



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:11 am GMT

PDB ID : 3G8E
Title : Crystal Structure of Rattus norvegicus Visfatin/PBEF/Nampt in Complex with an FK866-based inhibitor
Authors : Kang, G.B.; Bae, M.H.; Kim, M.K.; Im, I.; Kim, Y.C.; Eom, S.H.
Deposited on : 2009-02-12
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

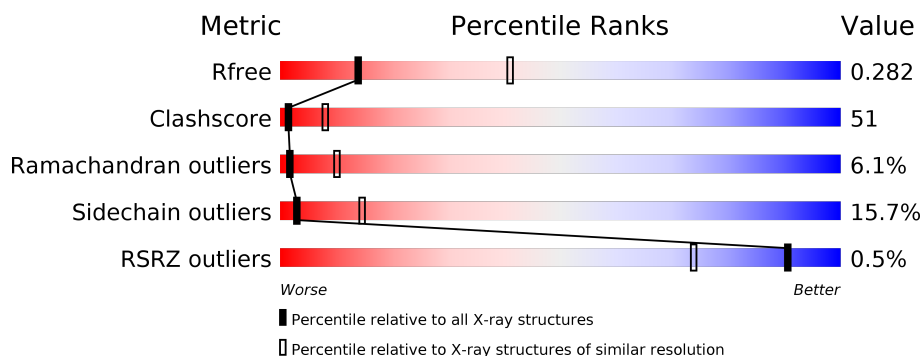
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	<div> <div></div> <div>31% 50% 12% • 6%</div> </div>
1	B	491	<div> <div></div> <div>34% 45% 14% • 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IS1	A	501	-	-	-	X
2	IS1	B	502	-	-	-	X

2 Entry composition [i](#)

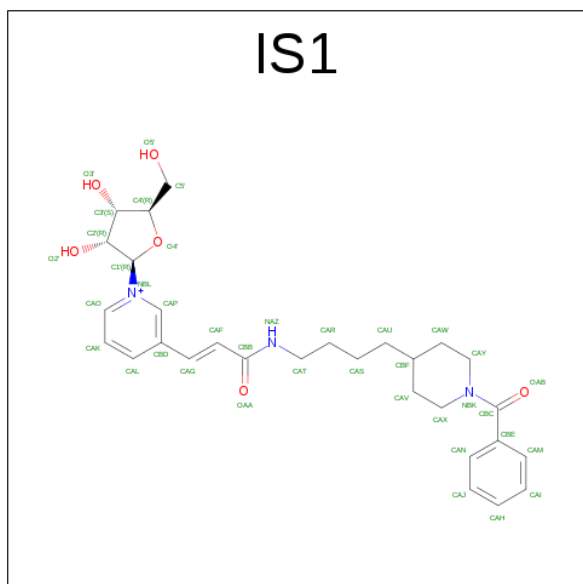
There are 2 unique types of molecules in this entry. The entry contains 7476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			
1	B	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			

- Molecule 2 is 3-[(1E)-3-OXO-3-({4-[1-(PHENYLCARBONYL)PIPERIDIN-4-YL]BUTYL}AMINO)PROP-1-EN-1-YL]-1-BETA-D-RIBOFURANOSYLPYRIDINIUM (three-letter code: IS1) (formula: C₂₉H₃₈N₃O₆).

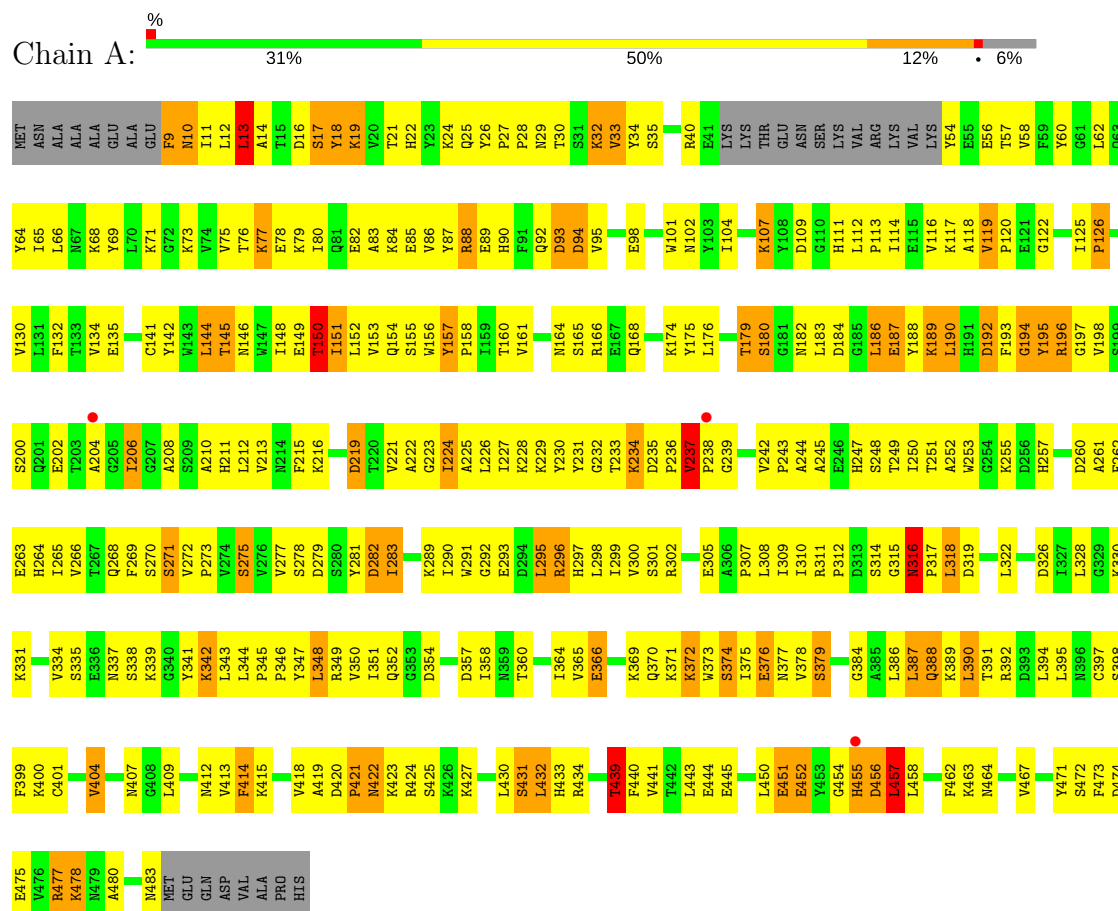


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	29	3	6		
2	B	1	Total	C	N	O	0	0
			38	29	3	6		

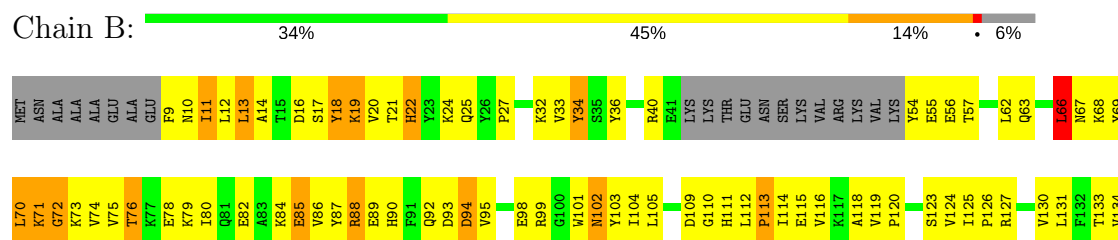
3 Residue-property plots

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

• Molecule 1: Nicotinamide phosphoribosyltransferase



• Molecule 1: Nicotinamide phosphoribosyltransferase



K423	K424	D354	A286	E135
E425	S425	G355	C287	N136
G426		I358	E288	T137
K427		N359	K289	D138
K428		T360	I290	P139
R429			W291	E140
			G292	C141
L430		I364	E293	Y142
S431		V365	D294	W143
L432		E366	L295	L144
H433		G367	R296	T145
		M368		N146
T439			T299	W147
F440		K371	V300	L148
		K372		E149
L443		W373	T304	T150
E444		S374	E305	I151
E445		I375	A306	L152
G446		E376	P307	V153
K447		N377	L308	Q154
G448		V378	I309	K155
D449		S379	I310	S155
L450		F380	R311	W156
E451		G381	P312	Y157
E452			D313	P158
Y453		G384	S314	G239
G454		A385		V161
H455		L386	L318	N164
D456		L387		S165
L457		Q388	V321	R166
L458		K389	L322	E167
		L390	K323	Q168
F462		T391	V324	K169
K463		R392	L325	K170
N464		D393	D326	I171
		L394	I327	L172
		L395	L328	A173
K469				K259
S470		S398	K331	F262
Y471		F399	F332	E263
S472		K400	P333	H264
F473			V334	I265
D474		V404		V266
E475		V405	N337	T267
		T406	S338	Q268
Q481		N407	K339	F269
L482		G408	G340	
N483		L409	Y341	V272
MET		G410	K342	P273
GLU		G411	L343	Y274
GLN		V411	L344	S275
ASP		N412	L345	V276
VAL		V413	P345	
ALA		F414	P346	Y195
PRO		K415	Y347	R196
HIS		V418	L348	G197
		A419	R349	V198
		D420	V350	L190
		F421	I351	
		N422	D282	Y195
			I283	R196
				G197
				V198
				L190

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 107.41Å 120.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 40.04 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 99.0 (40.04-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.91 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.299 0.269 , 0.282	Depositor DCC
R_{free} test set	1119 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7476	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6152e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IS1

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	0.53	2/3788 (0.1%)	0.81	4/5136 (0.1%)
1	B	0.45	0/3788	0.78	3/5136 (0.1%)
All	All	0.49	2/7576 (0.0%)	0.80	7/10272 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	LEU	CG-CD1	-7.57	1.23	1.51
1	A	432	LEU	C-O	-6.38	1.11	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	348	LEU	CA-CB-CG	5.68	128.38	115.30
1	B	66	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	455	HIS	N-CA-C	5.50	125.84	111.00
1	A	270	SER	N-CA-C	-5.41	96.38	111.00
1	B	344	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	13	LEU	CB-CG-CD1	-5.02	102.46	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3700	0	3665	397	0
1	B	3700	0	3665	390	0
2	A	38	0	37	15	0
2	B	38	0	37	8	0
All	All	7476	0	7404	753	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 51.

All (753) 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:432:LEU:O	1:A:457:LEU:CD1	1.90	1.19
1:A:19:LYS:HG3	1:A:22:HIS:CD2	1.80	1.15
1:A:432:LEU:O	1:A:457:LEU:HD13	1.46	1.12
1:A:148:ILE:HD13	1:A:152:LEU:HD12	1.32	1.11
1:B:179:THR:HG21	1:B:374:SER:HA	1.13	1.08
1:B:32:LYS:HD3	1:B:136:ASN:HD21	1.17	1.07
1:B:179:THR:CG2	1:B:374:SER:HA	1.86	1.04
1:A:13:LEU:HA	1:A:87:TYR:OH	1.56	1.04
1:B:391:THR:HG22	1:B:393:ASP:H	1.17	1.03
1:A:224:ILE:HG22	1:A:238:PRO:HG2	1.40	1.02
1:A:104:ILE:HD11	1:A:141:CYS:SG	2.03	0.99
1:A:224:ILE:CG2	1:A:238:PRO:HG2	1.93	0.97
1:A:433:HIS:HA	1:A:457:LEU:HD11	1.45	0.97
1:A:316:ASN:ND2	1:A:319:ASP:H	1.62	0.96
1:B:112:LEU:HD22	1:B:144:LEU:HD11	1.46	0.96
1:B:311:ARG:HG3	1:B:351:ILE:HG23	1.48	0.96
1:B:149:GLU:HG3	1:B:399:PHE:CD2	2.01	0.95
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.49	0.95
1:B:175:TYR:OH	1:B:366:GLU:HG2	1.67	0.95
1:B:482:LEU:HD23	1:B:483:ASN:H	1.28	0.94
1:A:179:THR:CG2	1:A:374:SER:HA	1.97	0.94
1:B:405:VAL:HA	1:B:410:GLY:HA2	1.51	0.93
1:A:179:THR:HG21	1:A:375:ILE:H	1.34	0.93
1:A:151:ILE:HD12	1:B:201:GLN:HE21	1.33	0.93
1:A:193:PHE:HD2	2:A:501:IS1:H2'	1.35	0.92
1:A:212:LEU:HD12	1:A:227:ILE:HD11	1.53	0.91
1:B:198:VAL:HG21	1:B:204:ALA:HB2	1.52	0.91
1:A:10:ASN:HB3	1:A:13:LEU:HD11	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HD13	1:A:152:LEU:CD1	2.01	0.89
1:B:337:ASN:HD22	1:B:339:LYS:H	1.13	0.89
1:B:198:VAL:HG11	1:B:387:LEU:HD12	1.55	0.89
1:B:179:THR:HG21	1:B:374:SER:CA	2.02	0.89
1:A:202:GLU:O	1:A:206:ILE:HD13	1.71	0.88
1:B:374:SER:OG	1:B:376:GLU:HG3	1.73	0.88
1:B:337:ASN:ND2	1:B:339:LYS:H	1.71	0.87
1:B:309:ILE:HD13	1:B:349:ARG:HB2	1.55	0.87
1:B:311:ARG:HH11	2:B:502:IS1:HAG	1.40	0.87
1:A:32:LYS:NZ	1:A:135:GLU:OE1	2.08	0.86
1:A:198:VAL:HG21	1:A:204:ALA:HB2	1.55	0.86
1:A:149:GLU:HG3	1:A:399:PHE:CD2	2.11	0.86
1:A:10:ASN:HB3	1:A:13:LEU:CD1	2.06	0.86
1:B:71:LYS:HE3	1:B:72:GLY:H	1.42	0.85
1:B:13:LEU:HA	1:B:87:TYR:OH	1.76	0.85
1:A:193:PHE:CD2	2:A:501:IS1:H2'	2.10	0.85
1:B:80:ILE:HG21	1:B:102:ASN:HD21	1.42	0.85
1:B:13:LEU:N	1:B:13:LEU:HD22	1.92	0.85
1:A:9:PHE:O	1:A:10:ASN:HB2	1.77	0.84
1:B:309:ILE:CD1	1:B:349:ARG:HB2	2.08	0.83
1:A:432:LEU:O	1:A:457:LEU:HD12	1.77	0.83
1:B:155:SER:O	1:B:158:PRO:HD2	1.79	0.83
1:B:32:LYS:HD3	1:B:136:ASN:ND2	1.93	0.83
1:A:365:VAL:HG12	1:A:375:ILE:HD12	1.60	0.83
1:B:13:LEU:HD22	1:B:13:LEU:H	1.43	0.83
1:A:243:PRO:HA	1:B:21:THR:HG21	1.61	0.82
1:A:388:GLN:HG3	1:A:389:LYS:H	1.44	0.82
1:A:84:LYS:O	1:A:85:GLU:HB3	1.78	0.82
1:A:326:ASP:O	1:A:330:LYS:HG3	1.78	0.82
1:B:405:VAL:HA	1:B:410:GLY:CA	2.08	0.82
1:B:113:PRO:HB2	1:B:137:THR:OG1	1.79	0.82
1:A:374:SER:HB3	1:A:376:GLU:HG3	1.62	0.82
1:B:323:LYS:O	1:B:327:ILE:HD13	1.80	0.81
1:A:175:TYR:OH	1:A:366:GLU:HG2	1.81	0.81
1:A:98:GLU:O	1:A:102:ASN:ND2	2.13	0.81
1:A:463:LYS:HG3	1:A:464:ASN:ND2	1.96	0.81
1:A:77:LYS:H	1:A:77:LYS:HE2	1.46	0.80
1:A:179:THR:HG23	1:A:374:SER:HA	1.60	0.80
1:A:10:ASN:CB	1:A:13:LEU:HD11	2.10	0.80
1:B:237:VAL:HG12	1:B:237:VAL:O	1.82	0.80
1:A:149:GLU:O	1:A:153:VAL:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:OH	1:B:164:ASN:ND2	2.16	0.79
1:A:151:ILE:HD12	1:B:201:GLN:NE2	1.98	0.79
1:A:421:PRO:C	1:A:423:LYS:H	1.87	0.78
1:B:32:LYS:HE2	1:B:135:GLU:HG3	1.65	0.78
1:A:206:ILE:HD12	1:A:226:LEU:CD1	2.14	0.78
1:A:12:LEU:HD11	1:A:80:ILE:HD13	1.64	0.78
1:A:272:VAL:HB	1:A:273:PRO:CD	2.14	0.77
2:A:501:IS1:HAXA	2:A:501:IS1:CAM	2.14	0.77
1:B:355:GLY:O	1:B:360:THR:HG21	1.85	0.77
1:B:93:ASP:OD1	1:B:94:ASP:N	2.18	0.77
1:B:71:LYS:HE3	1:B:72:GLY:N	1.99	0.77
1:A:19:LYS:CG	1:A:22:HIS:CD2	2.67	0.75
1:A:379:SER:HB3	2:A:501:IS1:CAI	2.16	0.75
1:A:112:LEU:HD22	1:A:144:LEU:HD11	1.67	0.75
1:B:308:LEU:HD21	1:B:310:ILE:HD11	1.69	0.75
1:B:482:LEU:HD23	1:B:483:ASN:N	2.01	0.75
1:B:156:TRP:CG	1:B:392:ARG:HG3	2.22	0.75
1:A:234:LYS:HD2	1:A:234:LYS:N	2.02	0.75
1:A:57:THR:HG22	1:A:395:LEU:HD13	1.69	0.74
1:B:57:THR:CG2	1:B:395:LEU:HD13	2.17	0.74
1:B:161:VAL:O	1:B:165:SER:HB2	1.85	0.74
1:A:224:ILE:HG22	1:A:238:PRO:CG	2.15	0.74
1:B:157:TYR:HB3	1:B:158:PRO:HD3	1.68	0.74
1:B:342:LYS:HG3	1:B:372:LYS:O	1.87	0.74
1:A:179:THR:HG21	1:A:374:SER:HA	1.70	0.73
1:B:103:TYR:CZ	1:B:140:GLU:HG3	2.23	0.73
1:A:316:ASN:HD21	1:A:319:ASP:H	1.35	0.73
1:B:311:ARG:NH1	2:B:502:IS1:HAG	2.02	0.73
1:B:450:LEU:O	1:B:452:GLU:HG2	1.88	0.73
1:A:343:LEU:HD12	1:A:377:ASN:OD1	1.88	0.73
1:B:296:ARG:NH1	1:B:331:LYS:O	2.22	0.73
1:B:413:VAL:O	1:B:414:PHE:HB3	1.89	0.72
1:B:165:SER:OG	1:B:211:HIS:HD2	1.71	0.72
1:A:251:THR:HG22	1:A:281:TYR:OH	1.89	0.72
1:A:145:THR:O	1:A:148:ILE:HG13	1.88	0.72
1:A:179:THR:HG21	1:A:375:ILE:N	2.03	0.72
1:B:113:PRO:O	1:B:137:THR:OG1	2.07	0.72
1:A:119:VAL:HG11	1:A:125:ILE:HD11	1.71	0.72
1:A:349:ARG:HH11	1:A:349:ARG:HG2	1.54	0.72
1:A:457:LEU:HD12	1:A:457:LEU:N	2.04	0.72
1:A:168:GLN:HG3	1:A:358:ILE:HD13	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:H	1:B:104:ILE:HD12	1.53	0.71
1:A:76:THR:OG1	1:A:79:LYS:HG3	1.90	0.71
1:A:157:TYR:HB3	1:A:158:PRO:HD3	1.71	0.71
1:B:373:TRP:O	1:B:374:SER:HB3	1.90	0.71
1:B:398:SER:OG	1:B:400:LYS:HE3	1.92	0.70
1:A:433:HIS:HA	1:A:457:LEU:CD1	2.19	0.70
1:A:316:ASN:ND2	1:A:319:ASP:N	2.37	0.70
1:B:429:ARG:NH1	1:B:446:GLY:HA3	2.07	0.69
1:B:439:THR:HG23	1:B:440:PHE:N	2.06	0.69
1:A:13:LEU:HA	1:A:87:TYR:HH	1.55	0.69
1:B:82:GLU:O	1:B:86:VAL:HG23	1.91	0.69
1:B:180:SER:HB2	1:B:376:GLU:OE1	1.92	0.69
1:B:71:LYS:HG2	1:B:72:GLY:H	1.57	0.69
1:A:182:ASN:HD22	1:A:184:ASP:H	1.38	0.69
1:A:421:PRO:O	1:A:423:LYS:N	2.26	0.69
1:B:10:ASN:HB3	1:B:13:LEU:HD21	1.73	0.69
1:B:263:GLU:HA	1:B:266:VAL:HG22	1.75	0.69
1:A:76:THR:HG23	1:A:79:LYS:HE3	1.76	0.68
1:A:14:ALA:HA	1:B:195:TYR:OH	1.93	0.68
1:B:413:VAL:HG12	1:B:414:PHE:N	2.09	0.68
1:A:120:PRO:HA	1:A:471:TYR:CZ	2.29	0.68
1:A:349:ARG:HG2	1:A:349:ARG:NH1	2.06	0.68
1:B:165:SER:OG	1:B:211:HIS:CD2	2.47	0.68
1:A:54:TYR:OH	1:A:164:ASN:ND2	2.26	0.68
1:A:263:GLU:HG3	1:A:298:LEU:CD1	2.23	0.68
1:A:176:LEU:HD22	1:A:182:ASN:O	1.94	0.67
1:A:431:SER:HB2	1:A:433:HIS:NE2	2.09	0.67
1:B:415:LYS:H	1:B:425:SER:HB3	1.57	0.67
1:A:299:ILE:HG23	1:A:300:VAL:H	1.59	0.67
1:B:325:LEU:HD11	1:B:368:MET:HE3	1.75	0.67
1:A:311:ARG:HG3	1:A:351:ILE:HG13	1.76	0.67
1:B:374:SER:OG	1:B:376:GLU:CG	2.42	0.67
1:A:89:GLU:OE2	1:B:238:PRO:HD2	1.94	0.67
1:B:56:GLU:O	1:B:56:GLU:HG3	1.94	0.67
1:B:71:LYS:CG	1:B:72:GLY:H	2.05	0.67
1:B:353:GLY:HA2	1:B:381:GLY:O	1.94	0.67
1:B:264:HIS:O	1:B:268:GLN:HG2	1.94	0.67
1:A:122:GLY:O	1:A:480:ALA:HB2	1.95	0.66
1:A:17:SER:OG	1:A:90:HIS:HE1	1.78	0.66
1:A:257:HIS:ND1	1:A:260:ASP:OD2	2.28	0.66
1:B:123:SER:HB3	1:B:125:ILE:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG23	1:B:152:LEU:N	2.11	0.66
1:A:10:ASN:CG	1:A:13:LEU:HD11	2.14	0.66
1:B:78:GLU:N	1:B:78:GLU:OE1	2.27	0.66
1:A:374:SER:CB	1:A:376:GLU:HG3	2.24	0.66
1:B:431:SER:HB2	1:B:433:HIS:NE2	2.10	0.66
1:A:189:LYS:NZ	1:A:376:GLU:HA	2.11	0.66
1:A:118:ALA:O	1:A:458:LEU:HA	1.94	0.66
1:A:252:ALA:O	1:B:27:PRO:HG3	1.96	0.66
1:B:311:ARG:NH1	2:B:502:IS1:CAG	2.59	0.66
1:B:337:ASN:HD22	1:B:337:ASN:C	1.98	0.66
1:B:57:THR:HG22	1:B:395:LEU:HD13	1.78	0.66
1:B:80:ILE:HD12	1:B:101:TRP:HB3	1.78	0.66
1:B:123:SER:HB3	1:B:125:ILE:HD11	1.77	0.65
1:A:221:VAL:HG21	1:B:13:LEU:HB2	1.78	0.65
1:B:153:VAL:C	1:B:155:SER:H	1.98	0.65
1:A:463:LYS:HG3	1:A:464:ASN:HD22	1.60	0.65
1:B:113:PRO:C	1:B:137:THR:OG1	2.35	0.65
1:A:179:THR:CG2	1:A:375:ILE:H	2.08	0.64
1:B:386:LEU:HD13	1:B:387:LEU:HD23	1.79	0.64
1:B:136:ASN:OD1	1:B:142:TYR:HA	1.97	0.64
1:B:413:VAL:CG1	1:B:414:PHE:N	2.60	0.64
1:B:198:VAL:HG12	1:B:387:LEU:HB3	1.78	0.64
1:A:264:HIS:O	1:A:268:GLN:HG2	1.96	0.64
1:A:9:PHE:HD2	1:A:9:PHE:N	1.96	0.64
1:A:299:ILE:HG23	1:A:300:VAL:N	2.13	0.64
1:B:289:LYS:HA	1:B:293:GLU:HG3	1.80	0.64
1:A:148:ILE:CD1	1:A:152:LEU:HD12	2.20	0.64
1:A:412:ASN:ND2	1:A:445:GLU:HG2	2.13	0.64
1:A:243:PRO:CA	1:B:21:THR:HG21	2.28	0.63
1:B:296:ARG:HA	1:B:299:ILE:HD12	1.79	0.63
1:B:56:GLU:HA	1:B:126:PRO:HA	1.80	0.63
1:A:206:ILE:HD12	1:A:226:LEU:HD11	1.79	0.63
1:B:198:VAL:HB	1:B:203:THR:CG2	2.29	0.63
1:A:221:VAL:O	1:A:224:ILE:HG13	1.98	0.63
1:B:70:LEU:HD21	1:B:151:ILE:HG21	1.79	0.63
1:B:113:PRO:CB	1:B:137:THR:OG1	2.45	0.63
1:A:420:ASP:OD2	1:A:423:LYS:HG3	1.98	0.63
1:B:116:VAL:HG13	1:B:134:VAL:HG22	1.79	0.63
1:B:283:ILE:CD1	1:B:312:PRO:HA	2.28	0.63
1:A:342:LYS:CB	1:A:342:LYS:HZ2	2.12	0.62
1:A:80:ILE:HD12	1:A:101:TRP:HB3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:CA	1:B:137:THR:HG23	2.29	0.62
1:B:304:THR:HG22	1:B:346:PRO:HB2	1.81	0.62
1:A:195:TYR:OH	1:B:14:ALA:HA	2.00	0.62
1:B:149:GLU:HG3	1:B:399:PHE:CE2	2.35	0.62
1:B:73:LYS:HG3	1:B:109:ASP:O	1.99	0.62
1:A:86:VAL:C	1:A:88:ARG:H	2.01	0.62
1:B:167:GLU:O	1:B:170:LYS:N	2.32	0.62
1:B:351:ILE:HD13	1:B:352:GLN:N	2.14	0.62
1:B:237:VAL:O	1:B:237:VAL:CG1	2.47	0.62
1:A:156:TRP:HH2	1:B:388:GLN:HE21	1.48	0.62
1:B:24:LYS:NZ	1:B:95:VAL:HG12	2.15	0.61
1:A:212:LEU:HD12	1:A:227:ILE:CD1	2.26	0.61
1:A:156:TRP:CB	1:A:392:ARG:HG3	2.30	0.61
1:B:182:ASN:C	1:B:182:ASN:HD22	2.03	0.61
1:B:75:VAL:CG1	1:B:80:ILE:HD11	2.30	0.61
1:B:198:VAL:CG1	1:B:387:LEU:HB3	2.31	0.61
1:A:300:VAL:HG13	1:A:347:TYR:CE2	2.34	0.61
1:B:311:ARG:HG3	1:B:351:ILE:CG2	2.25	0.61
1:A:193:PHE:CD2	2:A:501:IS1:C2'	2.82	0.61
1:B:413:VAL:CG1	1:B:414:PHE:H	2.13	0.61
1:A:432:LEU:CB	1:A:458:LEU:HD21	2.31	0.61
1:B:337:ASN:HD22	1:B:339:LYS:N	1.92	0.61
1:B:337:ASN:O	1:B:340:GLY:N	2.32	0.61
1:B:70:LEU:O	1:B:71:LYS:O	2.18	0.61
1:B:373:TRP:O	1:B:377:ASN:ND2	2.34	0.60
1:A:414:PHE:CD2	1:A:414:PHE:N	2.69	0.60
1:A:433:HIS:CD2	1:A:443:LEU:HD12	2.36	0.60
1:A:432:LEU:HB2	1:A:458:LEU:HD21	1.83	0.60
1:A:9:PHE:CD2	1:A:9:PHE:N	2.69	0.60
1:A:12:LEU:CD1	1:A:80:ILE:HD13	2.30	0.60
1:A:421:PRO:C	1:A:423:LYS:N	2.55	0.60
1:B:127:ARG:CZ	1:B:395:LEU:HA	2.32	0.60
1:B:24:LYS:HZ1	1:B:95:VAL:HG12	1.66	0.60
2:A:501:IS1:O2'	2:A:501:IS1:HAP	2.01	0.60
1:A:12:LEU:O	1:A:87:TYR:CE1	2.55	0.60
1:B:273:PRO:HG3	1:B:306:ALA:HA	1.84	0.60
1:B:350:VAL:HB	1:B:378:VAL:HG22	1.83	0.60
1:B:233:THR:HG22	1:B:235:ASP:HB2	1.82	0.60
1:B:365:VAL:HG12	1:B:375:ILE:HD12	1.85	0.59
1:A:272:VAL:HB	1:A:273:PRO:HD2	1.83	0.59
1:B:13:LEU:HA	1:B:87:TYR:HH	1.63	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HD23	1:B:395:LEU:N	2.17	0.59
1:B:12:LEU:HD21	1:B:80:ILE:HD13	1.85	0.59
1:B:13:LEU:N	1:B:13:LEU:CD2	2.64	0.58
1:B:155:SER:C	1:B:158:PRO:HD2	2.23	0.58
1:A:237:VAL:HG21	1:B:89:GLU:HB3	1.85	0.58
1:B:113:PRO:C	1:B:137:THR:HG1	2.06	0.58
1:A:9:PHE:CE2	1:A:69:TYR:HD2	2.21	0.58
1:B:134:VAL:HG21	1:B:152:LEU:CD1	2.33	0.58
1:A:80:ILE:CD1	1:A:101:TRP:HB3	2.33	0.58
1:B:332:PHE:HB3	1:B:333:PRO:HD2	1.85	0.58
1:B:86:VAL:C	1:B:88:ARG:H	2.07	0.58
1:A:153:VAL:C	1:A:155:SER:H	2.06	0.58
1:A:21:THR:HG21	1:B:243:PRO:HB3	1.84	0.58
1:A:388:GLN:HG3	1:A:389:LYS:N	2.16	0.58
1:A:414:PHE:HB2	1:A:425:SER:HB2	1.85	0.58
1:B:57:THR:HG21	1:B:395:LEU:HD13	1.84	0.58
1:A:309:ILE:CD1	1:A:349:ARG:HB2	2.33	0.58
1:B:32:LYS:O	1:B:404:VAL:HA	2.04	0.58
1:A:348:LEU:O	1:A:349:ARG:HG2	2.04	0.58
1:A:414:PHE:HD2	1:A:414:PHE:N	2.02	0.58
1:A:73:LYS:HG3	1:A:109:ASP:O	2.03	0.58
1:B:179:THR:CG2	1:B:374:SER:CA	2.73	0.58
1:B:300:VAL:HG13	1:B:347:TYR:CZ	2.39	0.57
1:A:87:TYR:CE2	1:B:221:VAL:HG11	2.40	0.57
1:A:427:LYS:HB2	1:A:427:LYS:HZ3	1.69	0.57
1:B:136:ASN:C	1:B:136:ASN:HD22	2.07	0.57
1:A:224:ILE:HA	1:A:227:ILE:HD12	1.86	0.57
1:A:473:PHE:O	1:A:477:ARG:HG2	2.04	0.57
1:A:75:VAL:CG1	1:A:80:ILE:HD11	2.34	0.57
1:A:212:LEU:HA	1:A:215:PHE:O	2.04	0.57
1:B:167:GLU:O	1:B:169:LYS:N	2.37	0.57
1:B:318:LEU:HB2	1:B:364:ILE:HD13	1.86	0.57
1:A:76:THR:CG2	1:A:79:LYS:HE3	2.33	0.57
1:A:318:LEU:HA	1:A:364:ILE:HD12	1.86	0.57
1:B:202:GLU:O	1:B:206:ILE:HG13	2.04	0.57
1:B:286:ALA:HA	1:B:290:ILE:HD12	1.87	0.57
1:A:371:LYS:O	1:A:372:LYS:HB2	2.05	0.57
1:A:9:PHE:CZ	1:A:69:TYR:HD2	2.23	0.57
1:A:84:LYS:C	1:A:86:VAL:H	2.08	0.57
1:A:357:ASP:OD2	1:A:360:THR:HB	2.05	0.57
1:A:413:VAL:HG13	1:B:251:THR:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.19	0.56
1:A:235:ASP:HB3	1:A:236:PRO:HD2	1.87	0.56
1:A:12:LEU:O	1:A:87:TYR:HE1	1.87	0.56
1:A:155:SER:C	1:A:157:TYR:N	2.58	0.56
1:A:242:VAL:HG22	2:A:501:IS1:HATA	1.88	0.56
1:B:84:LYS:HE3	1:B:98:GLU:OE1	2.05	0.56
1:A:193:PHE:HD2	2:A:501:IS1:C2'	2.14	0.56
1:A:28:PRO:O	1:A:29:ASN:HB2	2.04	0.56
1:B:63:GLN:OE1	1:B:470:SER:HA	2.06	0.56
1:A:189:LYS:HE2	1:A:378:VAL:O	2.05	0.56
1:A:309:ILE:HD13	1:A:349:ARG:HB2	1.88	0.56
1:B:283:ILE:HG23	1:B:283:ILE:O	2.04	0.56
1:B:115:GLU:HG3	1:B:463:LYS:HG2	1.87	0.56
1:B:149:GLU:O	1:B:153:VAL:HG23	2.06	0.56
1:B:80:ILE:CD1	1:B:101:TRP:HB3	2.36	0.56
1:B:373:TRP:O	1:B:374:SER:CB	2.51	0.56
1:B:242:VAL:HG22	2:B:502:IS1:HATA	1.88	0.56
1:B:262:PHE:O	1:B:266:VAL:HG22	2.05	0.56
1:A:148:ILE:HD12	1:A:148:ILE:C	2.25	0.55
1:A:19:LYS:C	1:A:21:THR:N	2.57	0.55
1:A:300:VAL:HG13	1:A:347:TYR:CZ	2.41	0.55
1:B:353:GLY:O	1:B:354:ASP:CB	2.55	0.55
1:B:114:ILE:N	1:B:137:THR:HG23	2.22	0.55
1:A:277:VAL:HG23	1:A:277:VAL:O	2.07	0.55
1:A:160:THR:HG23	1:A:394:LEU:HD23	1.87	0.55
1:B:186:LEU:O	1:B:188:TYR:N	2.40	0.55
1:B:272:VAL:C	1:B:306:ALA:HB1	2.27	0.55
1:A:418:VAL:HG13	1:A:419:ALA:N	2.21	0.55
1:B:142:TYR:CD1	1:B:143:TRP:N	2.75	0.55
1:B:198:VAL:HB	1:B:203:THR:HG22	1.88	0.55
1:A:25:GLN:HB2	1:B:249:THR:HB	1.89	0.55
1:B:424:ARG:HG2	1:B:425:SER:H	1.72	0.55
1:A:373:TRP:O	1:A:374:SER:C	2.44	0.55
1:B:231:TYR:O	1:B:472:SER:HA	2.07	0.55
1:A:57:THR:CG2	1:A:395:LEU:HD13	2.35	0.55
1:B:151:ILE:CG2	1:B:152:LEU:N	2.69	0.55
1:B:406:THR:O	1:B:406:THR:HG22	2.07	0.55
1:B:76:THR:O	1:B:80:ILE:HG12	2.06	0.55
1:A:317:PRO:HB2	1:A:364:ILE:HD11	1.89	0.55
1:A:35:SER:HB3	1:A:399:PHE:CE2	2.42	0.55
1:B:399:PHE:CD2	1:B:399:PHE:C	2.81	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:O	1:A:212:LEU:HG	2.07	0.55
1:A:316:ASN:C	1:A:316:ASN:HD22	2.10	0.54
1:B:344:LEU:CB	1:B:345:PRO:HD2	2.37	0.54
1:A:175:TYR:O	1:A:179:THR:HB	2.07	0.54
1:B:404:VAL:O	1:B:410:GLY:HA2	2.07	0.54
1:B:71:LYS:HG2	1:B:72:GLY:N	2.23	0.54
1:B:445:GLU:C	1:B:447:LYS:H	2.09	0.54
1:A:430:LEU:CD2	1:A:444:GLU:HG2	2.37	0.54
1:A:472:SER:OG	1:A:475:GLU:HG3	2.07	0.54
1:A:9:PHE:CZ	1:A:69:TYR:CD2	2.95	0.54
1:A:27:PRO:HA	1:B:253:TRP:CZ2	2.43	0.54
1:A:216:LYS:O	1:A:239:GLY:HA2	2.08	0.54
1:A:263:GLU:OE1	1:A:295:LEU:HD11	2.07	0.54
1:A:315:GLY:O	1:A:316:ASN:HB3	2.06	0.54
1:A:93:ASP:OD1	1:A:94:ASP:N	2.40	0.54
1:B:409:LEU:H	1:B:409:LEU:HD22	1.72	0.54
1:B:173:ALA:HB2	1:B:186:LEU:HD11	1.90	0.54
1:B:371:LYS:O	1:B:372:LYS:HB2	2.08	0.54
1:B:68:LYS:NZ	1:B:69:TYR:CZ	2.76	0.54
1:A:282:ASP:HA	1:B:418:VAL:HG22	1.90	0.54
1:B:180:SER:HB2	1:B:376:GLU:CD	2.27	0.54
1:B:311:ARG:HH11	2:B:502:IS1:CAG	2.14	0.54
1:B:313:ASP:O	1:B:313:ASP:CG	2.46	0.54
1:B:17:SER:OG	1:B:90:HIS:HE1	1.90	0.54
1:A:10:ASN:O	1:A:13:LEU:HD12	2.08	0.53
1:A:119:VAL:HG12	1:A:120:PRO:HD2	1.90	0.53
1:B:112:LEU:CD2	1:B:144:LEU:HD11	2.31	0.53
1:B:337:ASN:ND2	1:B:337:ASN:C	2.61	0.53
1:A:62:LEU:HD12	1:A:62:LEU:O	2.09	0.53
1:B:104:ILE:H	1:B:104:ILE:CD1	2.21	0.53
1:B:11:ILE:O	1:B:11:ILE:HD13	2.07	0.53
1:B:179:THR:HG23	1:B:341:TYR:CG	2.43	0.53
1:A:149:GLU:CG	1:A:399:PHE:CD2	2.90	0.53
1:B:333:PRO:O	1:B:345:PRO:HD3	2.08	0.53
1:A:86:VAL:C	1:A:88:ARG:N	2.62	0.53
1:A:198:VAL:HG11	1:A:387:LEU:HD12	1.90	0.53
1:B:146:ASN:O	1:B:149:GLU:N	2.24	0.53
1:B:321:VAL:CG2	1:B:352:GLN:HG3	2.38	0.53
1:B:138:ASP:C	1:B:138:ASP:OD2	2.47	0.53
1:B:105:LEU:HA	1:B:110:GLY:H	1.74	0.53
1:B:168:GLN:HA	1:B:171:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLU:HB2	1:B:295:LEU:HD22	1.91	0.52
1:A:251:THR:HB	1:B:413:VAL:HG13	1.91	0.52
1:A:318:LEU:CA	1:A:364:ILE:HD12	2.40	0.52
1:A:211:HIS:HD2	1:A:386:LEU:HD11	1.73	0.52
1:B:114:ILE:HG23	1:B:144:LEU:HD13	1.91	0.52
1:B:234:LYS:HD3	1:B:234:LYS:N	2.24	0.52
1:B:304:THR:HG22	1:B:346:PRO:CB	2.38	0.52
1:A:196:ARG:HH11	1:A:196:ARG:HB3	1.73	0.52
1:B:398:SER:CB	1:B:400:LYS:HE3	2.39	0.52
1:B:118:ALA:O	1:B:458:LEU:HA	2.08	0.52
1:A:413:VAL:CG1	1:A:414:PHE:N	2.72	0.52
1:A:292:GLY:C	1:A:293:GLU:HG2	2.29	0.52
1:B:190:LEU:O	1:B:211:HIS:HE1	1.93	0.52
1:B:391:THR:HG21	1:B:393:ASP:HB2	1.92	0.52
1:B:418:VAL:O	1:B:418:VAL:HG23	2.10	0.52
1:A:224:ILE:HG21	1:A:238:PRO:HG2	1.86	0.52
1:A:283:ILE:HD13	1:A:312:PRO:HB3	1.92	0.52
1:B:55:GLU:HA	1:B:127:ARG:HD3	1.91	0.52
1:A:374:SER:C	1:A:376:GLU:H	2.14	0.52
1:B:328:LEU:HD13	1:B:348:LEU:HD11	1.91	0.52
1:B:450:LEU:O	1:B:451:GLU:C	2.47	0.52
1:A:189:LYS:HG3	1:A:379:SER:HA	1.92	0.51
1:A:33:VAL:CG1	1:A:142:TYR:O	2.58	0.51
2:A:501:IS1:O2'	2:A:501:IS1:CAP	2.58	0.51
1:B:116:VAL:HG13	1:B:133:THR:O	2.10	0.51
1:B:136:ASN:ND2	1:B:136:ASN:C	2.63	0.51
1:B:19:LYS:HG3	1:B:22:HIS:CD2	2.45	0.51
1:A:82:GLU:O	1:A:86:VAL:HG23	2.10	0.51
1:B:198:VAL:HB	1:B:203:THR:HG21	1.93	0.51
1:A:32:LYS:O	1:A:404:VAL:HA	2.10	0.51
1:B:345:PRO:HB2	1:B:347:TYR:CZ	2.45	0.51
1:A:375:ILE:HG22	1:A:375:ILE:O	2.09	0.51
1:A:183:LEU:HD13	1:A:186:LEU:HD12	1.93	0.51
1:B:153:VAL:C	1:B:155:SER:N	2.64	0.51
1:A:242:VAL:HG11	2:A:501:IS1:HAW	1.92	0.51
1:A:189:LYS:HZ1	1:A:376:GLU:HA	1.73	0.51
1:A:130:VAL:CG1	1:A:432:LEU:HB2	2.40	0.51
1:A:472:SER:C	1:A:474:ASP:H	2.14	0.51
1:B:104:ILE:HD12	1:B:104:ILE:N	2.24	0.51
1:A:161:VAL:O	1:A:165:SER:HB3	2.11	0.51
1:A:375:ILE:CG2	1:A:375:ILE:O	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:O	1:A:66:LEU:HG	2.10	0.51
1:B:146:ASN:O	1:B:147:TRP:C	2.48	0.51
1:B:11:ILE:HG12	1:B:14:ALA:HB3	1.92	0.51
1:A:64:TYR:HD2	1:A:65:ILE:HG13	1.75	0.50
1:A:193:PHE:CD2	2:A:501:IS1:O2'	2.61	0.50
1:A:224:ILE:O	1:A:225:ALA:C	2.50	0.50
1:A:311:ARG:NH1	2:A:501:IS1:HAG	2.26	0.50
1:B:120:PRO:HA	1:B:471:TYR:CZ	2.46	0.50
1:B:171:ILE:HD12	1:B:171:ILE:H	1.76	0.50
1:B:388:GLN:HG3	1:B:389:LYS:H	1.75	0.50
1:A:73:LYS:HA	1:A:111:HIS:HD2	1.76	0.50
1:A:200:SER:OG	1:B:203:THR:OG1	2.26	0.50
1:A:144:LEU:O	1:A:145:THR:C	2.49	0.50
1:A:283:ILE:HG12	1:A:283:ILE:O	2.12	0.50
1:A:430:LEU:HA	1:A:443:LEU:O	2.11	0.50
1:A:68:LYS:HG2	1:A:68:LYS:O	2.10	0.50
1:B:430:LEU:CD2	1:B:444:GLU:HB3	2.41	0.50
1:A:211:HIS:CD2	1:A:386:LEU:HD11	2.47	0.50
1:A:253:TRP:CD1	1:A:261:ALA:HB2	2.47	0.50
1:B:375:ILE:O	1:B:375:ILE:HG22	2.12	0.50
1:B:40:ARG:HD3	1:B:400:LYS:HZ3	1.77	0.50
1:A:188:TYR:OH	1:A:216:LYS:NZ	2.43	0.49
1:A:221:VAL:HG23	1:A:222:ALA:N	2.27	0.49
1:B:73:LYS:HA	1:B:111:HIS:HD2	1.76	0.49
1:B:32:LYS:HB2	1:B:405:VAL:HB	1.93	0.49
1:B:472:SER:C	1:B:474:ASP:H	2.15	0.49
1:A:77:LYS:HG3	1:A:78:GLU:OE2	2.13	0.49
1:B:224:ILE:HD11	1:B:239:GLY:HA3	1.93	0.49
1:A:297:HIS:C	1:A:299:ILE:H	2.15	0.49
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.46	0.49
1:A:418:VAL:HG12	1:B:282:ASP:HA	1.93	0.49
1:A:146:ASN:H	1:A:146:ASN:HD22	1.59	0.49
1:A:60:TYR:O	1:A:158:PRO:HB2	2.11	0.49
1:B:103:TYR:HB3	1:B:104:ILE:HD12	1.94	0.49
1:A:450:LEU:O	1:A:452:GLU:N	2.45	0.49
1:B:409:LEU:HD13	1:B:409:LEU:N	2.28	0.49
1:A:316:ASN:ND2	1:A:316:ASN:C	2.66	0.49
1:B:391:THR:CG2	1:B:393:ASP:HB2	2.42	0.49
1:B:445:GLU:C	1:B:447:LYS:N	2.66	0.49
1:A:194:GLY:O	1:A:197:GLY:N	2.43	0.49
1:A:192:ASP:HB2	1:A:386:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:O	1:A:458:LEU:CA	2.58	0.49
1:A:278:SER:O	1:A:283:ILE:HG13	2.13	0.49
1:A:156:TRP:CG	1:A:392:ARG:HG3	2.47	0.49
1:B:114:ILE:HD11	1:B:462:PHE:CE2	2.48	0.49
1:A:160:THR:CG2	1:A:394:LEU:HD23	2.43	0.49
1:A:229:LYS:HD3	1:A:230:TYR:CE1	2.48	0.49
1:B:175:TYR:HB3	1:B:375:ILE:HG13	1.95	0.49
1:B:472:SER:OG	1:B:475:GLU:HG3	2.13	0.49
1:A:151:ILE:HG23	1:A:152:LEU:N	2.27	0.48
1:A:211:HIS:CD2	1:A:386:LEU:HD21	2.47	0.48
1:A:342:LYS:HD3	1:A:372:LYS:O	2.13	0.48
1:A:430:LEU:HD23	1:A:444:GLU:HA	1.94	0.48
1:B:125:ILE:HG22	1:B:126:PRO:O	2.13	0.48
1:A:229:LYS:O	1:A:229:LYS:HG2	2.12	0.48
1:A:432:LEU:C	1:A:457:LEU:HD13	2.23	0.48
1:B:251:THR:HG22	1:B:281:TYR:OH	2.13	0.48
1:B:12:LEU:CD2	1:B:80:ILE:HD13	2.43	0.48
1:A:247:HIS:HE1	1:A:279:ASP:OD2	1.96	0.48
1:B:364:ILE:HG21	1:B:380:PHE:HE2	1.77	0.48
1:B:158:PRO:HG3	1:B:206:ILE:CG2	2.43	0.48
1:A:249:THR:HB	1:B:25:GLN:HB2	1.96	0.48
1:B:263:GLU:HA	1:B:266:VAL:CG2	2.41	0.48
1:A:351:ILE:HA	1:A:379:SER:O	2.13	0.48
1:A:84:LYS:O	1:A:85:GLU:CB	2.53	0.48
1:A:219:ASP:HA	1:B:17:SER:OG	2.12	0.48
1:A:236:PRO:O	1:A:237:VAL:HG23	2.13	0.48
1:A:418:VAL:C	1:A:420:ASP:H	2.16	0.48
1:B:388:GLN:O	1:B:389:LYS:HB2	2.13	0.48
1:A:384:GLY:O	1:A:388:GLN:O	2.31	0.48
1:B:136:ASN:HD22	1:B:136:ASN:N	2.11	0.48
1:A:188:TYR:CE2	1:A:216:LYS:HB2	2.49	0.48
1:A:296:ARG:C	1:A:299:ILE:HG22	2.34	0.48
1:A:350:VAL:HB	1:A:378:VAL:HG22	1.94	0.48
1:B:430:LEU:HD22	1:B:444:GLU:HB3	1.95	0.48
1:A:196:ARG:NH1	1:B:16:ASP:OD2	2.42	0.48
1:B:342:LYS:CG	1:B:372:LYS:O	2.61	0.48
1:A:261:ALA:O	1:A:262:PHE:C	2.52	0.48
1:A:189:LYS:HZ3	1:A:376:GLU:HA	1.77	0.48
1:B:16:ASP:HB2	1:B:18:TYR:HE2	1.79	0.48
1:B:365:VAL:CG1	1:B:375:ILE:HD12	2.42	0.48
1:B:384:GLY:O	1:B:388:GLN:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:HIS:O	1:A:456:ASP:C	2.52	0.47
1:B:342:LYS:NZ	1:B:373:TRP:CE2	2.82	0.47
1:B:423:LYS:O	1:B:424:ARG:O	2.32	0.47
1:B:482:LEU:CD2	1:B:483:ASN:N	2.76	0.47
1:A:208:ALA:HB3	1:A:223:GLY:HA3	1.96	0.47
1:A:179:THR:HA	1:A:341:TYR:CE1	2.49	0.47
1:A:9:PHE:CD2	1:A:10:ASN:N	2.75	0.47
1:B:9:PHE:CE2	1:B:69:TYR:HD2	2.31	0.47
1:A:283:ILE:CD1	1:A:312:PRO:HA	2.43	0.47
1:A:299:ILE:C	1:A:301:SER:N	2.66	0.47
1:B:16:ASP:CB	1:B:18:TYR:HE2	2.26	0.47
1:B:17:SER:O	1:B:20:VAL:HG23	2.14	0.47
1:B:394:LEU:HD12	1:B:394:LEU:N	2.30	0.47
1:B:445:GLU:O	1:B:447:LYS:N	2.47	0.47
1:A:250:ILE:HD11	1:A:265:ILE:HD12	1.96	0.47
1:A:263:GLU:HG3	1:A:298:LEU:HD11	1.95	0.47
1:A:455:HIS:C	1:A:456:ASP:O	2.48	0.47
1:B:71:LYS:CG	1:B:72:GLY:N	2.77	0.47
1:A:281:TYR:O	1:A:282:ASP:C	2.53	0.47
1:A:292:GLY:O	1:A:293:GLU:HG2	2.14	0.47
1:A:392:ARG:HG2	1:A:397:CYS:HB2	1.96	0.47
1:A:56:GLU:HA	1:A:126:PRO:HA	1.96	0.47
1:B:443:LEU:HD11	1:B:453:TYR:CD1	2.49	0.47
1:A:153:VAL:O	1:A:155:SER:N	2.46	0.47
1:A:255:LYS:O	1:A:255:LYS:HD3	2.14	0.47
1:A:29:ASN:HB3	1:A:407:ASN:OD1	2.15	0.47
1:B:446:GLY:O	1:B:449:ASP:HB2	2.14	0.47
1:B:450:LEU:O	1:B:452:GLU:CG	2.59	0.47
1:A:337:ASN:ND2	1:A:339:LYS:HB2	2.29	0.47
1:B:114:ILE:HD11	1:B:462:PHE:HE2	1.79	0.47
1:A:17:SER:C	1:A:19:LYS:H	2.17	0.47
1:B:102:ASN:N	1:B:102:ASN:HD22	2.13	0.47
1:B:259:LYS:HE3	1:B:294:ASP:HB3	1.97	0.47
1:B:156:TRP:CD1	1:B:392:ARG:HG3	2.49	0.47
1:A:104:ILE:HD12	1:A:113:PRO:HD3	1.96	0.47
1:A:180:SER:HB2	1:A:376:GLU:OE1	2.15	0.47
1:A:68:LYS:HB2	1:A:230:TYR:CZ	2.50	0.47
1:B:275:SER:HB3	2:B:502:IS1:HAT	1.96	0.47
1:B:391:THR:HG22	1:B:392:ARG:N	2.29	0.47
1:A:68:LYS:HE3	1:A:69:TYR:OH	2.15	0.46
1:B:325:LEU:HD11	1:B:368:MET:CE	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LEU:O	1:B:395:LEU:CB	2.63	0.46
1:B:462:PHE:O	1:B:463:LYS:C	2.52	0.46
1:B:86:VAL:C	1:B:88:ARG:N	2.68	0.46
1:A:114:ILE:O	1:A:114:ILE:HG13	2.14	0.46
1:A:13:LEU:O	1:B:221:VAL:CG2	2.63	0.46
1:A:157:TYR:O	1:A:158:PRO:C	2.50	0.46
1:B:420:ASP:O	1:B:423:LYS:HB2	2.14	0.46
1:A:273:PRO:HG3	1:A:307:PRO:HD2	1.96	0.46
1:A:86:VAL:O	1:A:88:ARG:N	2.42	0.46
1:B:137:THR:HG21	1:B:464:ASN:OD1	2.16	0.46
1:B:233:THR:C	1:B:234:LYS:HD3	2.35	0.46
1:A:308:LEU:HG	1:A:308:LEU:O	2.13	0.46
1:A:418:VAL:HG11	1:B:282:ASP:OD2	2.16	0.46
1:B:415:LYS:H	1:B:425:SER:CB	2.28	0.46
1:B:455:HIS:CD2	1:B:455:HIS:N	2.84	0.46
1:A:262:PHE:O	1:A:266:VAL:HG22	2.16	0.46
1:A:26:TYR:O	1:A:27:PRO:C	2.47	0.46
1:A:35:SER:HA	1:A:401:CYS:HA	1.97	0.46
1:B:327:ILE:O	1:B:331:LYS:HG2	2.15	0.46
1:B:342:LYS:NZ	1:B:373:TRP:CZ2	2.84	0.46
1:B:391:THR:HB	1:B:394:LEU:CD1	2.46	0.46
1:A:192:ASP:C	1:A:192:ASP:OD1	2.54	0.46
1:B:153:VAL:O	1:B:155:SER:N	2.49	0.46
1:B:40:ARG:CG	1:B:400:LYS:HZ1	2.29	0.46
1:A:350:VAL:O	1:A:378:VAL:HA	2.16	0.46
1:A:83:ALA:O	1:A:86:VAL:HB	2.15	0.46
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.71	0.46
1:A:200:SER:HG	1:B:203:THR:HG1	1.59	0.46
1:B:56:GLU:OE2	1:B:124:VAL:HG12	2.15	0.46
1:A:17:SER:OG	1:A:90:HIS:CE1	2.65	0.46
1:A:289:LYS:HE3	1:A:289:LYS:HB2	1.75	0.46
1:A:92:GLN:O	1:A:93:ASP:HB2	2.16	0.46
1:B:311:ARG:NH1	2:B:502:IS1:HAP	2.31	0.46
1:A:151:ILE:CG2	1:A:152:LEU:N	2.78	0.45
1:A:299:ILE:HD12	1:A:308:LEU:HD23	1.99	0.45
1:B:171:ILE:HD12	1:B:171:ILE:N	2.31	0.45
1:A:467:VAL:O	1:A:467:VAL:HG12	2.16	0.45
1:B:18:TYR:CE2	1:B:19:LYS:HD3	2.52	0.45
1:B:447:LYS:C	1:B:449:ASP:N	2.69	0.45
1:A:427:LYS:NZ	1:A:427:LYS:HB2	2.26	0.45
1:B:243:PRO:HG3	1:B:269:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:THR:CG2	1:B:346:PRO:HB3	2.46	0.45
1:B:127:ARG:NH2	1:B:395:LEU:HA	2.31	0.45
1:B:86:VAL:O	1:B:88:ARG:N	2.44	0.45
1:A:208:ALA:HB3	1:A:223:GLY:CA	2.46	0.45
1:A:344:LEU:HB3	1:A:345:PRO:HD2	1.98	0.45
1:A:231:TYR:O	1:A:472:SER:HA	2.16	0.45
1:A:243:PRO:CB	1:B:21:THR:HG21	2.46	0.45
1:A:18:TYR:HD1	1:B:244:ALA:HB3	1.81	0.45
1:A:345:PRO:O	1:A:347:TYR:N	2.49	0.45
1:A:366:GLU:OE1	1:A:370:GLN:OE1	2.35	0.45
1:B:34:TYR:CD2	1:B:34:TYR:C	2.90	0.45
1:A:33:VAL:HG11	1:A:142:TYR:O	2.17	0.45
1:A:16:ASP:OD2	1:A:150:THR:CG2	2.65	0.45
1:A:275:SER:HA	1:A:309:ILE:O	2.16	0.45
1:B:138:ASP:HA	1:B:139:PRO:HD3	1.86	0.45
1:B:176:LEU:HD21	1:B:189:LYS:HE3	1.99	0.45
1:B:279:ASP:HB3	1:B:283:ILE:HD12	1.98	0.45
1:B:62:LEU:O	1:B:66:LEU:CB	2.66	0.45
1:A:119:VAL:HG11	1:A:125:ILE:CD1	2.43	0.44
1:A:374:SER:C	1:A:376:GLU:N	2.70	0.44
1:A:299:ILE:O	1:A:302:ARG:HG3	2.16	0.44
1:A:116:VAL:HB	1:A:462:PHE:HB3	1.99	0.44
1:B:153:VAL:O	1:B:156:TRP:HD1	1.99	0.44
1:A:19:LYS:C	1:A:21:THR:H	2.19	0.44
1:A:250:ILE:HD13	1:A:261:ALA:HB1	1.98	0.44
1:A:432:LEU:HD13	1:A:457:LEU:HD13	1.99	0.44
1:A:89:GLU:CD	1:B:236:PRO:O	2.55	0.44
1:B:211:HIS:CD2	1:B:386:LEU:HD21	2.53	0.44
1:B:432:LEU:HD13	1:B:457:LEU:HD12	1.98	0.44
1:A:244:ALA:HA	1:A:275:SER:O	2.18	0.44
1:A:414:PHE:CB	1:A:425:SER:HB2	2.47	0.44
1:B:308:LEU:HD21	1:B:310:ILE:CD1	2.45	0.44
1:B:311:ARG:CG	1:B:351:ILE:CG2	2.96	0.44
1:B:406:THR:O	1:B:407:ASN:HB2	2.18	0.44
1:A:257:HIS:HB3	1:A:260:ASP:HB2	1.99	0.44
1:A:379:SER:HB3	2:A:501:ISI:HAI	1.98	0.44
1:B:10:ASN:OD1	1:B:11:ILE:N	2.51	0.44
1:B:167:GLU:O	1:B:168:GLN:C	2.56	0.44
1:A:13:LEU:O	1:B:221:VAL:HG23	2.18	0.44
1:A:168:GLN:HG3	1:A:358:ILE:CD1	2.42	0.44
1:A:318:LEU:HD22	1:A:322:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLU:O	1:B:135:GLU:HG2	2.17	0.44
1:B:136:ASN:ND2	1:B:136:ASN:O	2.45	0.44
1:B:16:ASP:HB2	1:B:18:TYR:CE2	2.52	0.44
1:B:283:ILE:HD13	1:B:312:PRO:HA	1.97	0.44
2:A:501:IS1:HAXA	2:A:501:IS1:HAM	1.98	0.44
1:A:93:ASP:OD2	1:A:95:VAL:CG2	2.66	0.44
1:A:155:SER:C	1:A:157:TYR:H	2.21	0.44
1:A:84:LYS:HE3	1:A:98:GLU:OE1	2.17	0.44
1:B:472:SER:C	1:B:474:ASP:N	2.70	0.44
1:A:262:PHE:CD2	1:A:290:ILE:HG21	2.53	0.43
1:A:344:LEU:HB2	1:A:349:ARG:HH12	1.83	0.43
1:B:10:ASN:O	1:B:13:LEU:CD2	2.66	0.43
1:B:273:PRO:HG3	1:B:307:PRO:HD2	2.00	0.43
1:B:40:ARG:HD3	1:B:400:LYS:NZ	2.33	0.43
1:B:85:GLU:O	1:B:88:ARG:HB3	2.18	0.43
1:A:104:ILE:HD12	1:A:113:PRO:CD	2.48	0.43
1:A:134:VAL:HG11	1:A:148:ILE:HD11	1.99	0.43
1:A:157:TYR:HB3	1:A:158:PRO:CD	2.45	0.43
1:A:279:ASP:CG	1:A:279:ASP:O	2.54	0.43
1:A:314:SER:HB3	1:A:315:GLY:H	1.49	0.43
1:A:337:ASN:C	1:A:339:LYS:H	2.21	0.43
1:B:186:LEU:C	1:B:188:TYR:N	2.71	0.43
1:B:16:ASP:CB	1:B:18:TYR:CE2	3.01	0.43
1:A:273:PRO:HG3	1:A:305:GLU:O	2.17	0.43
1:A:337:ASN:O	1:A:339:LYS:N	2.51	0.43
1:B:13:LEU:CD2	1:B:13:LEU:H	2.21	0.43
1:B:203:THR:HG22	1:B:204:ALA:N	2.32	0.43
1:B:224:ILE:HA	1:B:227:ILE:HD12	1.99	0.43
1:A:10:ASN:OD1	1:A:12:LEU:HB2	2.17	0.43
1:A:291:TRP:CE2	1:A:310:ILE:HD11	2.52	0.43
1:A:387:LEU:HD22	1:A:387:LEU:HA	1.86	0.43
1:A:40:ARG:NE	1:A:422:ASN:O	2.51	0.43
1:A:433:HIS:HD2	1:A:443:LEU:HG	1.83	0.43
1:A:472:SER:C	1:A:474:ASP:N	2.71	0.43
1:A:9:PHE:CG	1:A:10:ASN:N	2.87	0.43
1:A:116:VAL:CG2	1:A:462:PHE:HB3	2.49	0.43
1:A:269:PHE:C	1:A:271:SER:N	2.65	0.43
1:B:309:ILE:HG21	1:B:351:ILE:HB	2.00	0.43
1:B:412:ASN:OD1	1:B:428:GLY:CA	2.66	0.43
1:A:311:ARG:HA	1:A:312:PRO:HD2	1.97	0.43
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:CG2	1:A:166:ARG:HD3	2.48	0.43
1:A:221:VAL:CG2	1:B:13:LEU:HB2	2.46	0.43
1:B:429:ARG:NH1	1:B:446:GLY:CA	2.79	0.43
1:A:68:LYS:HD3	1:A:69:TYR:CE1	2.54	0.43
1:B:449:ASP:C	1:B:451:GLU:N	2.72	0.43
1:B:12:LEU:O	1:B:87:TYR:CE1	2.72	0.43
1:A:296:ARG:O	1:A:299:ILE:HG22	2.19	0.42
1:A:315:GLY:O	1:A:316:ASN:CB	2.67	0.42
1:B:12:LEU:O	1:B:87:TYR:HE1	2.02	0.42
1:B:380:PHE:N	1:B:380:PHE:CD1	2.87	0.42
1:A:279:ASP:HB3	1:A:283:ILE:HD12	2.00	0.42
1:A:299:ILE:C	1:A:301:SER:H	2.23	0.42
1:A:328:LEU:HD13	1:A:348:LEU:HD11	2.01	0.42
1:B:56:GLU:OE2	1:B:124:VAL:CG1	2.67	0.42
1:B:374:SER:C	1:B:376:GLU:H	2.23	0.42
1:B:447:LYS:HB2	1:B:447:LYS:HE3	1.72	0.42
1:A:221:VAL:CG2	1:B:13:LEU:O	2.68	0.42
1:B:447:LYS:C	1:B:449:ASP:H	2.22	0.42
1:A:130:VAL:O	1:A:130:VAL:CG1	2.67	0.42
1:A:161:VAL:HB	1:A:210:ALA:CB	2.49	0.42
1:A:213:VAL:O	1:A:213:VAL:HG12	2.19	0.42
1:B:182:ASN:C	1:B:182:ASN:ND2	2.72	0.42
1:B:449:ASP:O	1:B:451:GLU:N	2.50	0.42
1:A:149:GLU:HG3	1:A:399:PHE:CE2	2.53	0.42
1:A:433:HIS:HB2	1:A:441:VAL:HG13	2.01	0.42
1:B:420:ASP:C	1:B:422:ASN:H	2.22	0.42
1:B:114:ILE:N	1:B:137:THR:CG2	2.83	0.42
1:B:130:VAL:HG13	1:B:130:VAL:O	2.19	0.42
1:A:21:THR:HG21	1:B:243:PRO:CB	2.48	0.42
1:B:394:LEU:O	1:B:395:LEU:HB2	2.19	0.42
1:A:311:ARG:HG3	1:A:351:ILE:CG1	2.46	0.42
1:A:439:THR:HB	1:A:440:PHE:H	1.35	0.42
1:B:36:TYR:HA	1:B:133:THR:HA	2.02	0.42
1:B:423:LYS:C	1:B:424:ARG:O	2.58	0.42
1:A:107:LYS:HB2	1:A:107:LYS:HZ2	1.82	0.42
1:A:351:ILE:HG13	1:A:351:ILE:O	2.20	0.42
1:B:136:ASN:ND2	1:B:136:ASN:N	2.67	0.42
1:A:206:ILE:N	1:A:206:ILE:CD1	2.82	0.41
1:A:158:PRO:HG3	1:A:206:ILE:CG2	2.49	0.41
1:A:351:ILE:HG22	1:A:379:SER:OG	2.19	0.41
1:B:19:LYS:HA	1:B:22:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:VAL:HG13	1:B:414:PHE:H	1.82	0.41
1:B:439:THR:HG23	1:B:440:PHE:H	1.79	0.41
1:A:130:VAL:O	1:A:130:VAL:HG13	2.20	0.41
1:A:160:THR:HG22	1:A:390:LEU:HG	2.02	0.41
1:B:289:LYS:HG3	1:B:290:ILE:N	2.35	0.41
1:B:311:ARG:NH1	2:B:502:IS1:CAP	2.83	0.41
1:A:153:VAL:C	1:A:155:SER:N	2.72	0.41
1:A:235:ASP:HB3	1:A:236:PRO:CD	2.50	0.41
1:A:248:SER:C	1:A:250:ILE:H	2.23	0.41
1:A:283:ILE:O	1:A:283:ILE:CG1	2.68	0.41
1:A:263:GLU:HB2	1:A:295:LEU:HD21	2.02	0.41
1:B:33:VAL:O	1:B:145:THR:HG21	2.20	0.41
1:A:243:PRO:HB3	1:B:21:THR:HG21	2.03	0.41
1:B:343:LEU:HD12	1:B:377:ASN:OD1	2.20	0.41
1:A:114:ILE:CG2	1:A:144:LEU:HD13	2.50	0.41
1:A:221:VAL:HG21	1:B:13:LEU:CB	2.48	0.41
1:A:418:VAL:CG1	1:A:419:ALA:N	2.83	0.41
1:B:337:ASN:ND2	1:B:339:LYS:N	2.53	0.41
1:B:429:ARG:HH11	1:B:446:GLY:HA3	1.81	0.41
1:A:12:LEU:HD22	1:A:101:TRP:CE2	2.54	0.41
1:A:117:LYS:O	1:A:132:PHE:HA	2.19	0.41
1:A:9:PHE:CE2	1:A:11:ILE:HD13	2.56	0.41
1:A:24:LYS:HB3	1:A:24:LYS:HE2	1.83	0.41
1:A:421:PRO:O	1:A:422:ASN:HB3	2.19	0.41
1:A:130:VAL:HG12	1:A:432:LEU:HB2	2.02	0.41
1:A:11:ILE:HG22	1:A:11:ILE:O	2.19	0.41
1:A:264:HIS:CG	1:A:264:HIS:O	2.73	0.41
1:A:390:LEU:HA	1:A:390:LEU:HD12	1.84	0.41
1:B:155:SER:HA	1:B:158:PRO:HD2	2.03	0.41
1:A:415:LYS:HG2	1:A:425:SER:OG	2.21	0.41
1:B:233:THR:CG2	1:B:235:ASP:HB2	2.51	0.41
1:B:279:ASP:N	1:B:283:ILE:HD12	2.36	0.41
1:B:313:ASP:O	1:B:314:SER:HB3	2.21	0.41
1:A:32:LYS:O	1:A:404:VAL:HG12	2.21	0.41
1:B:157:TYR:HB3	1:B:158:PRO:CD	2.44	0.41
1:B:155:SER:C	1:B:157:TYR:N	2.71	0.41
1:B:250:ILE:HD11	1:B:265:ILE:HD12	2.01	0.41
1:A:245:ALA:HA	1:B:25:GLN:OE1	2.21	0.41
1:A:233:THR:HG22	1:A:235:ASP:N	2.36	0.41
1:B:137:THR:H	1:B:137:THR:HG1	1.54	0.41
1:B:212:LEU:HD12	1:B:227:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLN:O	1:B:389:LYS:CB	2.68	0.41
1:A:18:TYR:CD2	1:B:219:ASP:OD2	2.74	0.41
1:A:202:GLU:O	1:A:206:ILE:CD1	2.58	0.41
1:A:227:ILE:H	1:A:227:ILE:HG13	1.76	0.41
1:B:155:SER:O	1:B:156:TRP:C	2.60	0.41
1:A:120:PRO:HA	1:A:471:TYR:OH	2.21	0.40
1:A:295:LEU:O	1:A:297:HIS:N	2.54	0.40
1:B:150:THR:O	1:B:151:ILE:C	2.59	0.40
1:B:54:TYR:OH	1:B:358:ILE:HG21	2.21	0.40
1:A:190:LEU:O	1:A:211:HIS:HE1	2.04	0.40
1:A:221:VAL:CG2	1:A:222:ALA:N	2.83	0.40
1:A:434:ARG:HB2	1:A:434:ARG:HE	1.75	0.40
1:B:113:PRO:HG2	1:B:113:PRO:O	2.22	0.40
1:B:19:LYS:O	1:B:22:HIS:HB2	2.21	0.40
1:B:412:ASN:HB3	1:B:427:LYS:HB3	2.03	0.40
1:B:66:LEU:HD11	1:B:462:PHE:HB2	2.03	0.40
1:A:360:THR:O	1:A:364:ILE:HG12	2.21	0.40
1:B:74:VAL:N	1:B:110:GLY:O	2.50	0.40
1:B:151:ILE:CG2	1:B:152:LEU:H	2.33	0.40
1:B:291:TRP:CD1	1:B:310:ILE:HD12	2.57	0.40
1:B:32:LYS:O	1:B:404:VAL:HG23	2.21	0.40
1:B:125:ILE:HD12	1:B:125:ILE:N	2.37	0.40
1:A:87:TYR:HE2	1:B:221:VAL:HG11	1.83	0.40
1:B:55:GLU:HA	1:B:127:ARG:CD	2.52	0.40
1:B:10:ASN:ND2	1:B:79:LYS:HB3	2.36	0.40
1:A:477:ARG:HB2	1:A:478:LYS:H	1.73	0.40
1:A:242:VAL:HG13	2:A:501:IS1:HAU	2.03	0.40
1:B:10:ASN:OD1	1:B:10:ASN:C	2.59	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	459/491 (94%)	372 (81%)	58 (13%)	29 (6%)	1	9
1	B	459/491 (94%)	371 (81%)	61 (13%)	27 (6%)	2	11
All	All	918/982 (94%)	743 (81%)	119 (13%)	56 (6%)	2	10

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	271	SER
1	A	282	ASP
1	B	71	LYS
1	B	72	GLY
1	B	282	ASP
1	B	354	ASP
1	B	414	PHE
1	B	424	ARG
1	B	452	GLU
1	A	154	GLN
1	A	187	GLU
1	A	237	VAL
1	A	338	SER
1	A	346	PRO
1	A	439	THR
1	A	451	GLU
1	A	454	GLY
1	B	22	HIS
1	B	67	ASN
1	B	168	GLN
1	B	187	GLU
1	B	195	TYR
1	B	463	LYS
1	A	17	SER
1	A	126	PRO
1	A	145	THR
1	A	150	THR
1	A	372	LYS
1	A	422	ASN
1	A	478	LYS
1	B	154	GLN
1	B	236	PRO
1	B	288	GLU
1	B	375	ILE

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Mol	Chain	Res	Type
1	A	232	GLY
1	A	316	ASN
1	A	456	ASP
1	A	477	ARG
1	B	113	PRO
1	B	338	SER
1	B	469	LYS
1	A	71	LYS
1	A	93	ASP
1	A	421	PRO
1	B	167	GLU
1	B	283	ILE
1	B	410	GLY
1	A	296	ARG
1	B	372	LYS
1	A	194	GLY
1	A	283	ILE
1	B	139	PRO
1	B	418	VAL
1	B	446	GLY
1	A	157	TYR

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	408/431 (95%)	345 (85%)	63 (15%)	3	15
1	B	408/431 (95%)	343 (84%)	65 (16%)	3	14
All	All	816/862 (95%)	688 (84%)	128 (16%)	3	14

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	13	LEU

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Mol	Chain	Res	Type
1	A	18	TYR
1	A	19	LYS
1	A	30	THR
1	A	32	LYS
1	A	33	VAL
1	A	34	TYR
1	A	77	LYS
1	A	88	ARG
1	A	94	ASP
1	A	107	LYS
1	A	119	VAL
1	A	144	LEU
1	A	150	THR
1	A	151	ILE
1	A	174	LYS
1	A	179	THR
1	A	180	SER
1	A	186	LEU
1	A	187	GLU
1	A	189	LYS
1	A	190	LEU
1	A	192	ASP
1	A	195	TYR
1	A	196	ARG
1	A	206	ILE
1	A	219	ASP
1	A	224	ILE
1	A	228	LYS
1	A	234	LYS
1	A	237	VAL
1	A	275	SER
1	A	295	LEU
1	A	316	ASN
1	A	318	LEU
1	A	331	LYS
1	A	334	VAL
1	A	335	SER
1	A	342	LYS
1	A	352	GLN
1	A	354	ASP
1	A	366	GLU
1	A	369	LYS

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Mol	Chain	Res	Type
1	A	374	SER
1	A	376	GLU
1	A	379	SER
1	A	387	LEU
1	A	388	GLN
1	A	390	LEU
1	A	391	THR
1	A	398	SER
1	A	400	LYS
1	A	404	VAL
1	A	409	LEU
1	A	414	PHE
1	A	424	ARG
1	A	431	SER
1	A	439	THR
1	A	451	GLU
1	A	452	GLU
1	A	457	LEU
1	A	483	ASN
1	B	11	ILE
1	B	13	LEU
1	B	18	TYR
1	B	19	LYS
1	B	34	TYR
1	B	66	LEU
1	B	70	LEU
1	B	76	THR
1	B	85	GLU
1	B	88	ARG
1	B	92	GLN
1	B	94	ASP
1	B	99	ARG
1	B	102	ASN
1	B	119	VAL
1	B	136	ASN
1	B	137	THR
1	B	138	ASP
1	B	144	LEU
1	B	150	THR
1	B	165	SER
1	B	180	SER
1	B	182	ASN

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Mol	Chain	Res	Type
1	B	186	LEU
1	B	190	LEU
1	B	195	TYR
1	B	203	THR
1	B	219	ASP
1	B	226	LEU
1	B	233	THR
1	B	235	ASP
1	B	237	VAL
1	B	275	SER
1	B	277	VAL
1	B	334	VAL
1	B	337	ASN
1	B	338	SER
1	B	342	LYS
1	B	344	LEU
1	B	351	ILE
1	B	352	GLN
1	B	354	ASP
1	B	360	THR
1	B	368	MET
1	B	376	GLU
1	B	386	LEU
1	B	387	LEU
1	B	389	LYS
1	B	390	LEU
1	B	395	LEU
1	B	399	PHE
1	B	406	THR
1	B	409	LEU
1	B	414	PHE
1	B	423	LYS
1	B	429	ARG
1	B	431	SER
1	B	432	LEU
1	B	449	ASP
1	B	451	GLU
1	B	452	GLU
1	B	453	TYR
1	B	455	HIS
1	B	481	GLN
1	B	482	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	81	GLN
1	A	90	HIS
1	A	92	GLN
1	A	102	ASN
1	A	111	HIS
1	A	146	ASN
1	A	164	ASN
1	A	182	ASN
1	A	211	HIS
1	A	316	ASN
1	A	388	GLN
1	A	396	ASN
1	B	22	HIS
1	B	81	GLN
1	B	90	HIS
1	B	102	ASN
1	B	111	HIS
1	B	129	ASN
1	B	136	ASN
1	B	164	ASN
1	B	168	GLN
1	B	182	ASN
1	B	201	GLN
1	B	211	HIS
1	B	214	ASN
1	B	337	ASN
1	B	370	GLN
1	B	422	ASN
1	B	455	HIS
1	B	459	HIS
1	B	481	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IS1	A	501	-	39,41,41	1.46	5 (12%)	48,55,55	2.23	9 (18%)
2	IS1	B	502	-	39,41,41	1.33	6 (15%)	48,55,55	2.18	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IS1	A	501	-	-	0/23/53/53	0/4/4/4
2	IS1	B	502	-	-	0/23/53/53	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IS1	O4'-C4'	-5.09	1.33	1.45
2	B	502	IS1	CAF-CBB	-5.06	1.38	1.48
2	A	501	IS1	CAF-CBB	-4.60	1.39	1.48
2	B	502	IS1	CBD-CAG	-2.81	1.39	1.47
2	A	501	IS1	CBD-CAG	-2.65	1.39	1.47
2	A	501	IS1	CAF-CAG	2.16	1.38	1.32
2	B	502	IS1	CBE-CBC	2.23	1.53	1.50
2	A	501	IS1	CBE-CBC	2.25	1.53	1.50
2	B	502	IS1	O5'-C5'	2.33	1.52	1.42
2	B	502	IS1	O4'-C1'	2.46	1.44	1.41
2	B	502	IS1	CAF-CAG	2.52	1.39	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IS1	C2'-C3'-C4'	-4.99	92.90	102.62
2	A	501	IS1	C4'-O4'-C1'	-3.61	105.92	109.77
2	A	501	IS1	CBD-CAG-CAF	-3.54	118.21	126.92
2	B	502	IS1	C4'-O4'-C1'	-3.40	106.16	109.77
2	B	502	IS1	CBD-CAG-CAF	-2.57	120.60	126.92
2	A	501	IS1	CAS-CAU-CBF	-2.33	103.41	115.82
2	A	501	IS1	CAR-CAT-NAZ	-2.25	105.72	112.18
2	B	502	IS1	CAU-CBF-CAV	-2.13	107.26	112.11
2	B	502	IS1	CAR-CAT-NAZ	-2.06	106.24	112.18
2	B	502	IS1	CAX-NBK-CAY	4.57	121.25	112.61
2	A	501	IS1	O3'-C3'-C4'	4.72	124.86	111.09
2	A	501	IS1	CAX-NBK-CAY	5.48	122.97	112.61
2	A	501	IS1	C5'-C4'-C3'	6.06	129.68	115.05
2	B	502	IS1	O4'-C4'-C5'	6.56	123.19	109.16
2	B	502	IS1	O3'-C3'-C4'	7.20	132.12	111.09
2	B	502	IS1	O2'-C2'-C1'	7.51	135.10	111.61
2	A	501	IS1	O3'-C3'-C2'	7.54	135.98	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IS1	15	0
2	B	502	IS1	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	463/491 (94%)	-0.07	3 (0%)	89 71	7, 33, 56, 78	0
1	B	463/491 (94%)	-0.10	2 (0%)	92 77	10, 32, 55, 79	0
All	All	926/982 (94%)	-0.08	5 (0%)	90 74	7, 33, 56, 79	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ASP	2.8
1	A	455	HIS	2.4
1	A	238	PRO	2.2
1	A	204	ALA	2.1
1	B	294	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	IS1	A	501	38/38	0.74	0.41	4.62	54,64,87,89	0
2	IS1	B	502	38/38	0.75	0.40	4.21	56,62,78,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.