



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:11 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 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/ValidationPDFNotes.html>

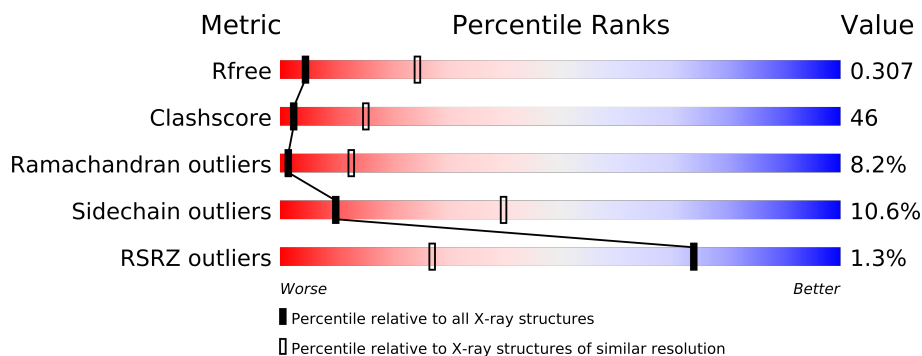
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	583	
1	B	583	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8476 atoms, of which 0 are hydrogen and 0 are deuterium.

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

T600	V631	T467	Q404	V325	SER	E174	G107
L601	Q532	P468	D405	G326	PHE	E175	V108
L602	P533	T469	E406	F327	PHE	S176	T109
L603	P534	P470	V407	L328	PRO	A177	F110
A604	N635	L471	D408	R329	LYS	A178	F111
R636	R636	F472	A410	T332	LYS	A179	A112
T637	T637	G473	L411	Y333	ASP	R180	I113
G638	G638	F474	L414	Y334	ASP	T181	E114
I639	I639	E475	L415	S334	ALA	L182	S115
K640	K640	R476	T416	W335	PHE	F183	A116
T641	T641	L477	L416	Q336	HIS	S184	Y117
C642	C642	H480	L417	F341	ARG	R185	L118
S643	S643	F481	V420	S258	SER	M186	P119
L644	L644	R482	D421	S259	SER	M187	Y120
T645	T645	V483	T422	F260	S264	I188	T121
G646	G646	Y484	N423	E350	V265	L189	V122
L648	L648	Y485	N424	E351	P266	G190	Q123
A649	A649	S486	V424	F352	H267	H191	K124
V650	V650	K487	E425	A353	F268	K192	S125
R651	R651	P488	S426	I356	R269	V193	S126
E652	E652	T489	R427	F359	A270	P194	G128
H653	H653	C490	L428	T363	E271	L200	R129
G654	G654	I493	A429	L366	L272	K201	F130
A655	A655	M494	L430	L367	H275	I202	D134
F656	F656	E495	D432	I368	Y276	R203	I135
I657	I657	Q496	N433	I369	G277	R204	M136
V662	V662	D497	M434	I369	S279	G207	T137
E663	E663	F498	E435	I369	G280	T208	F138
P664	P664	A499	G436	I369	G281	T209	S139
H665	H665	C500	Y437	Q370	G282	R210	S140
L668	L668	A501	T438	N373	L283	W216	E141
P669	P669	D502	V439	P374	R282	R217	I142
F670	F670	F503	D440	G375	S283	R218	R143
T671	T671	P504	L441	G376	G284	Y218	V144
S672	S672	P505	Q442	G377	Y285	V219	G145
N673	N673	V506	V443	V378	N286	G222	L148
D674	D674	V507	A444	L379	T290	VAL	L149
I675	I675	K509	E445	Y380	D291	GLY	V151
K578	K578	D510	L447	L381	T292	ASP	D152
G579	G579	N511	K448	Y382	G292	LEU	G153
Y580	Y580	D512	S449	A383	F293	ALA	A154
S681	S681	R513	F450	L384	V296	THR	P155
E582	E582	A514	G451	L385	I297	ILE	V156
Y583	Y583	L515	R452	T389	Q298	ALA	Q157
K586	K586	I516	Q453	P392	P299	PRO	D158
V591	V591	V517	V454	L393	V300	SER	V159
C592	C592	G518	L455	L394	I301	ILE	L160
Q593	Q593	A522	M456	E394	W302	ARG	A161
L594	L594	G523	C457	L395	S304	ALA	T162
I595	I595	A524	W458	H398	A310	PRO	L163
G596	G596	G525	S459	R399	Y311	GLN	Y164
N597	N597	G526	K460	M400	I312	LEU	H168
D598	D598	F527	T463	I401	S313	LYS	K169
G599	G599	V528	E464	L402	T403	SER	G170
		N530	S466			MET	T171
						ARG	

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.305 0.262 , 0.307	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 , 107.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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	0.47	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($^{\circ}$)	Ideal($^{\circ}$)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 46.

All (768) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:550:VAL:CG1	1:A:554:GLY:HA2	2.15	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/583 (91%)	397 (74%)	90 (17%)	46 (9%)	1	11
1	B	533/583 (91%)	404 (76%)	88 (16%)	41 (8%)	1	14
All	All	1066/1166 (91%)	801 (75%)	178 (17%)	87 (8%)	1	13

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	12	45
1	B	463/505 (92%)	410 (89%)	53 (11%)	8	36
All	All	926/1010 (92%)	828 (89%)	98 (11%)	10	40

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
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 ⓘ

There are no RNA chains 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, 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%)	0.16	9 (1%) 67 21	54, 107, 187, 198	0
1	B	537/583 (92%)	0.07	5 (0%) 81 37	43, 90, 169, 198	0
All	All	1074/1166 (92%)	0.12	14 (1%) 74 27	43, 98, 181, 198	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	LYS	3.8
1	A	604	ALA	3.3
1	B	554	GLY	2.8
1	B	536	ARG	2.6
1	A	600	THR	2.5
1	B	600	THR	2.5
1	A	215	LYS	2.4
1	A	197	ARG	2.3
1	A	213	ARG	2.3
1	A	320	GLY	2.3
1	A	136	MET	2.2
1	A	66	TRP	2.2
1	B	551	ARG	2.1
1	A	460	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.