	1:B:266:PRO:HD2	2.39	0.52
1:B:276:TYR:HE1	1:B:286:ASN:HB3	1.74	0.52
1:B:180:ARG:HH11	1:B:180:ARG:HB2	1.72	0.52
1:B:39:ALA:HB1	1:B:79:LEU:HD22	1.92	0.52
1:A:50:LEU:HD12	1:A:68:LEU:CD1	2.40	0.52
1:B:403:THR:O	1:B:405:ASP:N	2.43	0.52
1:B:56:PRO:CD	1:B:545:THR:HB	2.40	0.51
1:B:379:LEU:O	1:B:380:TYR:C	2.49	0.51
1:A:509:LYS:HG2	1:A:509:LYS:O	2.10	0.51
1:B:601:ILE:HG22	1:B:602:ILE:N	2.25	0.51
1:B:272:LEU:O	1:B:275:HIS:N	2.39	0.51
1:A:297:ILE:CD1	1:A:325:VAL:HG11	2.40	0.51
1:B:43:LEU:O	1:B:46:LEU:N	2.39	0.51
1:B:148:LEU:HD11	1:B:200:LEU:HD22	1.91	0.51
1:A:439:VAL:HG12	1:A:440:ASP:N	2.26	0.51
1:B:327:PHE:C	1:B:327:PHE:CD2	2.83	0.51
1:B:502:ASP:OD2	1:B:523:GLY:O	2.29	0.51
1:A:597:ASN:O	1:A:598:ASP:HB2	2.10	0.51
1:B:541:THR:CG2	1:B:542:CYS:N	2.72	0.51
1:A:451:GLY:O	1:A:454:VAL:CG2	2.57	0.51
1:B:334:SER:HB3	1:B:376:GLY:HA2	1.93	0.51
1:B:516:ILE:N	1:B:565:HIS:HD2	2.08	0.51
1:B:279:SER:O	1:B:280:GLY:C	2.48	0.51
1:B:50:LEU:HD13	1:B:66:TRP:HH2	1.76	0.50
1:A:59:TRP:CZ2	1:A:557:ILE:CB	2.94	0.50
1:A:406:GLU:N	1:A:406:GLU:OE2	2.44	0.50
1:A:402:LEU:HD21	1:A:454:VAL:HG12	1.92	0.50
1:B:381:LEU:HD13	1:B:385:LEU:HD12	1.92	0.50
1:B:264:MET:HE2	1:B:526:GLY:H	1.75	0.50
1:B:311:TYR:OH	1:B:327:PHE:HD1	1.92	0.50
1:B:470:PRO:HG2	1:B:473:GLY:HA2	1.93	0.50
1:B:56:PRO:HB2	1:B:60:LYS:HG2	1.94	0.50
1:A:132:PHE:HE1	1:A:148:LEU:HB2	1.76	0.50
1:A:494:ASN:H	1:A:494:ASN:HD22	1.57	0.50
1:A:297:ILE:HD11	1:A:325:VAL:HG12	1.92	0.50
1:B:450:PHE:C	1:B:452:ARG:N	2.64	0.50
1:B:398:HIS:HE2	1:B:503:PHE:HZ	1.59	0.50
1:A:98:ILE:C	1:A:100:GLY:H	2.15	0.50
1:A:398:HIS:CE1	1:A:549:ALA:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:TYR:C	1:A:376:GLY:HA3	2.31	0.50
1:B:328:LEU:HD22	1:B:329:ARG:N	2.27	0.50
1:A:113:ILE:O	1:A:114:GLU:C	2.50	0.50
1:A:516:ILE:CD1	1:A:516:ILE:H	2.23	0.50
1:B:143:ARG:NE	1:B:204:ARG:HH11	2.10	0.50
1:A:417:LEU:O	1:A:417:LEU:HD12	2.12	0.50
1:B:176:SER:O	1:B:179:LEU:HB2	2.12	0.50
1:B:311:TYR:CD1	1:B:311:TYR:C	2.85	0.50
1:A:427:ARG:O	1:A:431:GLY:O	2.29	0.49
1:B:161:ALA:C	1:B:163:LEU:H	2.16	0.49
1:B:144:VAL:CG1	1:B:145:GLY:N	2.74	0.49
1:B:186:MET:H	1:B:191:HIS:HD2	1.58	0.49
1:A:40:LEU:HD21	1:A:76:GLN:HG2	1.94	0.49
1:A:218:TYR:CG	1:A:219:VAL:N	2.80	0.49
1:A:441:LEU:C	1:A:441:LEU:HD13	2.33	0.49
1:A:366:LEU:HB2	1:A:485:TYR:CZ	2.47	0.49
1:A:444:ALA:O	1:A:448:LYS:HG3	2.13	0.49
1:B:450:PHE:O	1:B:452:ARG:N	2.45	0.49
1:B:333:TYR:OH	1:B:504:PHE:CG	2.65	0.49
1:A:265:VAL:CG1	1:A:266:PRO:HD2	2.42	0.49
1:A:390:ASP:HA	1:A:484:GLN:OE1	2.13	0.49
1:A:504:PHE:HB3	1:A:505:PRO:HD3	1.94	0.49
1:A:185:ARG:NH1	1:A:185:ARG:HG3	2.27	0.49
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.78	0.49
1:B:551:ARG:CB	1:B:555:ALA:HB3	2.37	0.49
1:A:339:GLU:O	1:A:340:ASP:HB2	2.12	0.49
1:B:50:LEU:HD13	1:B:66:TRP:CH2	2.48	0.49
1:B:118:LEU:HD21	1:B:216:TRP:HA	1.95	0.49
1:B:42:ASP:O	1:B:43:LEU:O	2.30	0.49
1:B:366:LEU:HD22	1:B:368:ILE:HD12	1.94	0.49
1:B:82:GLN:HG3	1:B:89:PHE:HE2	1.71	0.49
1:B:293:PHE:HZ	1:B:570:PHE:CE1	2.30	0.49
1:B:494:ASN:ND2	1:B:494:ASN:C	2.64	0.49
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.95	0.49
1:A:470:PRO:O	1:A:472:PHE:O	2.31	0.48
1:B:414:LEU:C	1:B:416:LEU:N	2.65	0.48
1:A:439:VAL:O	1:A:440:ASP:HB2	2.12	0.48
1:A:498:PHE:N	1:A:498:PHE:CD1	2.81	0.48
1:B:571:THR:O	1:B:574:ASP:HB2	2.13	0.48
1:B:463:ILE:HG13	1:B:464:GLU:N	2.27	0.48
1:A:76:GLN:O	1:A:77:GLN:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:C	1:B:368:ILE:HD12	2.33	0.48
1:B:269:TRP:O	1:B:270:ALA:C	2.50	0.48
1:B:403:THR:O	1:B:407:VAL:HG23	2.12	0.48
1:A:440:ASP:O	1:A:441:LEU:C	2.52	0.48
1:A:373:ASN:OD1	1:A:374:PRO:HD2	2.13	0.48
1:A:43:LEU:HD11	1:A:75:ALA:HB3	1.96	0.48
1:A:118:LEU:HG	1:A:216:TRP:CZ3	2.48	0.48
1:B:463:ILE:C	1:B:465:LEU:N	2.67	0.48
1:B:76:GLN:O	1:B:77:GLN:O	2.32	0.48
1:B:328:LEU:O	1:B:368:ILE:HA	2.13	0.48
1:B:568:LEU:HD22	1:B:583:TYR:HD1	1.77	0.48
1:A:556:PHE:HD2	1:A:556:PHE:C	2.16	0.48
1:B:179:LEU:O	1:B:180:ARG:C	2.51	0.48
1:B:463:ILE:C	1:B:465:LEU:H	2.16	0.48
1:B:352:PHE:CG	1:B:384:LEU:HD22	2.48	0.48
1:B:114:GLU:O	1:B:193:VAL:HG21	2.13	0.48
1:B:276:TYR:CE1	1:B:286:ASN:HB3	2.48	0.48
1:B:509:LYS:C	1:B:511:ASN:H	2.16	0.48
1:B:434:MET:O	1:B:435:GLU:C	2.52	0.48
1:A:280:GLY:O	1:A:281:LEU:C	2.52	0.48
1:B:143:ARG:NH2	1:B:204:ARG:NH1	2.62	0.48
1:B:499:ALA:HA	1:B:525:GLY:HA2	1.95	0.48
1:A:352:PHE:HD2	1:A:387:MET:HE2	1.69	0.48
1:B:430:LEU:HB2	1:B:439:VAL:HG11	1.96	0.48
1:B:327:PHE:HD2	1:B:328:LEU:N	2.11	0.47
1:B:89:PHE:O	1:B:92:GLN:HB2	2.14	0.47
1:A:387:MET:SD	1:A:480:HIS:HD2	2.37	0.47
1:A:487:LYS:HB3	1:A:488:PRO:CD	2.32	0.47
1:B:164:TYR:CE1	1:B:168:HIS:NE2	2.82	0.47
1:B:264:MET:SD	1:B:378:VAL:HG22	2.54	0.47
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.79	0.47
1:B:535:ASN:HD21	1:B:539:ILE:HB	1.78	0.47
1:A:372:ASN:H	1:A:494:ASN:HD21	1.62	0.47
1:A:457:CYS:SG	1:A:466:SER:HB2	2.54	0.47
1:B:368:ILE:CD1	1:B:489:ILE:HG23	2.44	0.47
1:A:493:ILE:HD13	1:A:516:ILE:CG2	2.45	0.47
1:B:122:VAL:HG12	1:B:123:GLN:H	1.79	0.47
1:A:601:ILE:HG22	1:A:602:ILE:N	2.29	0.47
1:B:259:LEU:O	1:B:527:PHE:CD2	2.68	0.47
1:A:586:LYS:O	1:A:590:LEU:HD12	2.14	0.47
1:B:114:GLU:HG2	1:B:193:VAL:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:HA	1:B:373:ASN:OD1	2.13	0.47
1:A:381:LEU:HD13	1:A:381:LEU:C	2.35	0.47
1:B:164:TYR:CD1	1:B:168:HIS:CD2	3.03	0.47
1:B:503:PHE:O	1:B:506:VAL:HG13	2.14	0.47
1:A:276:TYR:O	1:A:277:ALA:C	2.51	0.47
1:A:122:VAL:HG12	1:A:123:GLN:H	1.79	0.47
1:B:114:GLU:HG2	1:B:193:VAL:HG21	1.97	0.47
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.49	0.47
1:A:202:ILE:HG13	1:A:202:ILE:O	2.15	0.47
1:A:558:GLU:O	1:A:559:ASN:HB2	2.14	0.47
1:A:441:LEU:HD13	1:A:441:LEU:O	2.15	0.47
1:B:140:SER:OG	1:B:141:GLU:N	2.47	0.47
1:B:312:ILE:HG23	1:B:325:VAL:O	2.15	0.47
1:A:433:ASN:HD22	1:A:436:GLY:H	1.61	0.47
1:A:381:LEU:HD13	1:A:382:TYR:N	2.30	0.47
1:A:144:VAL:CG1	1:A:145:GLY:N	2.74	0.47
1:A:267:HIS:O	1:A:268:PHE:C	2.53	0.47
1:A:136:MET:SD	1:A:136:MET:N	2.88	0.47
1:A:503:PHE:O	1:A:507:VAL:HG23	2.15	0.47
1:B:505:PRO:O	1:B:506:VAL:C	2.53	0.47
1:B:503:PHE:O	1:B:506:VAL:CG1	2.62	0.47
1:B:143:ARG:HE	1:B:204:ARG:HH11	1.62	0.47
1:B:437:TYR:CE2	1:B:474:PHE:HE2	2.33	0.47
1:A:42:ASP:CG	1:A:535:ASN:HB2	2.35	0.46
1:A:176:SER:O	1:A:177:ALA:C	2.53	0.46
1:A:214:VAL:HG12	1:A:215:LYS:N	2.31	0.46
1:B:302:TRP:O	1:B:311:TYR:HB2	2.15	0.46
1:B:452:ARG:C	1:B:454:VAL:H	2.19	0.46
1:B:446:TYR:CE2	1:B:475:GLU:N	2.78	0.46
1:A:260:PHE:HA	1:A:527:PHE:CD2	2.50	0.46
1:A:182:LEU:HD22	1:A:183:PHE:CE1	2.49	0.46
1:B:444:ALA:O	1:B:448:LYS:HG3	2.15	0.46
1:B:401:ILE:O	1:B:401:ILE:HG22	2.15	0.46
1:B:441:LEU:HD23	1:B:441:LEU:C	2.35	0.46
1:A:302:TRP:CZ2	1:A:358:VAL:HG11	2.50	0.46
1:B:483:VAL:HG23	1:B:483:VAL:O	2.15	0.46
1:A:287:ILE:N	1:A:287:ILE:HD12	2.31	0.46
1:A:550:VAL:HG12	1:A:554:GLY:CA	2.22	0.46
1:B:60:LYS:HG3	1:B:101:LEU:HD22	1.98	0.46
1:A:373:ASN:HB3	1:A:501:ALA:HB2	1.96	0.46
1:A:457:CYS:CB	1:A:466:SER:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:O	1:A:55:ALA:C	2.54	0.46
1:A:602:ILE:CG2	1:A:603:LEU:H	2.29	0.46
1:B:264:MET:HE2	1:B:526:GLY:N	2.31	0.46
1:B:570:PHE:HE2	1:B:583:TYR:CD2	2.33	0.46
1:B:368:ILE:HD12	1:B:368:ILE:N	2.30	0.46
1:B:382:TYR:O	1:B:385:LEU:HB2	2.16	0.46
1:B:55:ALA:CB	1:B:56:PRO:CD	2.94	0.46
1:A:427:ARG:HA	1:A:439:VAL:CG1	2.35	0.46
1:A:402:LEU:N	1:A:402:LEU:CD1	2.79	0.46
1:A:317:ASP:HB2	1:A:318:GLY:H	1.58	0.46
1:A:94:LEU:O	1:A:95:ALA:C	2.54	0.46
1:B:503:PHE:O	1:B:504:PHE:C	2.53	0.46
1:B:204:ARG:CG	1:B:208:THR:HG23	2.46	0.46
1:B:137:THR:O	1:B:137:THR:CG2	2.64	0.45
1:B:506:VAL:HG13	1:B:507:VAL:H	1.82	0.45
1:B:601:ILE:H	1:B:601:ILE:HD12	1.82	0.45
1:A:467:THR:OG1	1:A:468:PRO:HD2	2.17	0.45
1:A:333:TYR:CE1	1:A:373:ASN:ND2	2.84	0.45
1:A:387:MET:CG	1:A:480:HIS:HD2	2.27	0.45
1:B:91:GLN:HA	1:B:110:PHE:CE2	2.51	0.45
1:B:117:TYR:CD2	1:B:217:ARG:CB	2.99	0.45
1:B:389:THR:CG2	1:B:393:LEU:HD11	2.43	0.45
1:A:100:GLY:C	1:A:102:ASN:N	2.69	0.45
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.77	0.45
1:A:54:TYR:O	1:A:54:TYR:CG	2.69	0.45
1:A:423:ASN:HA	1:A:441:LEU:HB2	1.98	0.45
1:B:118:LEU:HG	1:B:216:TRP:CZ3	2.51	0.45
1:B:143:ARG:NE	1:B:204:ARG:NH1	2.64	0.45
1:B:446:TYR:CD2	1:B:474:PHE:HA	2.52	0.45
1:B:293:PHE:HZ	1:B:570:PHE:HE1	1.64	0.45
1:B:59:TRP:C	1:B:61:GLU:N	2.69	0.45
1:A:407:VAL:HG12	1:A:411:LEU:HD11	1.98	0.45
1:B:76:GLN:O	1:B:77:GLN:C	2.54	0.45
1:A:102:ASN:HA	1:A:102:ASN:HD22	1.57	0.45
1:A:83:GLU:O	1:A:84:ASN:C	2.54	0.45
1:B:82:GLN:CG	1:B:89:PHE:HE2	2.28	0.45
1:B:506:VAL:HG13	1:B:507:VAL:N	2.32	0.45
1:B:55:ALA:HB3	1:B:56:PRO:HD3	1.97	0.45
1:A:403:THR:O	1:A:406:GLU:OE2	2.35	0.45
1:B:516:ILE:N	1:B:516:ILE:HD12	2.31	0.45
1:A:132:PHE:CE2	1:A:142:ILE:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:CD1	1:A:142:ILE:O	2.64	0.45
1:B:180:ARG:NH1	1:B:268:PHE:CZ	2.85	0.45
1:A:118:LEU:CD2	1:A:216:TRP:HA	2.47	0.45
1:A:443:VAL:O	1:A:446:TYR:HB2	2.17	0.45
1:A:395:LEU:HB2	1:A:475:GLU:O	2.17	0.45
1:A:197:ARG:HB3	1:A:213:ARG:HE	1.81	0.45
1:A:506:VAL:HB	1:A:562:VAL:CG2	2.43	0.45
1:A:410:ALA:HB2	1:A:454:VAL:HG21	1.98	0.45
1:A:136:MET:CE	1:A:281:LEU:HA	2.47	0.45
1:B:602:ILE:CG2	1:B:603:LEU:N	2.80	0.45
1:A:82:GLN:C	1:A:83:GLU:O	2.55	0.45
1:A:556:PHE:CD2	1:A:556:PHE:O	2.70	0.44
1:B:134:ASP:OD2	1:B:283:SER:HB2	2.18	0.44
1:B:366:LEU:HD22	1:B:368:ILE:CD1	2.47	0.44
1:A:410:ALA:CB	1:A:454:VAL:HG21	2.47	0.44
1:B:185:ARG:NH1	1:B:185:ARG:HG3	2.32	0.44
1:A:413:TRP:HA	1:A:413:TRP:CE3	2.53	0.44
1:A:427:ARG:CA	1:A:439:VAL:HG11	2.36	0.44
1:A:135:ILE:HD11	1:A:142:ILE:CG2	2.43	0.44
1:B:493:ILE:O	1:B:518:GLY:HA3	2.18	0.44
1:A:333:TYR:HB2	1:A:375:GLY:O	2.17	0.44
1:B:143:ARG:NH2	1:B:204:ARG:HH11	2.15	0.44
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.63	0.44
1:A:88:SER:O	1:A:91:GLN:HB2	2.17	0.44
1:B:302:TRP:CH2	1:B:304:SER:HB2	2.53	0.44
1:B:176:SER:O	1:B:179:LEU:N	2.50	0.44
1:A:539:ILE:H	1:A:539:ILE:HD12	1.82	0.44
1:B:186:MET:O	1:B:191:HIS:HB2	2.17	0.44
1:B:152:ASP:O	1:B:154:ALA:N	2.50	0.44
1:B:117:TYR:HD2	1:B:217:ARG:CB	2.31	0.44
1:A:603:LEU:HD23	1:A:603:LEU:O	2.17	0.44
1:B:568:LEU:HD22	1:B:583:TYR:CD1	2.52	0.44
1:A:498:PHE:O	1:A:501:ALA:HB3	2.17	0.44
1:B:550:VAL:HG23	1:B:551:ARG:N	2.30	0.44
1:A:297:ILE:HD11	1:A:325:VAL:HG11	1.97	0.44
1:A:151:VAL:HG12	1:A:152:ASP:OD2	2.18	0.44
1:A:539:ILE:N	1:A:539:ILE:HD12	2.32	0.44
1:B:108:VAL:CG1	1:B:109:THR:N	2.80	0.44
1:B:127:ASP:OD1	1:B:129:ARG:NH2	2.46	0.44
1:A:133:VAL:HB	1:A:285:TYR:CZ	2.53	0.44
1:A:276:TYR:CZ	1:A:286:ASN:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:VAL:O	1:A:358:VAL:CG1	2.66	0.44
1:A:49:LEU:HD11	1:A:531:VAL:HG11	2.00	0.44
1:A:574:ASP:HB3	1:A:580:TYR:HA	2.00	0.44
1:B:563:GLU:O	1:B:563:GLU:HG2	2.17	0.44
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.82	0.43
1:B:118:LEU:HA	1:B:119:PRO:HD2	1.76	0.43
1:A:373:ASN:HB3	1:A:501:ALA:CB	2.48	0.43
1:B:107:GLY:HA3	1:B:267:HIS:NE2	2.33	0.43
1:B:267:HIS:O	1:B:268:PHE:C	2.56	0.43
1:B:94:LEU:CD1	1:B:537:THR:HG21	2.48	0.43
1:A:533:PHE:C	1:A:533:PHE:CD1	2.91	0.43
1:B:168:HIS:NE2	1:B:170:GLY:HA2	2.33	0.43
1:A:503:PHE:C	1:A:506:VAL:HG12	2.39	0.43
1:B:77:GLN:O	1:B:78:LYS:C	2.57	0.43
1:A:50:LEU:HD21	1:A:98:ILE:CD1	2.48	0.43
1:B:111:PHE:CE2	1:B:540:LYS:CB	3.00	0.43
1:B:42:ASP:O	1:B:43:LEU:C	2.55	0.43
1:B:531:VAL:HG12	1:B:531:VAL:O	2.18	0.43
1:B:411:LEU:HD21	1:B:455:LEU:HD11	2.00	0.43
1:B:392:PRO:HA	1:B:477:ILE:O	2.18	0.43
1:A:591:VAL:O	1:A:595:ILE:HG12	2.17	0.43
1:A:122:VAL:CG1	1:A:123:GLN:N	2.78	0.43
1:A:511:ASN:O	1:A:512:ASP:HB2	2.19	0.43
1:B:138:PHE:HB3	1:B:139:SER:H	1.16	0.43
1:A:164:TYR:HB3	1:A:168:HIS:CD2	2.54	0.43
1:A:443:VAL:O	1:A:446:TYR:N	2.46	0.43
1:B:136:MET:HE2	1:B:281:LEU:C	2.39	0.43
1:A:498:PHE:O	1:A:501:ALA:N	2.51	0.43
1:B:116:ALA:CB	1:B:194:PRO:HD2	2.48	0.43
1:B:334:SER:O	1:B:336:GLN:N	2.52	0.43
1:A:138:PHE:O	1:A:139:SER:O	2.36	0.43
1:A:471:LEU:HD22	1:A:527:PHE:CE1	2.53	0.43
1:A:480:HIS:O	1:A:482:ARG:N	2.52	0.43
1:A:416:LEU:HD23	1:A:416:LEU:C	2.39	0.43
1:B:113:ILE:O	1:B:114:GLU:C	2.56	0.43
1:A:152:ASP:H	1:A:199:THR:HB	1.83	0.43
1:B:579:GLY:O	1:B:580:TYR:C	2.57	0.43
1:A:209:THR:O	1:A:210:ARG:HD3	2.17	0.43
1:B:420:VAL:HG13	1:B:425:GLU:HB3	2.00	0.43
1:B:516:ILE:HG22	1:B:564:PRO:HA	2.00	0.43
1:A:279:SER:O	1:A:280:GLY:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:PHE:HB3	1:B:505:PRO:CD	2.49	0.43
1:B:370:GLN:HB3	1:B:370:GLN:HE21	1.52	0.43
1:A:314:SER:HA	1:A:323:HIS:O	2.19	0.43
1:B:422:THR:O	1:B:423:ASN:C	2.57	0.43
1:B:380:TYR:O	1:B:383:ALA:HB3	2.19	0.43
1:A:352:PHE:CD2	1:A:384:LEU:HD22	2.54	0.43
1:A:160:LEU:O	1:A:163:LEU:N	2.50	0.43
1:B:416:LEU:O	1:B:417:LEU:HD23	2.19	0.43
1:A:260:PHE:HA	1:A:527:PHE:CE2	2.54	0.43
1:A:495:GLU:HG2	1:A:496:GLN:HG3	2.00	0.43
1:B:352:PHE:O	1:B:356:ILE:HG12	2.19	0.43
1:A:155:PRO:O	1:A:156:VAL:C	2.57	0.43
1:A:411:LEU:HD13	1:B:411:LEU:CD1	2.49	0.43
1:A:180:ARG:CD	1:A:496:GLN:HE21	2.23	0.43
1:B:296:VAL:HA	1:B:311:TYR:OH	2.19	0.43
1:A:592:CYS:HA	1:A:595:ILE:HG13	2.00	0.43
1:A:395:LEU:HG	1:A:476:LYS:HA	2.01	0.43
1:A:94:LEU:O	1:A:97:PHE:HB3	2.18	0.43
1:A:328:LEU:HD22	1:A:328:LEU:C	2.38	0.42
1:B:108:VAL:CG1	1:B:109:THR:H	2.32	0.42
1:A:371:THR:O	1:A:372:ASN:HB2	2.19	0.42
1:A:198:THR:O	1:A:213:ARG:HA	2.19	0.42
1:A:403:THR:N	1:A:406:GLU:OE2	2.47	0.42
1:A:492:LEU:N	1:A:492:LEU:CD2	2.82	0.42
1:A:87:THR:O	1:A:88:SER:C	2.57	0.42
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.59	0.42
1:A:492:LEU:HD23	1:A:492:LEU:N	2.34	0.42
1:A:315:VAL:HG11	1:A:588:LYS:HD2	2.01	0.42
1:B:48:HIS:CE1	1:B:52:VAL:HG21	2.55	0.42
1:A:467:THR:O	1:A:469:ILE:HG13	2.18	0.42
1:A:398:HIS:ND1	1:A:549:ALA:HA	2.35	0.42
1:A:399:ARG:NH2	1:A:465:LEU:HD23	2.34	0.42
1:B:155:PRO:O	1:B:156:VAL:C	2.58	0.42
1:A:171:THR:OG1	1:A:174:GLU:HG3	2.19	0.42
1:B:124:LYS:HG2	1:B:125:SER:O	2.19	0.42
1:A:65:GLY:O	1:A:66:TRP:C	2.58	0.42
1:A:264:MET:HE2	1:A:264:MET:HB2	1.80	0.42
1:A:466:SER:O	1:A:467:THR:C	2.58	0.42
1:A:523:GLY:O	1:A:524:ALA:O	2.37	0.42
1:B:551:ARG:HD2	1:B:552:GLU:HG3	2.01	0.42
1:B:471:LEU:O	1:B:472:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:O	1:B:76:GLN:N	2.53	0.42
1:A:212:VAL:HG12	1:A:213:ARG:N	2.35	0.42
1:B:458:TRP:O	1:B:458:TRP:CG	2.73	0.42
1:A:385:LEU:HD21	1:A:504:PHE:CD1	2.54	0.42
1:A:76:GLN:OE1	1:A:80:ARG:NH1	2.53	0.42
1:A:601:ILE:N	1:A:601:ILE:HD12	2.35	0.42
1:B:601:ILE:H	1:B:601:ILE:CD1	2.32	0.42
1:A:403:THR:O	1:A:407:VAL:HG23	2.19	0.41
1:B:489:ILE:HG22	1:B:490:CYS:N	2.34	0.41
1:A:136:MET:HG2	1:A:281:LEU:HD23	2.01	0.41
1:A:493:ILE:HD13	1:A:516:ILE:HG21	2.01	0.41
1:B:399:ARG:NE	1:B:465:LEU:HG	2.35	0.41
1:B:601:ILE:N	1:B:601:ILE:CD1	2.81	0.41
1:B:186:MET:CE	1:B:275:HIS:HB2	2.50	0.41
1:B:122:VAL:CG1	1:B:123:GLN:N	2.82	0.41
1:A:349:TRP:HB3	1:A:380:TYR:HE1	1.84	0.41
1:B:427:ARG:HG3	1:B:439:VAL:O	2.20	0.41
1:B:75:ALA:O	1:B:79:LEU:HD12	2.20	0.41
1:A:579:GLY:O	1:A:581:SER:N	2.53	0.41
1:A:462:ASP:C	1:A:464:GLU:N	2.73	0.41
1:A:533:PHE:O	1:A:533:PHE:CD1	2.74	0.41
1:A:138:PHE:O	1:A:139:SER:C	2.58	0.41
1:A:55:ALA:HB3	1:A:56:PRO:HD3	2.03	0.41
1:A:446:TYR:HB3	1:A:473:GLY:HA3	2.02	0.41
1:B:515:LEU:HA	1:B:565:HIS:CD2	2.56	0.41
1:B:382:TYR:O	1:B:383:ALA:C	2.59	0.41
1:B:416:LEU:HD21	1:B:429:ALA:HB1	2.02	0.41
1:A:358:VAL:O	1:A:358:VAL:HG12	2.20	0.41
1:A:197:ARG:HD3	1:A:213:ARG:HG2	2.02	0.41
1:B:489:ILE:CG2	1:B:490:CYS:N	2.83	0.41
1:B:452:ARG:O	1:B:453:GLN:C	2.57	0.41
1:A:464:GLU:O	1:A:465:LEU:CB	2.68	0.41
1:B:568:LEU:CD2	1:B:583:TYR:HD1	2.33	0.41
1:A:83:GLU:O	1:A:85:PRO:N	2.53	0.41
1:A:54:TYR:CE1	1:A:56:PRO:CG	3.03	0.41
1:A:529:PHE:HB2	1:A:544:LEU:O	2.20	0.41
1:B:499:ALA:O	1:B:500:CYS:C	2.59	0.41
1:B:73:VAL:O	1:B:74:SER:C	2.59	0.41
1:B:516:ILE:N	1:B:565:HIS:CD2	2.72	0.41
1:B:450:PHE:C	1:B:452:ARG:H	2.23	0.41
1:B:94:LEU:HD12	1:B:537:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ALA:HA	1:A:387:MET:HE3	2.03	0.41
1:A:204:ARG:HB2	1:A:208:THR:HG23	2.02	0.41
1:A:399:ARG:HB3	1:A:465:LEU:HG	2.01	0.41
1:B:45:PHE:C	1:B:45:PHE:CD2	2.94	0.41
1:B:152:ASP:C	1:B:154:ALA:N	2.73	0.41
1:A:498:PHE:O	1:A:499:ALA:C	2.59	0.41
1:A:307:LEU:HD23	1:A:348:PRO:HB3	2.02	0.41
1:B:59:TRP:CH2	1:B:557:ILE:O	2.73	0.41
1:A:260:PHE:O	1:A:262:SER:N	2.49	0.41
1:A:57:LYS:O	1:A:58:THR:C	2.58	0.41
1:B:516:ILE:HG22	1:B:564:PRO:CB	2.50	0.41
1:A:177:ALA:O	1:A:178:ALA:C	2.58	0.41
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.78	0.41
1:B:571:THR:HG21	1:B:582:GLU:OE1	2.21	0.41
1:B:139:SER:O	1:B:140:SER:O	2.39	0.41
1:B:218:TYR:CG	1:B:219:VAL:N	2.89	0.41
1:B:297:ILE:HD12	1:B:298:GLY:N	2.36	0.41
1:B:136:MET:HE1	1:B:281:LEU:HD23	2.01	0.41
1:A:447:LEU:O	1:A:450:PHE:HB3	2.21	0.41
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.88	0.41
1:B:204:ARG:CB	1:B:208:THR:HG23	2.50	0.41
1:B:271:GLU:O	1:B:272:LEU:C	2.59	0.41
1:A:269:TRP:O	1:A:271:GLU:N	2.53	0.41
1:A:395:LEU:HD21	1:A:477:ILE:CD1	2.50	0.41
1:A:149:LEU:HB2	1:A:201:LYS:O	2.21	0.41
1:A:523:GLY:CA	1:A:560:ILE:CG2	2.92	0.40
1:A:454:VAL:C	1:A:455:LEU:HD23	2.42	0.40
1:B:417:LEU:HB3	1:B:448:LYS:HD2	2.02	0.40
1:B:123:GLN:NE2	1:B:285:TYR:HE2	2.19	0.40
1:A:112:ALA:O	1:A:113:ILE:HD13	2.20	0.40
1:A:188:SER:HB3	1:A:271:GLU:OE2	2.21	0.40
1:A:417:LEU:CD1	1:A:448:LYS:HG2	2.52	0.40
1:A:54:TYR:CE2	1:A:101:LEU:HD13	2.56	0.40
1:B:114:GLU:HG2	1:B:193:VAL:HB	2.04	0.40
1:A:55:ALA:O	1:A:57:LYS:N	2.55	0.40
1:A:439:VAL:HG12	1:A:440:ASP:H	1.86	0.40
1:B:136:MET:CE	1:B:283:SER:H	2.27	0.40
1:A:180:ARG:CB	1:A:180:ARG:CZ	2.99	0.40
1:B:501:ALA:O	1:B:505:PRO:CD	2.68	0.40
1:B:39:ALA:CB	1:B:79:LEU:HD22	2.51	0.40
1:A:265:VAL:HG12	1:A:266:PRO:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:HIS:CE1	1:B:482:ARG:HB2	2.56	0.40
1:B:54:TYR:CE1	1:B:56:PRO:CG	3.02	0.40
1:A:333:TYR:CD2	1:A:381:LEU:HB2	2.56	0.40
1:A:98:ILE:C	1:A:100:GLY:N	2.75	0.40
1:A:186:MET:CE	1:A:275:HIS:HB2	2.51	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	533/583 (91%)	397 (74%)	90 (17%)	46 (9%)	1	7
1	B	533/583 (91%)	404 (76%)	88 (16%)	41 (8%)	1	9
All	All	1066/1166 (91%)	801 (75%)	178 (17%)	87 (8%)	1	8

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	136	MET
1	A	139	SER
1	A	261	TYR
1	A	268	PHE
1	A	283	SER
1	A	317	ASP
1	A	524	ALA
1	A	552	GLU
1	A	559	ASN
1	B	43	LEU
1	B	44	SER
1	B	57	LYS

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Mol	Chain	Res	Type
1	B	77	GLN
1	B	114	GLU
1	B	140	SER
1	B	259	LEU
1	B	268	PHE
1	B	335	TRP
1	B	453	GLN
1	B	465	LEU
1	B	552	GLU
1	B	555	ALA
1	B	556	PHE
1	B	557	ILE
1	B	596	ASN
1	B	598	ASP
1	B	601	ILE
1	A	59	TRP
1	A	66	TRP
1	A	83	GLU
1	A	276	TYR
1	A	280	GLY
1	A	281	LEU
1	A	331	PRO
1	A	404	GLN
1	A	465	LEU
1	A	521	THR
1	A	557	ILE
1	A	580	TYR
1	A	596	ASN
1	A	598	ASP
1	B	62	GLN
1	B	78	LYS
1	B	156	VAL
1	B	281	LEU
1	B	404	GLN
1	B	415	THR
1	B	578	LYS
1	A	144	VAL
1	A	270	ALA
1	A	343	PRO
1	A	405	ASP
1	A	440	ASP
1	A	556	PHE

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Mol	Chain	Res	Type
1	A	560	ILE
1	B	34	LEU
1	B	119	PRO
1	B	188	SER
1	B	283	SER
1	B	464	GLU
1	A	99	GLY
1	A	145	GLY
1	B	207	GLY
1	B	510	ASP
1	A	55	ALA
1	A	204	ARG
1	A	460	LYS
1	A	499	ALA
1	A	572	ALA
1	A	601	ILE
1	B	52	VAL
1	B	55	ALA
1	B	144	VAL
1	B	427	ARG
1	B	505	PRO
1	A	77	GLN
1	A	164	TYR
1	A	504	PHE
1	A	56	PRO
1	A	481	PRO
1	B	69	VAL
1	B	454	VAL
1	B	506	VAL
1	B	408	VAL
1	A	348	PRO
1	A	374	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	463/505 (92%)	418 (90%)	45 (10%)	10	38
1	B	463/505 (92%)	410 (89%)	53 (11%)	7	29
All	All	926/1010 (92%)	828 (89%)	98 (11%)	8	33

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	43	LEU
1	A	45	PHE
1	A	68	LEU
1	A	70	GLN
1	A	84	ASN
1	A	86	SER
1	A	102	ASN
1	A	117	TYR
1	A	136	MET
1	A	138	PHE
1	A	139	SER
1	A	162	THR
1	A	208	THR
1	A	268	PHE
1	A	269	TRP
1	A	272	LEU
1	A	290	THR
1	A	300	VAL
1	A	315	VAL
1	A	317	ASP
1	A	325	VAL
1	A	328	LEU
1	A	366	LEU
1	A	370	GLN
1	A	381	LEU
1	A	421	ASP
1	A	438	THR
1	A	446	TYR
1	A	454	VAL
1	A	459	SER
1	A	465	LEU
1	A	474	PHE
1	A	483	VAL
1	A	492	LEU

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Mol	Chain	Res	Type
1	A	494	ASN
1	A	498	PHE
1	A	503	PHE
1	A	513	ARG
1	A	519	THR
1	A	536	ARG
1	A	548	LEU
1	A	550	VAL
1	A	552	GLU
1	A	556	PHE
1	B	41	GLN
1	B	43	LEU
1	B	45	PHE
1	B	59	TRP
1	B	70	GLN
1	B	84	ASN
1	B	96	ASP
1	B	102	ASN
1	B	110	PHE
1	B	113	ILE
1	B	136	MET
1	B	137	THR
1	B	138	PHE
1	B	142	ILE
1	B	143	ARG
1	B	182	LEU
1	B	184	SER
1	B	189	LEU
1	B	268	PHE
1	B	269	TRP
1	B	281	LEU
1	B	283	SER
1	B	290	THR
1	B	291	ASP
1	B	300	VAL
1	B	327	PHE
1	B	363	THR
1	B	366	LEU
1	B	370	GLN
1	B	381	LEU
1	B	400	MET
1	B	404	GLN

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Mol	Chain	Res	Type
1	B	405	ASP
1	B	406	GLU
1	B	409	ASP
1	B	447	LEU
1	B	458	TRP
1	B	494	ASN
1	B	498	PHE
1	B	503	PHE
1	B	513	ARG
1	B	515	LEU
1	B	529	PHE
1	B	532	GLN
1	B	543	SER
1	B	550	VAL
1	B	551	ARG
1	B	552	GLU
1	B	553	HIS
1	B	556	PHE
1	B	563	GLU
1	B	571	THR
1	B	586	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	102	ASN
1	A	105	HIS
1	A	123	GLN
1	A	286	ASN
1	A	370	GLN
1	A	433	ASN
1	A	442	GLN
1	A	480	HIS
1	A	494	ASN
1	A	496	GLN
1	A	532	GLN
1	A	565	HIS
1	A	596	ASN
1	B	84	ASN
1	B	102	ASN
1	B	105	HIS

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Mol	Chain	Res	Type
1	B	123	GLN
1	B	191	HIS
1	B	274	ASN
1	B	275	HIS
1	B	362	ASN
1	B	419	ASN
1	B	494	ASN
1	B	496	GLN
1	B	530	ASN
1	B	565	HIS
1	B	596	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	537/583 (92%)	0.37	50 (9%)	11	9	54, 107, 187, 198	0
1	B	537/583 (92%)	0.21	20 (3%)	45	38	43, 90, 169, 198	0
All	All	1074/1166 (92%)	0.29	70 (6%)	22	18	43, 98, 181, 198	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	THR	6.4
1	B	554	GLY	5.6
1	A	66	TRP	5.3
1	B	600	THR	5.0
1	A	604	ALA	4.9
1	A	320	GLY	4.3
1	B	604	ALA	3.6
1	B	63	TYR	3.6
1	A	101	LEU	3.5
1	A	601	ILE	3.5
1	B	64	LEU	3.4
1	A	136	MET	3.3
1	B	460	LYS	3.2
1	A	116	ALA	3.2
1	A	214	VAL	3.2
1	A	142	ILE	3.2
1	A	420	VAL	3.2
1	B	551	ARG	3.2
1	A	120	TYR	3.1
1	B	555	ALA	3.1
1	B	417	LEU	3.1
1	B	603	LEU	3.1
1	A	212	VAL	3.0
1	A	141	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	197	ARG	2.9
1	B	66	TRP	2.8
1	A	558	GLU	2.8
1	A	216	TRP	2.8
1	A	64	LEU	2.7
1	A	135	ILE	2.7
1	B	536	ARG	2.7
1	A	213	ARG	2.7
1	A	63	TYR	2.7
1	A	202	ILE	2.6
1	A	318	GLY	2.6
1	A	198	THR	2.6
1	A	553	HIS	2.5
1	B	216	TRP	2.5
1	A	319	ASP	2.4
1	A	203	ARG	2.4
1	A	462	ASP	2.4
1	A	201	LYS	2.4
1	A	602	ILE	2.4
1	A	407	VAL	2.4
1	A	337	ASP	2.3
1	A	444	ALA	2.3
1	A	460	LYS	2.3
1	A	402	LEU	2.3
1	A	258	SER	2.3
1	A	49	LEU	2.3
1	A	132	PHE	2.3
1	B	79	LEU	2.3
1	B	101	LEU	2.2
1	A	131	TYR	2.2
1	B	552	GLU	2.2
1	B	602	ILE	2.2
1	A	544	LEU	2.2
1	A	119	PRO	2.1
1	A	559	ASN	2.1
1	A	297	ILE	2.1
1	A	323	HIS	2.1
1	A	167	ASN	2.1
1	B	320	GLY	2.1
1	A	118	LEU	2.1
1	A	215	LYS	2.1
1	A	46	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	420	VAL	2.1
1	B	167	ASN	2.0
1	A	183	PHE	2.0
1	A	97	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.