



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:39 AM GMT

PDB ID : 2BAN
Title : Crystal structure of HIV-1 reverse transcriptase (RT) in complex with JANSSEN-R157208
Authors : Das, K.; Arnold, E.
Deposited on : 2005-10-14
Resolution : 2.95 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

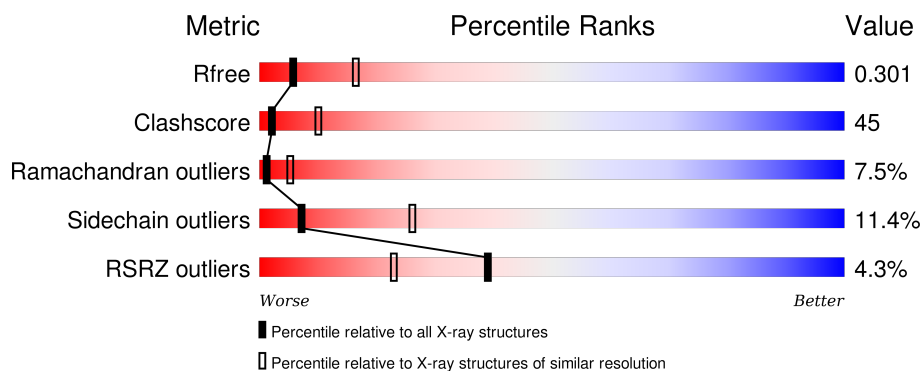
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	560	<div> <div>2%</div> <div>34%</div> <div>52%</div> <div>11%</div> <div>..</div> </div>
2	B	430	<div> <div>7%</div> <div>37%</div> <div>50%</div> <div>12%</div> <div>.</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
4	357	A	562	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7922 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 Reverse transcriptase P66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4431	2864	733	827	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called Reverse transcriptase P51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3465	2256	570	633	6			

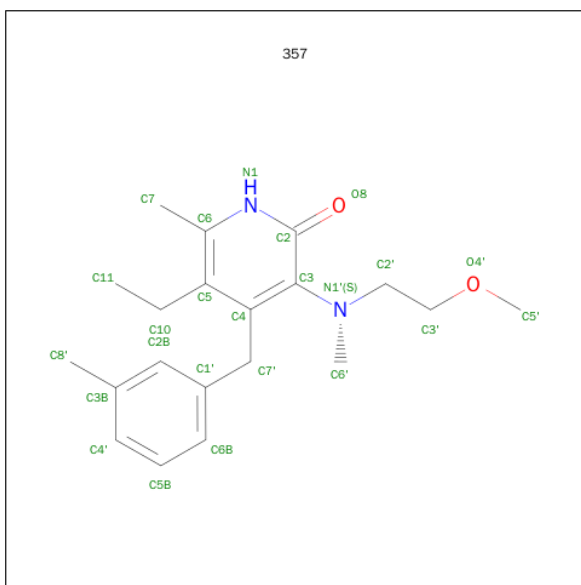
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-ETHYL-3-[(2-METHOXYETHYL)METHYLAMINO]-6-METHYL-4-(3-METHYLBENZYL)PYRIDIN-2(1H)-ONE (three-letter code: 357) (formula: C₂₀H₂₈N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	20	2	2		

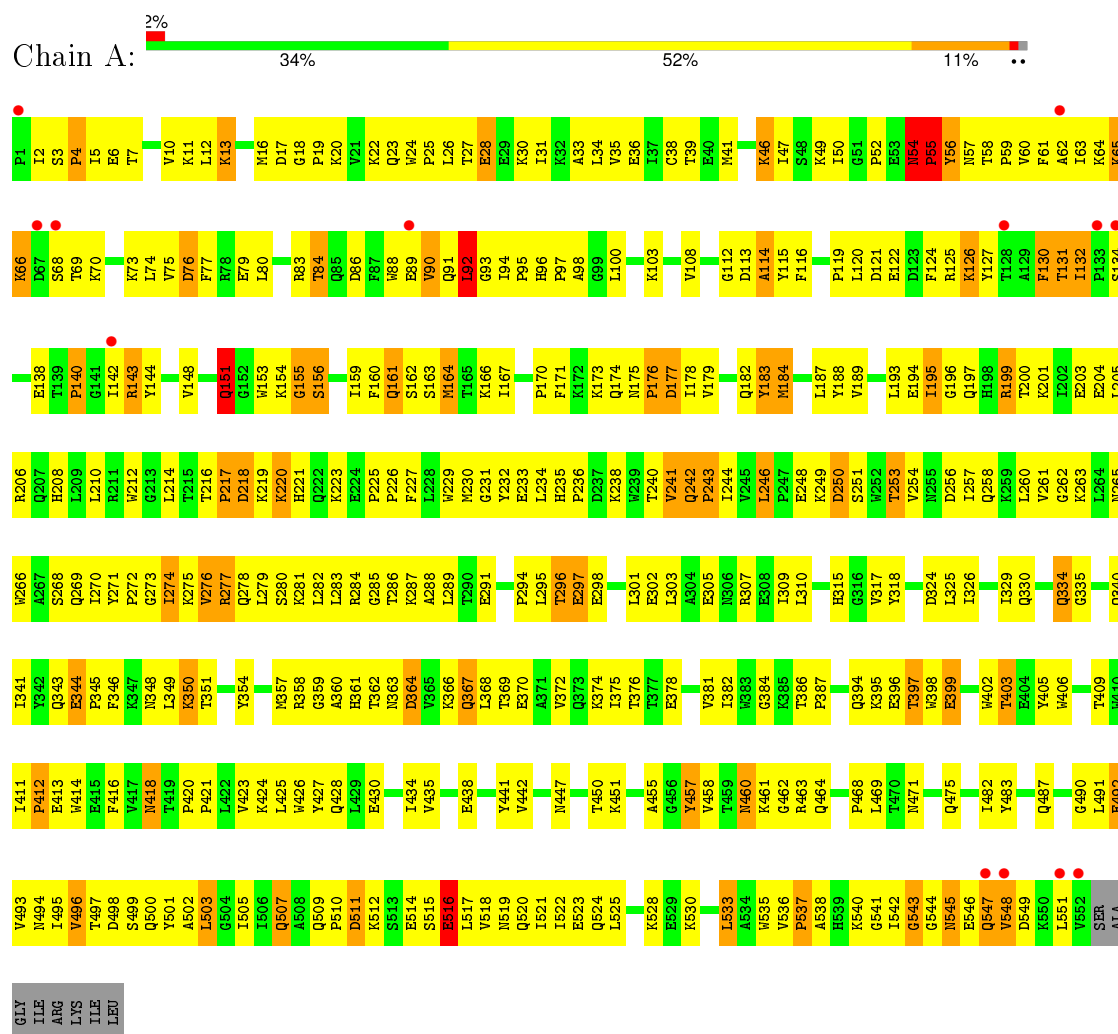
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0

3 Residue-property plots

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

• Molecule 1: Reverse transcriptase P66 subunit



F416	L349	T286	Q222	D86
V417	K350		K223	F87
N418			E224	W88
T419	K353	L289	P225	E89
P420	Y354	T290	F226	F160
A421	A355	V292	P227	Q161
L422	K356	I293	L228	S162
V423	K357	P294	W229	S163
K424	K358	L295	P230	M164
L425	G359	T296	W231	T165
W426	A360	E297	Y232	K166
Y427	H361	E298		I167
GLN	T362	A299	E235	L100
LEU	N363	E300	P236	K101
GLU	D364	L301	D237	K102
	V365	E302	K238	K103
	K366		W239	K104
	Q367	E305	T240	S105
	L368	N306	V241	V106
	T369	K307	Q242	T107
	E370	E308	I244	V108
	A371	I309	V245	V111
	V372	L310	P247	G112
	Q373	K311	E248	D113
	K374	E312	R249	A114
	I375	P313	D250	Y115
	T376	V314	S251	F116
	T377	H315	W252	S117
	E378	G316	T253	V118
	S379	V317	V254	F124
	I380	V318	N255	R125
	V381	D320	D256	K126
	G384	P321	I257	Y127
	K385	S322	Q258	Y128
	T386	K323	K259	I195
	P387	D324	L260	G196
	K388	L325	V261	F130
		I326	G262	T131
	P392		K263	I132
	I393	I329	L264	I135
	Q394	Q330	N265	N136
	K395	K331	W266	N137
	W398	G333		E138
	E399	Q334	Y271	T139
	T400	G335	P272	P140
	W401	Q336	G273	G141
	W402	K337	I274	I142
		T338	K275	R143
	W406	V339	V276	Y144
	Q407	Q340	R277	Q145
	A408	I341	Q278	Y146
	T409	V342	L279	
	W410	Q343	S280	L149
	I411	E344	K281	P150
	P412	P345	L282	Q151
	E413	F346	L283	G152
	W414	K347	R284	W153
	E415	N348	G285	K154
				G155

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.24Å 69.43Å 104.45Å 90.00° 106.49° 90.00°	Depositor
Resolution (Å)	19.86 – 2.95 32.37 – 2.95	Depositor EDS
% Data completeness (in resolution range)	91.9 (19.86-2.95) 93.8 (32.37-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.305 0.243 , 0.301	Depositor DCC
R_{free} test set	1533 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 31024 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7922	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 357, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/4546	0.78	5/6185 (0.1%)
2	B	0.49	0/3566	0.77	1/4856 (0.0%)
All	All	0.46	0/8112	0.78	6/11041 (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
2	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	55	PRO	N-CA-C	10.91	140.47	112.10
1	A	26	LEU	N-CA-C	7.64	131.63	111.00
1	A	54	ASN	N-CA-C	5.32	125.35	111.00
1	A	55	PRO	CA-C-N	-5.15	105.87	117.20
2	B	89	GLU	N-CA-C	-5.09	97.25	111.00
1	A	151	GLN	N-CA-C	5.07	124.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	232	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4431	0	4413	429	0
2	B	3465	0	3456	297	0
3	A	1	0	0	0	0
4	A	24	0	28	6	0
5	A	1	0	0	0	0
All	All	7922	0	7897	711	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 45.

All (711) 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:362:THR:HG22	1:A:363:ASN:H	1.08	1.18
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.06	1.15
1:A:132:ILE:HG13	1:A:142:ILE:HB	1.30	1.13
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.31	1.11
1:A:54:ASN:HB2	1:A:55:PRO:HD3	1.32	1.07
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.14	1.06
1:A:241:VAL:HG11	1:A:266:TRP:NE1	1.71	1.02
1:A:242:GLN:HB2	1:A:243:PRO:HD3	1.34	1.02
1:A:131:THR:HG23	1:A:143:ARG:HD2	1.39	1.02
1:A:241:VAL:CG1	1:A:266:TRP:HE1	1.78	0.97
1:A:362:THR:HG22	1:A:363:ASN:N	1.79	0.97
1:A:362:THR:CG2	1:A:363:ASN:H	1.80	0.94
2:B:276:VAL:H	2:B:277:ARG:HH11	0.96	0.94
1:A:35:VAL:HG22	1:A:132:ILE:HD12	1.50	0.94
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.47	0.93
1:A:161:GLN:HG2	1:A:182:GLN:HE21	1.31	0.93
1:A:218:ASP:C	1:A:220:LYS:H	1.63	0.92
2:B:11:LYS:HD3	2:B:11:LYS:H	1.35	0.92
2:B:87:PHE:O	2:B:91:GLN:HB2	1.70	0.90
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.16	0.90
2:B:149:LEU:HD22	2:B:156:SER:HA	1.51	0.89
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.54	0.88
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.54	0.87
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.71	0.87
1:A:164:MET:HE3	1:A:187:LEU:HD11	1.57	0.87
1:A:240:THR:HG22	1:A:241:VAL:H	1.38	0.87
2:B:277:ARG:O	2:B:281:LYS:HG3	1.75	0.86
1:A:460:ASN:ND2	1:A:461:LYS:H	1.73	0.86
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.10	0.86
1:A:270:ILE:O	1:A:272:PRO:HD3	1.76	0.85
1:A:460:ASN:HD22	1:A:461:LYS:H	1.22	0.85
1:A:249:LYS:HG3	1:A:250:ASP:H	1.40	0.85
2:B:276:VAL:N	2:B:277:ARG:HH11	1.74	0.85
2:B:277:ARG:CD	2:B:277:ARG:H	1.90	0.84
1:A:195:ILE:H	1:A:195:ILE:HD12	1.40	0.84
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.59	0.84
1:A:54:ASN:HB2	1:A:55:PRO:CD	2.08	0.84
1:A:90:VAL:HG23	1:A:91:GLN:H	1.44	0.83
1:A:231:GLY:O	1:A:241:VAL:HG13	1.78	0.82
2:B:241:VAL:HG13	2:B:243:PRO:HD3	1.62	0.82
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.15	0.82
1:A:64:LYS:HE2	1:A:68:SER:HA	1.62	0.82
1:A:450:THR:O	1:A:451:LYS:HG2	1.79	0.82
1:A:233:GLU:CD	1:A:242:GLN:HE21	1.83	0.82
1:A:27:THR:CG2	1:A:30:LYS:HB2	2.09	0.81
2:B:78:ARG:HD3	2:B:412:PRO:O	1.79	0.81
1:A:74:LEU:HD12	1:A:75:VAL:H	1.45	0.81
1:A:132:ILE:CG1	1:A:142:ILE:HB	2.10	0.81
2:B:139:THR:HB	2:B:140:PRO:HD2	1.63	0.80
2:B:276:VAL:H	2:B:277:ARG:NH1	1.78	0.80
2:B:306:ASN:ND2	2:B:309:ILE:HD12	1.97	0.79
2:B:350:LYS:HE3	2:B:378:GLU:OE1	1.82	0.79
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.63	0.79
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.12	0.79
2:B:275:LYS:HA	2:B:277:ARG:NH1	1.98	0.79
2:B:235:HIS:HB2	2:B:238:LYS:HE3	1.64	0.79
2:B:125:ARG:O	2:B:127:TYR:N	2.16	0.79
2:B:241:VAL:HG22	2:B:242:GLN:H	1.48	0.78
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.48	0.78
2:B:253:THR:HG22	2:B:292:VAL:HG22	1.65	0.78
2:B:156:SER:N	2:B:157:PRO:HD2	1.99	0.78
1:A:74:LEU:HD12	1:A:75:VAL:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:GLU:O	2:B:226:PRO:HD3	1.84	0.78
1:A:279:LEU:H	1:A:279:LEU:HD12	1.49	0.78
2:B:284:ARG:NH1	2:B:284:ARG:HG3	1.90	0.77
2:B:149:LEU:HD21	2:B:159:ILE:HD12	1.66	0.77
2:B:31:ILE:O	2:B:35:VAL:HG23	1.83	0.77
2:B:206:ARG:HE	2:B:217:PRO:HB2	1.48	0.77
2:B:296:THR:HG22	2:B:297:GLU:N	2.00	0.77
2:B:11:LYS:HD3	2:B:11:LYS:N	1.97	0.77
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.15	0.76
1:A:218:ASP:C	1:A:220:LYS:N	2.38	0.76
2:B:156:SER:H	2:B:157:PRO:HD2	1.50	0.76
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.21	0.76
2:B:128:THR:OG1	2:B:146:TYR:HB2	1.86	0.76
1:A:460:ASN:ND2	1:A:461:LYS:N	2.34	0.75
1:A:23:GLN:O	1:A:25:PRO:HD3	1.86	0.75
2:B:296:THR:CG2	2:B:297:GLU:H	1.99	0.75
1:A:66:LYS:C	1:A:68:SER:H	1.89	0.75
2:B:314:VAL:HG12	2:B:315:HIS:H	1.49	0.75
1:A:195:ILE:H	1:A:195:ILE:CD1	2.00	0.74
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.22	0.74
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.69	0.74
1:A:511:ASP:OD1	1:A:512:LYS:HG2	1.87	0.74
2:B:278:GLN:NE2	2:B:281:LYS:HD2	2.02	0.74
2:B:101:LYS:O	2:B:236:PRO:HB2	1.87	0.74
2:B:66:LYS:C	2:B:68:SER:H	1.90	0.73
2:B:277:ARG:HD3	2:B:277:ARG:H	1.53	0.73
2:B:149:LEU:CD2	2:B:156:SER:HA	2.19	0.72
1:A:92:LEU:HG	1:A:93:GLY:N	2.05	0.72
1:A:278:GLN:HG2	1:A:302:GLU:OE2	1.89	0.72
1:A:317:VAL:HG12	1:A:348:ASN:O	1.90	0.72
1:A:242:GLN:HB2	1:A:243:PRO:CD	2.16	0.71
2:B:28:GLU:HG2	2:B:32:LYS:HE3	1.72	0.71
2:B:340:GLN:HG2	2:B:426:TRP:CZ2	2.24	0.71
2:B:174:GLN:O	2:B:176:PRO:HD3	1.89	0.71
2:B:281:LYS:HA	2:B:284:ARG:NH1	2.06	0.71
2:B:253:THR:O	2:B:257:ILE:HG22	1.90	0.70
2:B:166:LYS:HE2	2:B:212:TRP:HH2	1.57	0.70
1:A:240:THR:HG22	1:A:241:VAL:N	2.07	0.69
2:B:253:THR:H	2:B:256:ASP:HB2	1.57	0.69
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.74	0.69
1:A:161:GLN:HG2	1:A:182:GLN:NE2	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SER:HA	1:A:166:LYS:HE3	1.74	0.69
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.58	0.69
2:B:241:VAL:HG22	2:B:242:GLN:N	2.06	0.68
1:A:242:GLN:CB	1:A:243:PRO:HD3	2.19	0.68
2:B:296:THR:CG2	2:B:297:GLU:N	2.55	0.68
1:A:487:GLN:HG3	1:A:524:GLN:HE22	1.58	0.68
2:B:7:THR:O	2:B:9:PRO:HD3	1.94	0.68
1:A:64:LYS:HE2	1:A:68:SER:CA	2.24	0.68
1:A:242:GLN:O	1:A:244:ILE:HG13	1.94	0.68
1:A:195:ILE:HD12	1:A:195:ILE:N	2.08	0.67
2:B:306:ASN:HD22	2:B:309:ILE:HD12	1.60	0.67
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.95	0.67
2:B:380:ILE:O	2:B:384:GLY:HA2	1.95	0.67
2:B:314:VAL:HG12	2:B:315:HIS:N	2.09	0.67
2:B:279:LEU:HD12	2:B:299:ALA:HB1	1.77	0.67
4:A:562:357:H5'1	2:B:138:GLU:HB3	1.77	0.67
2:B:12:LEU:HA	2:B:84:THR:HG22	1.75	0.67
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.77	0.67
2:B:66:LYS:HZ1	2:B:218:ASP:HB2	1.59	0.66
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.76	0.66
1:A:210:LEU:HA	1:A:214:LEU:O	1.96	0.66
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.90	0.66
1:A:296:THR:HG22	1:A:297:GLU:N	2.11	0.66
1:A:59:PRO:HB2	1:A:61:PHE:CE1	2.31	0.65
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.78	0.65
1:A:20:LYS:HG2	1:A:56:TYR:HB3	1.77	0.65
1:A:493:VAL:HG22	1:A:494:ASN:N	2.11	0.65
1:A:65:LYS:HE2	1:A:66:LYS:CA	2.26	0.65
1:A:65:LYS:HE2	1:A:66:LYS:HA	1.79	0.65
2:B:296:THR:HG22	2:B:297:GLU:H	1.58	0.65
1:A:297:GLU:OE1	1:A:297:GLU:N	2.30	0.65
2:B:219:LYS:NZ	2:B:219:LYS:HB3	2.12	0.65
2:B:349:LEU:HD23	2:B:349:LEU:N	2.11	0.65
1:A:60:VAL:C	1:A:61:PHE:HD1	2.00	0.65
1:A:298:GLU:H	1:A:298:GLU:CD	2.00	0.64
1:A:41:MET:HB2	1:A:47:ILE:HD11	1.79	0.64
1:A:138:GLU:HG3	1:A:138:GLU:O	1.98	0.64
1:A:398:TRP:CH2	1:A:411:ILE:HD11	2.32	0.64
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.80	0.64
1:A:521:ILE:O	1:A:525:LEU:HG	1.97	0.64
1:A:265:ASN:O	1:A:268:SER:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:O	2:B:284:ARG:HA	1.97	0.64
1:A:28:GLU:H	1:A:28:GLU:CD	2.02	0.64
2:B:366:LYS:O	2:B:370:GLU:HG3	1.98	0.63
1:A:358:ARG:C	1:A:360:ALA:H	2.02	0.63
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.32	0.63
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.29	0.63
2:B:277:ARG:CD	2:B:277:ARG:N	2.58	0.63
1:A:286:THR:HG22	1:A:288:ALA:H	1.64	0.63
2:B:373:GLN:HE22	2:B:407:GLN:H	1.45	0.63
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.80	0.63
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.81	0.63
1:A:324:ASP:O	1:A:326:ILE:HD12	1.98	0.63
1:A:537:PRO:HB2	1:A:541:GLY:HA3	1.81	0.63
1:A:276:VAL:O	1:A:276:VAL:HG12	1.98	0.63
1:A:430:GLU:CD	1:A:530:LYS:HE3	2.20	0.62
1:A:96:HIS:CE1	1:A:350:LYS:HD2	2.34	0.62
1:A:277:ARG:HD2	1:A:334:GLN:HB2	1.81	0.62
1:A:509:GLN:N	1:A:510:PRO:HD3	2.14	0.62
2:B:66:LYS:O	2:B:68:SER:N	2.33	0.62
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.81	0.62
2:B:1:PRO:HD2	2:B:117:SER:HA	1.82	0.62
1:A:17:ASP:O	1:A:83:ARG:HD3	1.98	0.62
2:B:17:ASP:O	2:B:83:ARG:NH1	2.33	0.62
2:B:146:TYR:CG	2:B:150:PRO:HG3	2.35	0.62
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.82	0.61
2:B:1:PRO:CD	2:B:117:SER:HA	2.29	0.61
1:A:235:HIS:CD2	1:A:238:LYS:HG3	2.35	0.61
1:A:434:ILE:H	1:A:494:ASN:HD21	1.48	0.61
1:A:286:THR:HG21	1:A:291:GLU:OE1	2.00	0.61
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.35	0.61
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.35	0.61
2:B:335:GLY:O	2:B:355:ALA:HA	2.01	0.61
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.81	0.61
1:A:503:LEU:HD11	1:A:507:GLN:OE1	2.00	0.61
2:B:421:PRO:HG2	2:B:422:LEU:H	1.65	0.60
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.83	0.60
1:A:126:LYS:HB3	1:A:126:LYS:NZ	2.16	0.60
1:A:108:VAL:O	1:A:108:VAL:HG23	2.00	0.60
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.83	0.60
1:A:441:TYR:O	1:A:548:VAL:HG11	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:N	1:A:219:LYS:HD2	2.16	0.60
1:A:49:LYS:HA	1:A:143:ARG:O	2.01	0.60
1:A:495:ILE:HB	1:A:533:LEU:HD22	1.83	0.60
2:B:213:GLY:C	2:B:215:THR:H	2.05	0.60
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.84	0.60
1:A:170:PRO:HB2	1:A:174:GLN:NE2	2.16	0.60
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.37	0.60
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.32	0.60
2:B:100:LEU:HD11	2:B:106:VAL:CG1	2.32	0.60
1:A:132:ILE:HG13	1:A:142:ILE:CB	2.20	0.59
2:B:371:ALA:O	2:B:375:ILE:HG13	2.02	0.59
1:A:19:PRO:O	1:A:56:TYR:HB2	2.02	0.59
2:B:281:LYS:HG2	2:B:284:ARG:CZ	2.32	0.59
2:B:365:VAL:HG12	2:B:366:LYS:N	2.17	0.59
2:B:275:LYS:O	2:B:302:GLU:CD	2.41	0.59
2:B:277:ARG:N	2:B:277:ARG:HD2	2.17	0.59
2:B:326:ILE:HG21	2:B:342:TYR:CE1	2.37	0.59
1:A:426:TRP:O	1:A:427:TYR:HB3	2.03	0.59
1:A:451:LYS:HE3	1:A:471:ASN:ND2	2.17	0.59
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.32	0.59
1:A:124:PHE:O	1:A:124:PHE:CD2	2.55	0.59
1:A:460:ASN:N	1:A:460:ASN:HD22	2.00	0.59
1:A:540:LYS:HE3	2:B:265:ASN:HD21	1.68	0.59
1:A:238:LYS:HE2	1:A:315:HIS:HB2	1.85	0.58
2:B:154:LYS:HG2	2:B:184:MET:HG2	1.83	0.58
1:A:57:ASN:ND2	1:A:58:THR:H	2.01	0.58
1:A:499:SER:OG	1:A:502:ALA:HB3	2.02	0.58
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.04	0.58
1:A:244:ILE:HD13	1:A:310:LEU:HD22	1.86	0.58
1:A:201:LYS:HA	1:A:204:GLU:HG3	1.85	0.58
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.39	0.58
2:B:166:LYS:HE2	2:B:212:TRP:CH2	2.38	0.58
1:A:46:LYS:HE2	1:A:116:PHE:O	2.03	0.58
1:A:19:PRO:O	1:A:56:TYR:CB	2.52	0.58
2:B:206:ARG:NE	2:B:217:PRO:HB2	2.19	0.58
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.39	0.58
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.39	0.57
1:A:420:PRO:HA	1:A:421:PRO:C	2.24	0.57
1:A:34:LEU:CD1	1:A:132:ILE:HG22	2.35	0.57
1:A:188:TYR:CD2	4:A:562:357:H6'	2.39	0.57
2:B:66:LYS:C	2:B:68:SER:N	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LEU:O	1:A:520:GLN:HB2	2.04	0.57
1:A:34:LEU:HD12	1:A:132:ILE:HG22	1.86	0.57
1:A:242:GLN:O	1:A:244:ILE:N	2.35	0.57
1:A:545:ASN:HA	1:A:548:VAL:HG23	1.85	0.57
1:A:33:ALA:O	1:A:36:GLU:HB3	2.04	0.57
1:A:164:MET:CE	1:A:187:LEU:HD11	2.32	0.57
2:B:91:GLN:C	2:B:91:GLN:HE21	2.07	0.57
2:B:266:TRP:HH2	2:B:426:TRP:CZ3	2.22	0.57
1:A:490:GLY:O	1:A:492:GLU:N	2.37	0.57
1:A:460:ASN:HD22	1:A:461:LYS:N	1.92	0.57
1:A:296:THR:HG22	1:A:298:GLU:OE1	2.05	0.57
2:B:297:GLU:OE1	2:B:297:GLU:HA	2.04	0.56
2:B:373:GLN:NE2	2:B:407:GLN:H	2.02	0.56
1:A:108:VAL:CG1	1:A:188:TYR:CD2	2.86	0.56
1:A:94:ILE:HD13	1:A:230:MET:HG3	1.87	0.56
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.39	0.56
1:A:284:ARG:HG3	1:A:285:GLY:N	2.19	0.56
2:B:156:SER:N	2:B:157:PRO:CD	2.68	0.56
2:B:423:VAL:O	2:B:423:VAL:HG12	2.06	0.56
1:A:394:GLN:HG2	1:A:397:THR:OG1	2.04	0.56
2:B:279:LEU:HA	2:B:299:ALA:HB1	1.88	0.56
1:A:350:LYS:HB3	1:A:350:LYS:NZ	2.21	0.56
1:A:457:TYR:CD2	1:A:457:TYR:C	2.79	0.56
2:B:385:LYS:HG3	2:B:385:LYS:O	2.05	0.56
1:A:131:THR:OG1	1:A:143:ARG:NE	2.35	0.56
1:A:406:TRP:CZ2	2:B:418:ASN:O	2.59	0.56
1:A:254:VAL:O	1:A:258:GLN:HG3	2.05	0.56
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.36	0.56
2:B:248:GLU:HA	2:B:307:ARG:NH2	2.20	0.56
1:A:537:PRO:O	1:A:541:GLY:O	2.24	0.56
1:A:542:ILE:CG1	1:A:546:GLU:HA	2.36	0.56
2:B:419:THR:O	2:B:421:PRO:HD3	2.06	0.56
1:A:223:LYS:O	1:A:223:LYS:HG3	2.06	0.56
1:A:487:GLN:HG3	1:A:524:GLN:NE2	2.21	0.55
2:B:201:LYS:O	2:B:204:GLU:HB3	2.06	0.55
1:A:219:LYS:C	1:A:221:HIS:H	2.09	0.55
2:B:259:LYS:O	2:B:263:LYS:HD3	2.06	0.55
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.88	0.55
2:B:419:THR:O	2:B:419:THR:HG23	2.06	0.55
2:B:252:TRP:O	2:B:292:VAL:HG13	2.07	0.55
2:B:311:LYS:O	2:B:313:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:LYS:HE2	2:B:252:TRP:CZ3	2.42	0.55
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.37	0.55
1:A:376:THR:HG23	1:A:386:THR:HG22	1.88	0.55
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.88	0.55
2:B:278:GLN:HE22	2:B:281:LYS:HD2	1.71	0.55
2:B:296:THR:O	2:B:300:GLU:HB2	2.07	0.55
1:A:210:LEU:O	1:A:210:LEU:HD12	2.06	0.55
1:A:41:MET:HB2	1:A:47:ILE:CD1	2.37	0.55
1:A:402:TRP:CE3	1:A:403:THR:HA	2.42	0.55
1:A:382:ILE:O	2:B:136:ASN:HB2	2.05	0.55
2:B:348:ASN:C	2:B:349:LEU:HD23	2.26	0.55
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.72	0.55
1:A:235:HIS:HD2	1:A:238:LYS:HG3	1.70	0.55
2:B:282:LEU:HD13	2:B:296:THR:OG1	2.06	0.55
2:B:213:GLY:O	2:B:215:THR:N	2.40	0.55
2:B:23:GLN:NE2	2:B:24:TRP:O	2.40	0.55
1:A:84:THR:HG23	1:A:124:PHE:CZ	2.42	0.54
1:A:399:GLU:OE1	1:A:402:TRP:NE1	2.39	0.54
1:A:496:VAL:HG12	1:A:496:VAL:O	2.06	0.54
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.33	0.54
1:A:344:GLU:HG3	1:A:345:PRO:HD2	1.88	0.54
1:A:96:HIS:NE2	1:A:350:LYS:HD2	2.23	0.54
1:A:277:ARG:HH11	1:A:334:GLN:HB2	1.73	0.54
1:A:317:VAL:HG13	1:A:349:LEU:HD23	1.90	0.54
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.43	0.54
1:A:194:GLU:O	1:A:196:GLY:N	2.41	0.54
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.38	0.54
2:B:315:HIS:C	2:B:317:VAL:H	2.11	0.54
2:B:66:LYS:NZ	2:B:218:ASP:HB2	2.23	0.54
1:A:515:SER:O	1:A:517:LEU:N	2.41	0.54
1:A:162:SER:O	1:A:166:LYS:HG3	2.08	0.54
1:A:427:TYR:OH	1:A:509:GLN:HA	2.09	0.54
1:A:298:GLU:N	1:A:298:GLU:CD	2.60	0.54
1:A:368:LEU:O	1:A:372:VAL:HG23	2.07	0.54
2:B:274:ILE:HG22	2:B:274:ILE:O	2.07	0.53
2:B:261:VAL:HG21	2:B:283:LEU:HD11	1.90	0.53
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.90	0.53
2:B:241:VAL:CG2	2:B:242:GLN:H	2.19	0.53
1:A:73:LYS:HG2	1:A:74:LEU:N	2.23	0.53
2:B:337:TRP:HE1	2:B:367:GLN:HG2	1.73	0.53
2:B:209:LEU:HB3	2:B:215:THR:OG1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LEU:O	2:B:80:LEU:HD12	2.08	0.53
1:A:362:THR:CG2	1:A:363:ASN:N	2.49	0.53
1:A:234:LEU:HD22	4:A:562:357:H111	1.90	0.53
1:A:23:GLN:HE21	1:A:24:TRP:H	1.57	0.53
1:A:398:TRP:CZ3	1:A:411:ILE:HD11	2.43	0.53
2:B:22:LYS:HD3	2:B:24:TRP:CZ3	2.42	0.53
1:A:301:LEU:O	1:A:305:GLU:HG3	2.09	0.53
2:B:343:GLN:O	2:B:344:GLU:HG2	2.08	0.53
2:B:329:ILE:HD11	2:B:375:ILE:HD12	1.91	0.53
2:B:277:ARG:H	2:B:277:ARG:HD2	1.67	0.52
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.44	0.52
1:A:115:TYR:HD1	1:A:115:TYR:H	1.57	0.52
1:A:54:ASN:CB	1:A:55:PRO:CD	2.77	0.52
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.43	0.52
2:B:249:LYS:HG2	2:B:252:TRP:CE2	2.44	0.52
1:A:112:GLY:C	1:A:114:ALA:H	2.13	0.52
1:A:277:ARG:HH11	1:A:334:GLN:CB	2.22	0.52
2:B:183:TYR:HE2	2:B:184:MET:SD	2.32	0.52
1:A:269:GLN:O	1:A:351:THR:N	2.31	0.52
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.92	0.52
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.39	0.52
1:A:425:LEU:HD13	1:A:428:GLN:OE1	2.10	0.52
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.43	0.52
2:B:395:LYS:O	2:B:399:GLU:HG3	2.10	0.52
2:B:168:LEU:HD13	2:B:180:ILE:HD12	1.91	0.52
1:A:233:GLU:OE1	1:A:235:HIS:NE2	2.41	0.52
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.44	0.52
1:A:517:LEU:O	1:A:520:GLN:N	2.43	0.52
2:B:326:ILE:CG2	2:B:342:TYR:CE1	2.93	0.52
2:B:276:VAL:HG22	2:B:276:VAL:O	2.09	0.51
2:B:125:ARG:C	2:B:127:TYR:H	2.13	0.51
1:A:296:THR:CG2	1:A:297:GLU:N	2.73	0.51
2:B:90:VAL:HG12	2:B:91:GLN:N	2.25	0.51
2:B:194:GLU:O	2:B:195:ILE:C	2.48	0.51
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.92	0.51
2:B:50:ILE:HG21	2:B:54:ASN:HD22	1.75	0.51
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.74	0.51
1:A:411:ILE:O	1:A:412:PRO:O	2.27	0.51
1:A:62:ALA:O	1:A:63:ILE:HD13	2.10	0.51
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.75	0.51
1:A:164:MET:HE3	1:A:187:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.46	0.51
2:B:115:TYR:O	2:B:117:SER:N	2.43	0.51
1:A:542:ILE:HG12	1:A:546:GLU:HA	1.93	0.51
1:A:54:ASN:CB	1:A:55:PRO:HD3	2.19	0.51
1:A:424:LYS:HD3	1:A:426:TRP:CH2	2.46	0.51
2:B:320:ASP:OD1	2:B:322:SER:OG	2.20	0.51
2:B:276:VAL:N	2:B:277:ARG:NH1	2.48	0.51
1:A:134:SER:CB	1:A:140:PRO:HD3	2.41	0.51
1:A:358:ARG:O	1:A:360:ALA:N	2.43	0.50
1:A:153:TRP:O	1:A:156:SER:HB2	2.11	0.50
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.93	0.50
1:A:233:GLU:OE2	1:A:242:GLN:HG3	2.11	0.50
2:B:245:VAL:HG22	2:B:246:LEU:O	2.11	0.50
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.92	0.50
1:A:116:PHE:O	1:A:148:VAL:HG11	2.11	0.50
1:A:460:ASN:C	1:A:462:GLY:H	2.14	0.50
1:A:3:SER:CB	1:A:5:ILE:HG13	2.37	0.50
2:B:174:GLN:O	2:B:176:PRO:CD	2.57	0.50
1:A:276:VAL:CG1	1:A:276:VAL:O	2.60	0.50
2:B:332:GLN:HB3	2:B:336:GLN:O	2.11	0.50
2:B:314:VAL:HB	2:B:317:VAL:CG2	2.42	0.50
2:B:94:ILE:HD11	2:B:158:ALA:HA	1.92	0.50
2:B:151:GLN:O	2:B:153:TRP:N	2.45	0.50
1:A:279:LEU:HD12	1:A:279:LEU:N	2.24	0.50
1:A:240:THR:CG2	1:A:241:VAL:H	2.08	0.50
1:A:108:VAL:HG13	1:A:227:PHE:CE1	2.47	0.50
1:A:167:ILE:O	1:A:170:PRO:HD2	2.12	0.50
1:A:183:TYR:C	1:A:183:TYR:CD2	2.85	0.50
1:A:113:ASP:O	1:A:114:ALA:C	2.50	0.50
2:B:376:THR:O	2:B:379:SER:N	2.45	0.50
1:A:77:PHE:O	1:A:80:LEU:HB3	2.12	0.50
2:B:249:LYS:NZ	2:B:249:LYS:HB3	2.27	0.50
1:A:275:LYS:O	1:A:276:VAL:HG23	2.12	0.50
2:B:406:TRP:CZ2	2:B:412:PRO:HD2	2.47	0.50
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.11	0.50
2:B:66:LYS:NZ	2:B:218:ASP:CB	2.75	0.50
1:A:434:ILE:HG21	1:A:492:GLU:CG	2.41	0.49
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.47	0.49
2:B:315:HIS:O	2:B:317:VAL:N	2.45	0.49
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.46	0.49
2:B:132:ILE:HB	2:B:142:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:VAL:HB	2:B:149:LEU:HD13	1.93	0.49
1:A:57:ASN:CG	1:A:58:THR:H	2.13	0.49
1:A:98:ALA:HB2	1:A:350:LYS:HG3	1.93	0.49
1:A:195:ILE:O	1:A:199:ARG:HD3	2.11	0.49
1:A:65:LYS:HE2	1:A:66:LYS:N	2.28	0.49
1:A:2:ILE:HG22	1:A:3:SER:N	2.27	0.49
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.27	0.49
1:A:238:LYS:HE2	1:A:315:HIS:CB	2.43	0.49
1:A:286:THR:HG22	1:A:287:LYS:N	2.28	0.49
2:B:115:TYR:C	2:B:117:SER:H	2.15	0.49
1:A:138:GLU:O	1:A:140:PRO:HD3	2.13	0.49
1:A:92:LEU:CG	1:A:93:GLY:N	2.70	0.49
2:B:235:HIS:O	2:B:238:LYS:HG2	2.13	0.49
2:B:198:HIS:O	2:B:201:LYS:N	2.46	0.49
2:B:28:GLU:HA	2:B:31:ILE:HD12	1.94	0.49
1:A:460:ASN:HA	2:B:286:THR:O	2.13	0.49
1:A:58:THR:HG22	1:A:76:ASP:O	2.12	0.49
1:A:246:LEU:H	1:A:246:LEU:HD23	1.78	0.49
2:B:282:LEU:HG	2:B:293:ILE:HD11	1.94	0.49
1:A:175:ASN:N	1:A:176:PRO:HD3	2.27	0.48
1:A:317:VAL:HG22	1:A:318:TYR:H	1.77	0.48
1:A:542:ILE:O	1:A:543:GLY:O	2.31	0.48
1:A:233:GLU:CD	1:A:242:GLN:NE2	2.61	0.48
1:A:482:ILE:O	1:A:483:TYR:C	2.50	0.48
1:A:413:GLU:OE2	1:A:413:GLU:HA	2.12	0.48
1:A:542:ILE:O	1:A:542:ILE:HG23	2.13	0.48
2:B:139:THR:HB	2:B:140:PRO:CD	2.34	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.95	0.48
2:B:84:THR:O	2:B:86:ASP:N	2.46	0.48
1:A:242:GLN:CB	1:A:243:PRO:CD	2.87	0.48
2:B:100:LEU:HD11	2:B:106:VAL:HG13	1.93	0.48
2:B:279:LEU:HA	2:B:299:ALA:CB	2.42	0.48
1:A:223:LYS:C	1:A:225:PRO:HD3	2.34	0.48
1:A:366:LYS:O	1:A:370:GLU:HG3	2.13	0.48
2:B:65:LYS:HD2	2:B:72:ARG:HG3	1.95	0.48
1:A:340:GLN:HA	1:A:351:THR:HA	1.96	0.48
1:A:249:LYS:HG3	1:A:250:ASP:OD2	2.14	0.48
1:A:402:TRP:CD2	1:A:403:THR:N	2.81	0.48
1:A:253:THR:HG23	1:A:256:ASP:H	1.79	0.48
1:A:457:TYR:HD2	1:A:457:TYR:C	2.15	0.48
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:HG22	1:A:297:GLU:H	1.76	0.48
2:B:279:LEU:CD1	2:B:299:ALA:HB1	2.43	0.48
1:A:90:VAL:HG23	1:A:91:GLN:N	2.22	0.48
2:B:260:LEU:HG	2:B:264:LEU:HD12	1.94	0.48
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.95	0.48
2:B:28:GLU:O	2:B:32:LYS:HG3	2.13	0.48
1:A:163:SER:HA	1:A:166:LYS:CE	2.42	0.48
2:B:425:LEU:HA	2:B:427:TYR:HD1	1.79	0.48
2:B:284:ARG:NH1	2:B:284:ARG:CG	2.67	0.47
1:A:451:LYS:HE3	1:A:471:ASN:HD22	1.78	0.47
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.49	0.47
1:A:178:ILE:HD11	1:A:201:LYS:HG3	1.96	0.47
1:A:345:PRO:HB2	1:A:346:PHE:CD1	2.49	0.47
2:B:281:LYS:HG2	2:B:284:ARG:NH2	2.29	0.47
1:A:270:ILE:HG13	1:A:270:ILE:O	2.14	0.47
1:A:234:LEU:HB3	4:A:562:357:H111	1.96	0.47
1:A:521:ILE:HG22	1:A:521:ILE:O	2.14	0.47
2:B:213:GLY:C	2:B:215:THR:N	2.67	0.47
2:B:167:ILE:O	2:B:170:PRO:HD2	2.14	0.47
1:A:384:GLY:O	2:B:27:THR:HG23	2.14	0.47
1:A:179:VAL:O	1:A:179:VAL:HG23	2.15	0.47
1:A:17:ASP:OD2	1:A:56:TYR:HE2	1.96	0.47
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.96	0.47
1:A:406:TRP:CZ2	2:B:419:THR:HB	2.49	0.47
2:B:210:LEU:HA	2:B:215:THR:O	2.15	0.47
1:A:178:ILE:CG2	1:A:189:VAL:HG13	2.44	0.47
1:A:10:VAL:HG12	1:A:11:LYS:N	2.29	0.47
1:A:108:VAL:CG1	1:A:227:PHE:CE1	2.98	0.47
1:A:95:PRO:HA	2:B:136:ASN:O	2.13	0.47
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.80	0.47
1:A:493:VAL:CG2	1:A:494:ASN:N	2.77	0.47
2:B:194:GLU:O	2:B:197:GLN:N	2.47	0.47
2:B:131:THR:CG2	2:B:141:GLY:HA3	2.45	0.47
1:A:56:TYR:N	1:A:56:TYR:CD1	2.72	0.47
1:A:130:PHE:HE1	1:A:144:TYR:HB2	1.74	0.47
1:A:46:LYS:HD2	1:A:46:LYS:N	2.29	0.47
1:A:455:ALA:HB2	1:A:469:LEU:HD11	1.96	0.47
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.50	0.47
1:A:218:ASP:O	1:A:220:LYS:N	2.47	0.47
1:A:92:LEU:HG	1:A:93:GLY:H	1.80	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:THR:HG23	2:B:297:GLU:H	1.80	0.46
1:A:296:THR:CG2	1:A:297:GLU:H	2.27	0.46
1:A:326:ILE:HD12	1:A:326:ILE:N	2.30	0.46
1:A:277:ARG:O	1:A:281:LYS:HB2	2.14	0.46
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.97	0.46
1:A:2:ILE:CG2	1:A:3:SER:N	2.78	0.46
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.45	0.46
2:B:314:VAL:CG1	2:B:315:HIS:N	2.78	0.46
1:A:294:PRO:O	1:A:296:THR:N	2.48	0.46
1:A:115:TYR:HE2	1:A:156:SER:HB3	1.80	0.46
1:A:12:LEU:O	1:A:13:LYS:C	2.54	0.46
1:A:79:GLU:O	1:A:83:ARG:NH1	2.49	0.46
1:A:161:GLN:NE2	1:A:161:GLN:C	2.69	0.46
1:A:59:PRO:HB2	1:A:61:PHE:HE1	1.80	0.46
1:A:270:ILE:HD11	1:A:315:HIS:O	2.16	0.46
2:B:11:LYS:CD	2:B:11:LYS:N	2.75	0.46
1:A:175:ASN:O	1:A:177:ASP:N	2.46	0.46
1:A:3:SER:OG	1:A:212:TRP:O	2.34	0.46
2:B:326:ILE:HG21	2:B:342:TYR:HE1	1.81	0.46
1:A:547:GLN:HE21	1:A:547:GLN:CA	2.28	0.46
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.28	0.46
1:A:381:VAL:O	2:B:136:ASN:HA	2.16	0.46
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.16	0.46
2:B:149:LEU:HB3	2:B:156:SER:HB3	1.98	0.46
1:A:354:TYR:CD1	1:A:374:LYS:HD2	2.39	0.46
1:A:277:ARG:NH2	1:A:281:LYS:HE2	2.31	0.46
1:A:27:THR:O	1:A:31:ILE:N	2.47	0.46
1:A:283:LEU:O	1:A:284:ARG:C	2.54	0.46
2:B:30:LYS:HB3	2:B:62:ALA:HB3	1.98	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.15	0.46
1:A:279:LEU:HD21	1:A:303:LEU:HD13	1.98	0.46
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.63	0.46
2:B:365:VAL:O	2:B:367:GLN:N	2.49	0.46
2:B:314:VAL:CG1	2:B:315:HIS:H	2.24	0.45
1:A:253:THR:O	1:A:257:ILE:HG13	2.16	0.45
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.16	0.45
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.34	0.45
1:A:170:PRO:HG2	1:A:171:PHE:H	1.80	0.45
2:B:160:PHE:O	2:B:161:GLN:C	2.54	0.45
1:A:175:ASN:C	1:A:177:ASP:H	2.20	0.45
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:LYS:HE2	2:B:378:GLU:OE2	2.15	0.45
2:B:295:LEU:CB	2:B:300:GLU:HG2	2.46	0.45
2:B:100:LEU:HD11	2:B:106:VAL:HG11	1.98	0.45
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.80	0.45
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.79	0.45
1:A:164:MET:HB3	1:A:182:GLN:HE22	1.82	0.45
1:A:493:VAL:HG22	1:A:494:ASN:H	1.80	0.45
1:A:246:LEU:HD12	1:A:303:LEU:HD11	1.99	0.45
1:A:398:TRP:CD1	1:A:399:GLU:N	2.84	0.45
1:A:12:LEU:O	1:A:13:LYS:O	2.34	0.45
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.51	0.45
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.98	0.45
2:B:94:ILE:HA	2:B:95:PRO:HD2	1.75	0.45
2:B:128:THR:CB	2:B:146:TYR:HB2	2.47	0.45
1:A:511:ASP:CG	1:A:512:LYS:HG2	2.37	0.45
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.99	0.45
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.98	0.45
1:A:34:LEU:CB	1:A:132:ILE:HG21	2.47	0.45
1:A:5:ILE:HD13	1:A:167:ILE:HD11	1.99	0.45
2:B:39:THR:O	2:B:43:LYS:HG3	2.16	0.45
1:A:155:GLY:O	1:A:159:ILE:HD12	2.17	0.45
2:B:23:GLN:HG3	2:B:131:THR:O	2.17	0.45
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.97	0.45
1:A:19:PRO:O	1:A:56:TYR:HB3	2.17	0.45
1:A:249:LYS:HG3	1:A:250:ASP:N	2.21	0.45
1:A:250:ASP:N	1:A:250:ASP:OD2	2.50	0.45
1:A:394:GLN:O	1:A:396:GLU:N	2.50	0.45
1:A:216:THR:HB	1:A:217:PRO:HD2	1.99	0.45
1:A:100:LEU:HD21	4:A:562:357:H8'1	1.99	0.44
2:B:162:SER:O	2:B:164:MET:N	2.49	0.44
1:A:358:ARG:C	1:A:360:ALA:N	2.67	0.44
1:A:12:LEU:CD1	1:A:127:TYR:CE2	3.01	0.44
1:A:17:ASP:CG	1:A:18:GLY:N	2.70	0.44
1:A:122:GLU:O	1:A:125:ARG:HG3	2.18	0.44
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.52	0.44
1:A:134:SER:CB	1:A:140:PRO:CD	2.96	0.44
1:A:405:TYR:O	2:B:331:LYS:HD3	2.18	0.44
2:B:401:TRP:O	2:B:402:TRP:C	2.56	0.44
1:A:468:PRO:C	1:A:469:LEU:HG	2.37	0.44
1:A:151:GLN:HE21	1:A:151:GLN:HA	1.82	0.44
1:A:130:PHE:N	1:A:130:PHE:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PHE:O	2:B:125:ARG:C	2.56	0.44
1:A:537:PRO:O	1:A:541:GLY:HA3	2.18	0.44
1:A:350:LYS:HB3	1:A:350:LYS:HZ2	1.81	0.44
2:B:369:THR:HA	2:B:398:TRP:HH2	1.83	0.44
2:B:183:TYR:C	2:B:183:TYR:CD2	2.91	0.44
1:A:94:ILE:CG2	1:A:229:TRP:CH2	3.01	0.44
1:A:522:ILE:O	1:A:525:LEU:N	2.50	0.44
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.48	0.44
2:B:125:ARG:C	2:B:127:TYR:N	2.66	0.44
1:A:12:LEU:HD11	1:A:127:TYR:CD2	2.53	0.44
1:A:543:GLY:C	1:A:545:ASN:H	2.19	0.44
2:B:164:MET:C	2:B:166:LYS:N	2.70	0.44
2:B:1:PRO:HB2	2:B:2:ILE:H	1.62	0.44
1:A:430:GLU:OE1	1:A:530:LYS:HE3	2.18	0.43
1:A:303:LEU:O	1:A:307:ARG:HG3	2.19	0.43
2:B:295:LEU:HB2	2:B:300:GLU:HG2	2.00	0.43
2:B:66:LYS:HZ2	2:B:218:ASP:HB3	1.82	0.43
2:B:363:ASN:HB3	2:B:366:LYS:HB3	2.00	0.43
1:A:273:GLY:O	1:A:274:ILE:C	2.55	0.43
2:B:214:LEU:O	2:B:214:LEU:HG	2.18	0.43
2:B:249:LYS:HE2	2:B:252:TRP:CE3	2.53	0.43
2:B:423:VAL:HG13	2:B:426:TRP:HE3	1.83	0.43
2:B:1:PRO:C	2:B:2:ILE:HG13	2.38	0.43
2:B:96:HIS:HE1	2:B:381:VAL:O	2.01	0.43
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.28	0.43
2:B:91:GLN:CA	2:B:91:GLN:HE21	2.32	0.43
2:B:305:GLU:OE2	2:B:309:ILE:HD11	2.18	0.43
2:B:257:ILE:O	2:B:260:LEU:HB3	2.18	0.43
1:A:350:LYS:HE3	1:A:378:GLU:OE2	2.18	0.43
1:A:116:PHE:HA	1:A:148:VAL:HG21	2.00	0.43
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.52	0.43
1:A:399:GLU:HG3	1:A:402:TRP:HE1	1.83	0.43
1:A:193:LEU:HB3	1:A:197:GLN:HG3	2.01	0.43
2:B:241:VAL:CG2	2:B:242:GLN:N	2.76	0.43
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.53	0.43
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.54	0.43
2:B:151:GLN:C	2:B:153:TRP:N	2.71	0.43
2:B:153:TRP:O	2:B:155:GLY:N	2.43	0.43
1:A:402:TRP:CZ3	1:A:403:THR:HA	2.54	0.43
2:B:379:SER:OG	2:B:387:PRO:HD3	2.19	0.43
2:B:358:ARG:O	2:B:362:THR:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.54	0.43
1:A:100:LEU:HD11	4:A:562:357:C8'	2.49	0.43
2:B:349:LEU:O	2:B:350:LYS:HB2	2.19	0.43
1:A:334:GLN:HB3	1:A:334:GLN:HE21	1.68	0.43
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.84	0.43
1:A:154:LYS:O	1:A:156:SER:N	2.50	0.43
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.54	0.43
2:B:426:TRP:HD1	2:B:426:TRP:O	2.01	0.43
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.43
1:A:277:ARG:HH21	1:A:281:LYS:HE2	1.84	0.43
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.49	0.43
1:A:22:LYS:HD2	1:A:22:LYS:HA	1.69	0.43
1:A:543:GLY:C	1:A:545:ASN:N	2.73	0.42
2:B:219:LYS:HZ3	2:B:219:LYS:HB3	1.84	0.42
1:A:514:GLU:N	1:A:514:GLU:OE1	2.51	0.42
1:A:248:GLU:HB3	1:A:307:ARG:NH2	2.34	0.42
2:B:398:TRP:O	2:B:402:TRP:HD1	2.01	0.42
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.54	0.42
1:A:138:GLU:CG	1:A:138:GLU:O	2.64	0.42
2:B:249:LYS:HG2	2:B:252:TRP:CZ2	2.54	0.42
2:B:418:ASN:O	2:B:419:THR:HB	2.18	0.42
1:A:201:LYS:CA	1:A:204:GLU:HG3	2.50	0.42
2:B:376:THR:O	2:B:377:THR:C	2.57	0.42
1:A:69:THR:HG22	1:A:69:THR:O	2.19	0.42
2:B:306:ASN:HD22	2:B:309:ILE:CD1	2.28	0.42
1:A:540:LYS:HE3	2:B:265:ASN:ND2	2.32	0.42
2:B:346:PHE:CD1	2:B:346:PHE:N	2.87	0.42
2:B:332:GLN:CB	2:B:336:GLN:O	2.67	0.42
1:A:34:LEU:HB2	1:A:132:ILE:HG21	2.01	0.42
1:A:507:GLN:O	1:A:509:GLN:HG3	2.19	0.42
1:A:3:SER:HB2	1:A:5:ILE:HD12	2.00	0.42
2:B:353:LYS:O	2:B:353:LYS:HG2	2.20	0.42
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.53	0.42
1:A:171:PHE:C	1:A:173:LYS:N	2.73	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.42
2:B:388:LYS:HA	2:B:413:GLU:O	2.19	0.42
1:A:94:ILE:HG23	1:A:229:TRP:CZ2	2.55	0.42
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.55	0.42
2:B:43:LYS:C	2:B:45:GLY:H	2.20	0.42
1:A:233:GLU:OE2	1:A:242:GLN:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:CD	1:A:125:ARG:HH11	2.24	0.41
1:A:91:GLN:O	1:A:92:LEU:C	2.58	0.41
1:A:325:LEU:HD22	1:A:341:ILE:HG21	2.02	0.41
2:B:181:TYR:CD1	2:B:182:GLN:N	2.88	0.41
2:B:278:GLN:HE21	2:B:278:GLN:CA	2.32	0.41
2:B:340:GLN:CG	2:B:426:TRP:CZ2	3.00	0.41
1:A:126:LYS:HZ3	1:A:126:LYS:HB3	1.82	0.41
2:B:275:LYS:HG2	2:B:277:ARG:HD3	2.02	0.41
2:B:118:VAL:O	2:B:149:LEU:HD12	2.19	0.41
1:A:260:LEU:HD11	1:A:303:LEU:HD11	2.01	0.41
2:B:28:GLU:HG3	2:B:135:ILE:HD11	2.02	0.41
2:B:206:ARG:HH11	2:B:206:ARG:HG3	1.85	0.41
1:A:515:SER:O	1:A:516:GLU:C	2.59	0.41
1:A:277:ARG:NH1	1:A:334:GLN:HB2	2.35	0.41
1:A:120:LEU:O	1:A:121:ASP:C	2.58	0.41
1:A:50:ILE:O	1:A:143:ARG:HB3	2.21	0.41
1:A:83:ARG:NH1	1:A:83:ARG:CG	2.83	0.41
2:B:178:ILE:HD11	2:B:201:LYS:CG	2.50	0.41
1:A:334:GLN:HG2	1:A:334:GLN:H	1.65	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.20	0.41
2:B:165:THR:O	2:B:169:GLU:HB2	2.20	0.41
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.87	0.41
1:A:249:LYS:HG2	1:A:251:SER:OG	2.21	0.41
2:B:241:VAL:CG1	2:B:243:PRO:HD3	2.43	0.41
2:B:253:THR:OG1	2:B:256:ASP:OD2	2.24	0.41
1:A:88:TRP:O	1:A:89:GLU:C	2.59	0.41
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.20	0.41
1:A:55:PRO:HB2	1:A:56:TYR:H	1.54	0.41
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.88	0.41
2:B:392:PRO:HA	2:B:417:VAL:HG22	2.03	0.41
1:A:66:LYS:O	1:A:68:SER:N	2.54	0.41
2:B:339:TYR:C	2:B:340:GLN:OE1	2.59	0.41
1:A:183:TYR:CE1	1:A:229:TRP:NE1	2.89	0.41
1:A:183:TYR:CD2	1:A:184:MET:HG3	2.55	0.41
1:A:261:VAL:O	1:A:262:GLY:C	2.59	0.41
2:B:188:TYR:CD1	2:B:188:TYR:N	2.88	0.41
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.51	0.41
2:B:164:MET:O	2:B:166:LYS:N	2.53	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.81	0.41
2:B:246:LEU:HD12	2:B:307:ARG:HG2	2.02	0.41
1:A:516:GLU:HG2	1:A:517:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.84	0.41
2:B:345:PRO:C	2:B:346:PHE:CD1	2.95	0.41
1:A:132:ILE:HD11	1:A:142:ILE:HG21	2.02	0.41
2:B:160:PHE:O	2:B:162:SER:N	2.54	0.41
1:A:402:TRP:CE3	1:A:402:TRP:C	2.94	0.41
1:A:280:SER:C	1:A:282:LEU:N	2.74	0.41
1:A:416:PHE:CZ	1:A:418:ASN:HA	2.56	0.41
1:A:56:TYR:O	1:A:143:ARG:NH2	2.53	0.40
1:A:173:LYS:O	1:A:176:PRO:HD3	2.20	0.40
2:B:319:TYR:O	2:B:321:PRO:HD3	2.22	0.40
2:B:183:TYR:CD1	2:B:380:ILE:HG23	2.57	0.40
1:A:60:VAL:O	1:A:61:PHE:HD1	2.02	0.40
1:A:402:TRP:CE3	1:A:403:THR:N	2.89	0.40
2:B:2:ILE:O	2:B:2:ILE:HG22	2.21	0.40
1:A:126:LYS:HZ2	1:A:126:LYS:HB3	1.85	0.40
1:A:197:GLN:HA	1:A:200:THR:OG1	2.21	0.40
1:A:27:THR:O	1:A:27:THR:HG23	2.21	0.40
2:B:151:GLN:C	2:B:153:TRP:H	2.24	0.40
2:B:426:TRP:CD1	2:B:426:TRP:O	2.74	0.40
2:B:253:THR:CG2	2:B:292:VAL:HG22	2.44	0.40
2:B:205:LEU:O	2:B:206:ARG:C	2.58	0.40
1:A:317:VAL:HG22	1:A:318:TYR:N	2.36	0.40
1:A:275:LYS:O	1:A:276:VAL:CG2	2.69	0.40
2:B:255:ASN:O	2:B:259:LYS:HG3	2.21	0.40
1:A:263:LYS:HB2	1:A:263:LYS:HE3	1.80	0.40
2:B:221:HIS:HD2	2:B:229:TRP:CB	2.34	0.40
2:B:155:GLY:O	2:B:159:ILE:HG13	2.21	0.40
2:B:340:GLN:HB3	2:B:348:ASN:HD22	1.87	0.40
2:B:423:VAL:HG13	2:B:426:TRP:CE3	2.55	0.40
1:A:344:GLU:HG3	1:A:345:PRO:CD	2.51	0.40
1:A:103:LYS:HE2	1:A:179:VAL:HG21	2.02	0.40
2:B:167:ILE:HA	2:B:212:TRP:CE3	2.57	0.40
1:A:458:VAL:HG13	1:A:464:GLN:HG2	2.02	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	550/560 (98%)	414 (75%)	100 (18%)	36 (6%)	1	7
2	B	425/430 (99%)	313 (74%)	75 (18%)	37 (9%)	1	4
All	All	975/990 (98%)	727 (75%)	175 (18%)	73 (8%)	1	5

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	90	VAL
1	A	114	ALA
1	A	242	GLN
1	A	357	MET
1	A	491	LEU
1	A	516	GLU
2	B	116	PHE
2	B	126	LYS
2	B	195	ILE
2	B	220	LYS
2	B	421	PRO
1	A	66	LYS
1	A	195	ILE
1	A	276	VAL
1	A	295	LEU
1	A	296	THR
1	A	412	PRO
1	A	543	GLY
2	B	12	LEU
2	B	18	GLY
2	B	67	ASP
2	B	85	GLN
2	B	103	LYS
2	B	154	LYS

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Mol	Chain	Res	Type
2	B	163	SER
2	B	174	GLN
2	B	214	LEU
2	B	284	ARG
2	B	296	THR
2	B	314	VAL
2	B	316	GLY
2	B	366	LYS
2	B	376	THR
2	B	377	THR
1	A	92	LEU
1	A	151	GLN
1	A	220	LYS
1	A	289	LEU
1	A	395	LYS
1	A	528	LYS
2	B	161	GLN
2	B	240	THR
2	B	272	PRO
2	B	355	ALA
1	A	16	MET
1	A	54	ASN
1	A	70	LYS
1	A	503	LEU
1	A	538	ALA
2	B	2	ILE
2	B	68	SER
1	A	140	PRO
1	A	241	VAL
1	A	359	GLY
2	B	176	PRO
2	B	345	PRO
1	A	176	PRO
1	A	309	ILE
2	B	111	VAL
2	B	313	PRO
2	B	412	PRO
2	B	419	THR
1	A	52	PRO
1	A	155	GLY
1	A	243	PRO
1	A	274	ILE

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Mol	Chain	Res	Type
2	B	231	GLY
1	A	4	PRO
1	A	13	LYS
2	B	217	PRO
2	B	225	PRO
2	B	241	VAL

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	477/500 (95%)	418 (88%)	59 (12%)	6	22
2	B	375/392 (96%)	337 (90%)	38 (10%)	9	32
All	All	852/892 (96%)	755 (89%)	97 (11%)	7	26

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	39	THR
1	A	46	LYS
1	A	55	PRO
1	A	56	TYR
1	A	65	LYS
1	A	76	ASP
1	A	84	THR
1	A	92	LEU
1	A	126	LYS
1	A	130	PHE
1	A	131	THR
1	A	132	ILE
1	A	143	ARG
1	A	156	SER
1	A	161	GLN
1	A	164	MET

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Mol	Chain	Res	Type
1	A	177	ASP
1	A	183	TYR
1	A	184	MET
1	A	199	ARG
1	A	203	GLU
1	A	217	PRO
1	A	218	ASP
1	A	246	LEU
1	A	250	ASP
1	A	253	THR
1	A	277	ARG
1	A	297	GLU
1	A	334	GLN
1	A	344	GLU
1	A	350	LYS
1	A	361	HIS
1	A	364	ASP
1	A	367	GLN
1	A	387	PRO
1	A	397	THR
1	A	399	GLU
1	A	403	THR
1	A	409	THR
1	A	414	TRP
1	A	418	ASN
1	A	457	TYR
1	A	460	ASN
1	A	492	GLU
1	A	496	VAL
1	A	497	THR
1	A	500	GLN
1	A	507	GLN
1	A	511	ASP
1	A	516	GLU
1	A	523	GLU
1	A	533	LEU
1	A	537	PRO
1	A	545	ASN
1	A	547	GLN
1	A	548	VAL
1	A	549	ASP
1	A	551	LEU

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Mol	Chain	Res	Type
2	B	11	LYS
2	B	23	GLN
2	B	50	ILE
2	B	67	ASP
2	B	86	ASP
2	B	91	GLN
2	B	113	ASP
2	B	126	LYS
2	B	142	ILE
2	B	149	LEU
2	B	164	MET
2	B	169	GLU
2	B	176	PRO
2	B	201	LYS
2	B	207	GLN
2	B	211	ARG
2	B	212	TRP
2	B	218	ASP
2	B	219	LYS
2	B	221	HIS
2	B	232	TYR
2	B	249	LYS
2	B	250	ASP
2	B	284	ARG
2	B	290	THR
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	307	ARG
2	B	310	LEU
2	B	315	HIS
2	B	324	ASP
2	B	334	GLN
2	B	342	TYR
2	B	348	ASN
2	B	367	GLN
2	B	369	THR
2	B	386	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	151	GLN
1	A	161	GLN
1	A	174	GLN
1	A	182	GLN
1	A	197	GLN
1	A	242	GLN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	340	GLN
1	A	367	GLN
1	A	418	ASN
1	A	460	ASN
1	A	471	ASN
1	A	494	ASN
1	A	509	GLN
1	A	519	ASN
1	A	545	ASN
1	A	547	GLN
2	B	54	ASN
2	B	91	GLN
2	B	96	HIS
2	B	161	GLN
2	B	207	GLN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	357	A	562	-	23,25,25	1.73	5 (21%)	25,34,34	1.35	5 (20%)

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
4	357	A	562	-	-	0/14/14/14	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	562	357	C2B-C3B	2.25	1.42	1.38
4	A	562	357	C5-C4	2.50	1.44	1.40
4	A	562	357	C2B-C1'	2.59	1.43	1.39
4	A	562	357	C3-C4	2.63	1.44	1.40
4	A	562	357	C5-C6	3.63	1.43	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	562	357	C6'-N1'-C2'	-3.75	104.74	115.31
4	A	562	357	C3-C2-N1	-2.12	120.20	123.46
4	A	562	357	C7'-C4-C5	2.10	121.94	119.87
4	A	562	357	C2-N1-C6	2.51	123.04	117.82
4	A	562	357	C5'-O4'-C3'	2.64	130.44	113.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	562	357	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	552/560 (98%)	0.02	13 (2%) 62 41	46, 94, 118, 126	0
2	B	427/430 (99%)	0.12	29 (6%) 20 11	38, 80, 120, 127	0
All	All	979/990 (98%)	0.06	42 (4%) 39 23	38, 90, 119, 127	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ILE	10.5
2	B	231	GLY	6.8
2	B	3	SER	6.6
2	B	225	PRO	6.1
1	A	133	PRO	5.8
1	A	547	GLN	5.6
1	A	552	VAL	4.4
2	B	227	PHE	4.4
1	A	551	LEU	4.1
2	B	230	MET	4.1
2	B	229	TRP	3.9
2	B	226	PRO	3.8
2	B	360	ALA	3.6
2	B	409	THR	3.3
2	B	228	LEU	3.1
2	B	310	LEU	3.1
2	B	1	PRO	3.1
2	B	410	TRP	3.0
1	A	68	SER	3.0
1	A	134	SER	2.8
1	A	548	VAL	2.7
2	B	224	GLU	2.7
1	A	128	THR	2.6
1	A	142	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	223	LYS	2.5
2	B	408	ALA	2.5
2	B	357	MET	2.4
2	B	279	LEU	2.4
2	B	222	GLN	2.3
2	B	186	ASP	2.3
2	B	359	GLY	2.3
1	A	1	PRO	2.2
1	A	89	GLU	2.2
2	B	299	ALA	2.2
2	B	295	LEU	2.1
2	B	5	ILE	2.1
2	B	4	PRO	2.1
2	B	294	PRO	2.1
2	B	252	TRP	2.1
2	B	185	ASP	2.0
1	A	62	ALA	2.0
1	A	67	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(Å ²)	Q<0.9
4	357	A	562	24/24	0.96	0.38	3.62	72,79,87,89	0
3	MN	A	561	1/1	0.92	0.14	-	85,85,85,85	0

6.5 Other polymers

There are no such residues in this entry.