



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:42 PM GMT

PDB ID : 1UWB
Title : TYR 181 CYS HIV-1 RT/8-CL TIBO
Authors : Das, K.; Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on : 1996-11-21
Resolution : 3.20 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

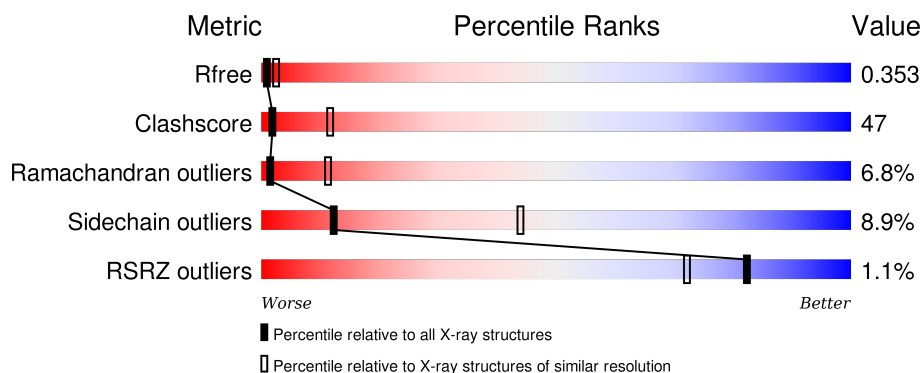
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	558	<div> <div></div> <div> <div></div> <div>36%</div> <div>56%</div> <div>8%</div> </div> </div>
2	B	427	<div> <div></div> <div> <div></div> <div>29%</div> <div>56%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7822 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4365	2822	725	812	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	TYR	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

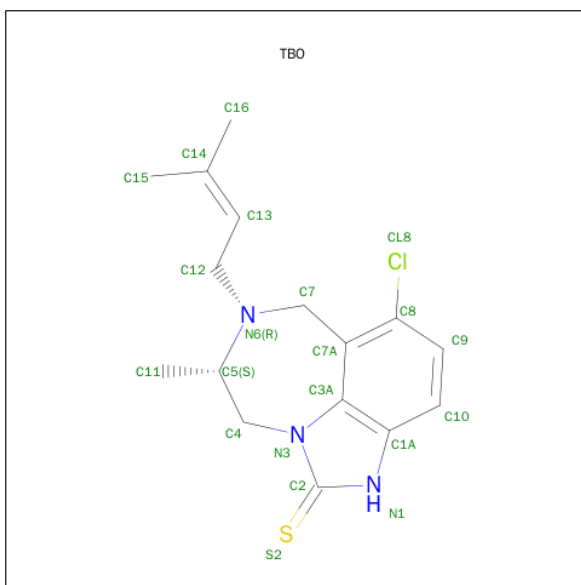
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3436	2234	567	629	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	CYS	TYR	ENGINEERED	UNP P03366
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is 5-CHLORO-8-METHYL-7-(3-METHYL-BUT-2-ENYL)-6,7,8,9-TETRAHYDRO-2H-2,7,9A-TRIAZA-BENZO[CD]AZULENE-1-THIONE (three-letter code: TBO) (formula: C₁₆H₂₀ClN₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	S	0	0
			21	16	1	3	1		

T400	T338	G273	E303	T139	L74
W401	Y339	I274	E204	P140	V75
W402	Q340	L279	L205	G141	D76
W403	I341	L280	Q207	I142	F77
E404	Y342	K281	E208	R143	R78
W405	Q343	L282	L209	Y144	E79
W406	E344	L283	L210	Q145	L80
Q407	P345	L284	G213	Y146	N81
W410	F346	G285	L214	N147	K82
L411	K347	T286	T215	V148	R83
P412	N348	T287	T216	L149	T84
W413	L349	K288	P217	G152	Q85
W414	K350	L289	D218	W153	D86
F415	T351	T290	E224	K154	F87
F416	G352	E291	S156	G155	W88
V417	K353	V292	P157	S157	E89
F421	A354	T293	P225	Y90	Q91
K424	R356	P294	P226	L92	A158
L425	M357	L295	W229	G93	G93
W426	K358	T296	M230	F160	I94
Y427	G359	E297	G231	Q161	P95
		E298	Y232	S162	H96
		A299	E233	S163	P97
	N363	E300	L234	M164	A98
	D364	L301	H235	T165	G99
	W365	E302	W239	K166	L100
	K366	L303	G239	I167	K101
	Q367	A304	T240	L168	K102
	L368	E305	V241	E169	K103
	T369	K306	Q242	P170	K104
	E370	R307	P243	F171	
	A371	E308	V245	A172	T107
	V372	L310	L246	K173	V108
	Q373	K311	D250	P176	L109
	I375	V314	S251	D177	D110
	T376	H315	W252	I178	V111
	T377	G316	T253	V179	Y115
	E378	V317	V254	C181	F116
	S379	V318	N255	D185	V118
	I380	V319	D256	D186	
	V381	D320	I257	L187	E122
	I382	P321	Q258	Y188	D123
	W383	S322	K259	V189	F124
	G384	K323	L260	K125	R125
	K385	D324	V261	Q190	K126
	T386	I325	G262	S191	Y127
	P387	L326	K263	D192	T128
	K388	A327	L264	L193	A129
	F389	G328	N265	E194	F130
	K390	I329	W266	T195	I131
	L391	Q330	A267	G196	I132
	E392	K331	S268	Q197	P133
	I393	Q332	Q269	H198	S134
	Q394	G333	I270	A199	I135
	K395	Q336	Y271	K201	N136
	E396	W337	P272	I202	I137
	T397				E138
	W398				
	E399				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.70Å 69.20Å 104.90Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20 14.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.0 ((Not available)-3.20) 85.0 (14.98-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.274 , 0.360 0.275 , 0.353	Depositor DCC
R_{free} test set	1059 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 14.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 21825 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7822	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.55	0/4479	0.78	3/6108 (0.0%)
2	B	0.60	0/3534	0.85	5/4812 (0.1%)
All	All	0.57	0/8013	0.81	8/10920 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	LYS	N-CA-C	6.92	129.68	111.00
1	A	517	LEU	CA-CB-CG	5.82	128.69	115.30
2	B	226	PRO	N-CA-CB	5.54	109.95	103.30
2	B	225	PRO	N-CA-CB	5.50	109.89	103.30
2	B	260	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	24	TRP	N-CA-C	-5.45	96.30	111.00
2	B	295	LEU	N-CA-C	5.30	125.33	111.00
2	B	332	GLN	N-CA-C	5.19	125.02	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	4365	0	4260	397	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3436	0	3401	363	0
3	A	21	0	20	8	0
All	All	7822	0	7681	736	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 47.

All (736) 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:60:VAL:HA	1:A:75:VAL:HG22	1.39	1.03
2:B:180:ILE:HG23	2:B:189:VAL:HG22	1.41	1.00
1:A:272:PRO:HA	1:A:351:THR:HG21	1.43	0.99
1:A:318:TYR:CE2	3:A:559:TBO:H10	2.03	0.93
2:B:12:LEU:HA	2:B:84:THR:HG22	1.48	0.92
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.51	0.91
1:A:543:GLY:H	2:B:284:ARG:HA	1.33	0.91
2:B:340:GLN:HB3	2:B:351:THR:HG22	1.54	0.90
1:A:373:GLN:NE2	2:B:397:THR:HA	1.87	0.90
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.51	0.89
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.37	0.89
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.53	0.89
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.55	0.88
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.09	0.88
2:B:263:LYS:HE2	2:B:425:LEU:HD13	1.58	0.86
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.11	0.85
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.59	0.85
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.42	0.84
1:A:543:GLY:HA2	1:A:546:GLU:HB3	1.61	0.83
1:A:63:ILE:HG22	1:A:64:LYS:H	1.43	0.82
1:A:399:GLU:HA	1:A:402:TRP:NE1	1.94	0.81
1:A:51:GLY:H	1:A:52:PRO:HD2	1.43	0.81
1:A:253:THR:HA	1:A:292:VAL:HA	1.63	0.81
2:B:258:GLN:HG2	2:B:283:LEU:HD13	1.61	0.81
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.63	0.81
2:B:344:GLU:HB2	2:B:347:LYS:HB2	1.62	0.80
1:A:341:ILE:HD13	1:A:350:LYS:HB3	1.62	0.80
2:B:326:ILE:HD12	2:B:388:LYS:HE2	1.63	0.80
2:B:132:ILE:CG2	2:B:142:ILE:HB	2.11	0.80
1:A:101:LYS:HD3	1:A:321:PRO:HD3	1.63	0.80
1:A:257:ILE:HD11	1:A:295:LEU:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ILE:HG23	2:B:142:ILE:HB	1.62	0.80
2:B:328:GLU:O	2:B:339:TYR:HA	1.81	0.79
2:B:306:ASN:HA	2:B:309:ILE:HB	1.64	0.79
2:B:79:GLU:O	2:B:83:ARG:HG3	1.82	0.79
1:A:164:MET:SD	1:A:168:LEU:HD21	2.23	0.78
1:A:542:ILE:HG23	1:A:545:ASN:HB2	1.66	0.78
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.13	0.78
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.84	0.78
1:A:240:THR:CG2	1:A:315:HIS:HA	2.13	0.77
1:A:8:VAL:O	1:A:121:ASP:HB2	1.85	0.77
2:B:379:SER:HA	2:B:383:TRP:CZ3	2.20	0.77
1:A:106:VAL:HG12	1:A:107:THR:H	1.50	0.77
1:A:227:PHE:O	1:A:233:GLU:HA	1.86	0.76
1:A:317:VAL:HG23	1:A:349:LEU:HD13	1.66	0.76
2:B:79:GLU:HG3	2:B:83:ARG:HD2	1.66	0.76
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.67	0.76
1:A:267:ALA:HB1	1:A:271:TYR:CD2	2.21	0.75
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.21	0.75
1:A:398:TRP:HE1	1:A:411:ILE:HG12	1.50	0.75
1:A:427:TYR:OH	1:A:509:GLN:HA	1.86	0.74
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.69	0.74
2:B:425:LEU:HD12	2:B:427:TYR:HB3	1.69	0.74
2:B:319:TYR:O	2:B:321:PRO:HD3	1.87	0.74
1:A:543:GLY:HA3	2:B:284:ARG:O	1.88	0.74
2:B:65:LYS:HD2	2:B:407:GLN:HG2	1.70	0.73
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.70	0.73
1:A:503:LEU:O	1:A:507:GLN:HG3	1.86	0.73
1:A:239:TRP:HB3	1:A:318:TYR:HE1	1.53	0.73
1:A:459:THR:OG1	1:A:463:ARG:HB3	1.88	0.73
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.23	0.73
1:A:503:LEU:HD13	1:A:535:TRP:CB	2.18	0.73
2:B:281:LYS:HA	2:B:284:ARG:HG3	1.71	0.72
2:B:254:VAL:O	2:B:258:GLN:HG3	1.90	0.72
2:B:61:PHE:CE1	2:B:76:ASP:HB2	2.24	0.72
1:A:301:LEU:O	1:A:305:GLU:HB2	1.88	0.72
1:A:99:GLY:HA2	1:A:383:TRP:NE1	2.03	0.71
2:B:366:LYS:O	2:B:369:THR:HG22	1.91	0.71
2:B:164:MET:SD	2:B:168:LEU:HD11	2.30	0.71
2:B:257:ILE:O	2:B:261:VAL:HG23	1.90	0.71
1:A:169:GLU:O	1:A:172:LYS:HG3	1.91	0.71
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.21	0.70
1:A:256:ASP:HA	1:A:259:LYS:HE3	1.73	0.70
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.70
2:B:116:PHE:HA	2:B:148:VAL:HG21	1.74	0.70
2:B:198:HIS:O	2:B:202:ILE:HG12	1.92	0.70
1:A:246:LEU:HG	1:A:310:LEU:HD22	1.74	0.70
1:A:443:ASP:CB	1:A:548:VAL:HB	2.21	0.70
2:B:257:ILE:O	2:B:260:LEU:HB3	1.92	0.69
2:B:252:TRP:O	2:B:292:VAL:HA	1.93	0.69
2:B:260:LEU:O	2:B:264:LEU:HG	1.93	0.69
2:B:84:THR:HG21	2:B:124:PHE:CZ	2.26	0.69
1:A:474:ASN:O	1:A:478:GLU:HG3	1.92	0.69
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.73	0.69
2:B:241:VAL:HG13	2:B:351:THR:OG1	1.93	0.69
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.75	0.69
1:A:478:GLU:O	1:A:481:ALA:HB3	1.92	0.69
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.27	0.69
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.27	0.69
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.55	0.69
1:A:239:TRP:O	1:A:240:THR:HG23	1.92	0.69
1:A:443:ASP:HB2	1:A:548:VAL:HB	1.74	0.68
1:A:92:LEU:HD11	2:B:22:LYS:HE3	1.74	0.68
2:B:23:GLN:HG3	2:B:133:PRO:HG3	1.75	0.68
2:B:261:VAL:HA	2:B:264:LEU:HD12	1.75	0.68
2:B:205:LEU:O	2:B:205:LEU:HD12	1.92	0.68
1:A:397:THR:HG21	1:A:424:LYS:HA	1.76	0.68
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.76	0.68
2:B:201:LYS:O	2:B:204:GLU:HB3	1.93	0.68
1:A:232:TYR:HA	1:A:241:VAL:HG22	1.74	0.68
1:A:128:THR:HG21	1:A:150:PRO:HG2	1.75	0.68
2:B:398:TRP:O	2:B:402:TRP:HD1	1.76	0.68
2:B:125:ARG:HE	2:B:147:ASN:HA	1.59	0.68
2:B:166:LYS:O	2:B:170:PRO:HD2	1.94	0.67
1:A:521:ILE:O	1:A:525:LEU:HG	1.94	0.67
2:B:108:VAL:HA	2:B:187:LEU:O	1.94	0.67
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.24	0.67
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.30	0.67
1:A:90:VAL:HG23	1:A:91:GLN:H	1.58	0.67
1:A:326:ILE:O	1:A:341:ILE:HA	1.94	0.67
1:A:188:TYR:CB	3:A:559:TBO:H122	2.25	0.67
2:B:107:THR:HA	2:B:232:TYR:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ARG:O	2:B:202:ILE:HB	1.94	0.67
2:B:323:LYS:HB2	2:B:343:GLN:OE1	1.93	0.67
1:A:398:TRP:CE2	1:A:402:TRP:CD1	2.84	0.66
1:A:198:HIS:O	1:A:202:ILE:HG12	1.96	0.66
1:A:399:GLU:HA	1:A:402:TRP:HE1	1.58	0.66
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.31	0.66
1:A:31:ILE:HG21	1:A:134:SER:O	1.96	0.66
1:A:419:THR:HB	1:A:420:PRO:HD2	1.78	0.66
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.61	0.66
2:B:326:ILE:O	2:B:341:ILE:HA	1.96	0.66
1:A:398:TRP:NE1	1:A:411:ILE:HG12	2.11	0.66
2:B:393:ILE:HG12	2:B:394:GLN:N	2.11	0.66
2:B:40:GLU:O	2:B:43:LYS:HB3	1.96	0.65
1:A:240:THR:HG21	1:A:315:HIS:HA	1.76	0.65
1:A:207:GLN:HB3	1:A:211:ARG:HH12	1.59	0.65
2:B:101:LYS:HD2	2:B:382:ILE:HG23	1.79	0.65
2:B:128:THR:CB	2:B:146:TYR:HB2	2.27	0.65
2:B:115:TYR:HD2	2:B:156:SER:HB3	1.61	0.65
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.78	0.65
1:A:303:LEU:HD21	1:A:307:ARG:HH21	1.60	0.65
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.65
2:B:271:TYR:O	2:B:274:ILE:HG22	1.97	0.65
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.33	0.64
2:B:163:SER:O	2:B:167:ILE:HG12	1.98	0.64
2:B:160:PHE:HE2	2:B:164:MET:HG2	1.63	0.64
1:A:514:GLU:CD	1:A:514:GLU:H	2.00	0.64
2:B:379:SER:HA	2:B:383:TRP:CE3	2.32	0.64
2:B:99:GLY:HA2	2:B:102:LYS:HD2	1.80	0.64
1:A:146:TYR:CE2	1:A:150:PRO:HA	2.33	0.64
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.80	0.63
1:A:260:LEU:O	1:A:264:LEU:HG	1.98	0.63
2:B:380:ILE:O	2:B:384:GLY:N	2.31	0.63
1:A:188:TYR:CG	3:A:559:TBO:H122	2.33	0.63
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.34	0.63
2:B:329:ILE:HD11	2:B:375:ILE:HD11	1.79	0.63
2:B:257:ILE:HD13	2:B:283:LEU:HB3	1.81	0.63
1:A:439:THR:HA	1:A:494:ASN:HB2	1.79	0.63
1:A:241:VAL:HG11	1:A:266:TRP:NE1	2.11	0.63
2:B:378:GLU:O	2:B:381:VAL:HB	1.99	0.63
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.80	0.62
2:B:5:ILE:HG22	2:B:6:GLU:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:PHE:HD2	2:B:152:GLY:HA3	1.64	0.62
1:A:101:LYS:HD3	1:A:321:PRO:CD	2.28	0.62
1:A:479:LEU:HA	1:A:482:ILE:HD12	1.81	0.62
1:A:194:GLU:O	1:A:197:GLN:N	2.31	0.62
1:A:331:LYS:O	1:A:421:PRO:HG2	1.99	0.62
1:A:466:VAL:HG12	1:A:467:VAL:N	2.15	0.62
1:A:398:TRP:O	1:A:401:TRP:HB3	1.99	0.62
1:A:445:ALA:O	1:A:477:THR:HG21	1.99	0.62
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.33	0.62
2:B:160:PHE:CE2	2:B:164:MET:HG2	2.34	0.62
1:A:304:ALA:HA	1:A:307:ARG:HB2	1.81	0.62
1:A:341:ILE:O	1:A:349:LEU:HB3	1.99	0.62
1:A:478:GLU:O	1:A:482:ILE:HG13	2.00	0.61
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.82	0.61
1:A:500:GLN:HA	1:A:500:GLN:OE1	1.98	0.61
1:A:482:ILE:O	1:A:485:ALA:HB3	2.00	0.61
1:A:239:TRP:HB3	1:A:318:TYR:CE1	2.36	0.61
2:B:292:VAL:HG12	2:B:294:PRO:HD3	1.83	0.61
1:A:509:GLN:N	1:A:510:PRO:HD3	2.16	0.61
1:A:442:VAL:HG21	1:A:485:ALA:HB2	1.83	0.61
1:A:372:VAL:HA	1:A:375:ILE:HD12	1.82	0.61
2:B:330:GLN:HB2	2:B:332:GLN:HE22	1.65	0.61
2:B:115:TYR:HE2	2:B:157:PRO:N	1.99	0.61
2:B:99:GLY:HA2	2:B:102:LYS:CD	2.31	0.61
2:B:27:THR:HG23	2:B:30:LYS:H	1.65	0.60
2:B:261:VAL:HG22	2:B:279:LEU:HD23	1.83	0.60
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.36	0.60
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.65	0.60
1:A:368:LEU:O	1:A:371:ALA:HB3	2.02	0.60
2:B:143:ARG:HH11	2:B:143:ARG:HG2	1.67	0.60
1:A:373:GLN:HE21	2:B:397:THR:HA	1.67	0.60
1:A:90:VAL:HG23	1:A:91:GLN:N	2.15	0.60
2:B:315:HIS:O	2:B:317:VAL:N	2.35	0.60
2:B:31:ILE:HD13	2:B:133:PRO:O	2.02	0.60
1:A:63:ILE:HG22	1:A:64:LYS:N	2.16	0.60
1:A:317:VAL:HG11	1:A:347:LYS:HE3	1.82	0.60
2:B:375:ILE:O	2:B:378:GLU:HG2	2.02	0.60
1:A:441:TYR:O	1:A:548:VAL:HG11	2.02	0.60
1:A:34:LEU:HD22	1:A:60:VAL:HG12	1.82	0.59
2:B:379:SER:HA	2:B:383:TRP:HZ3	1.65	0.59
2:B:354:TYR:HD2	2:B:371:ALA:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:CD2	2:B:325:LEU:H	2.15	0.59
1:A:92:LEU:HD11	2:B:22:LYS:CE	2.32	0.59
1:A:268:SER:O	1:A:351:THR:HB	2.03	0.59
1:A:37:ILE:O	1:A:41:MET:HG3	2.02	0.59
1:A:195:ILE:CG2	1:A:199:ARG:HH12	2.16	0.59
1:A:400:THR:O	1:A:404:GLU:HG3	2.02	0.59
1:A:106:VAL:HG12	1:A:107:THR:N	2.17	0.59
1:A:51:GLY:N	1:A:52:PRO:HD2	2.16	0.59
1:A:492:GLU:HG2	1:A:530:LYS:HD2	1.85	0.59
2:B:239:TRP:HB2	2:B:350:LYS:HE3	1.84	0.59
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.66	0.59
1:A:398:TRP:CE2	1:A:402:TRP:HD1	2.20	0.59
1:A:498:ASP:HB3	1:A:545:ASN:HD21	1.68	0.58
2:B:296:THR:HB	2:B:299:ALA:HB3	1.84	0.58
1:A:95:PRO:HG3	2:B:137:ASN:O	2.03	0.58
1:A:503:LEU:HD22	1:A:535:TRP:CG	2.38	0.58
1:A:480:GLN:HE22	1:A:483:TYR:HD2	1.51	0.58
1:A:482:ILE:HG23	1:A:495:ILE:HG21	1.85	0.58
2:B:342:TYR:HB3	2:B:348:ASN:CA	2.34	0.58
1:A:468:PRO:C	1:A:469:LEU:HG	2.22	0.58
2:B:32:LYS:O	2:B:35:VAL:HG22	2.04	0.58
2:B:64:LYS:HB3	2:B:68:SER:HA	1.85	0.58
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.85	0.58
1:A:123:ASP:O	1:A:126:LYS:HE3	2.01	0.58
1:A:269:GLN:O	1:A:351:THR:N	2.35	0.58
1:A:56:TYR:O	1:A:129:ALA:HB3	2.04	0.58
1:A:257:ILE:CD1	1:A:295:LEU:HD11	2.32	0.58
1:A:40:GLU:O	1:A:44:GLU:HG2	2.04	0.58
2:B:320:ASP:CG	2:B:323:LYS:HG2	2.23	0.58
1:A:163:SER:HA	1:A:166:LYS:HD2	1.85	0.58
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.18	0.57
1:A:325:LEU:HD11	1:A:383:TRP:HB2	1.85	0.57
1:A:447:ASN:HB3	1:A:450:THR:HG1	1.69	0.57
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.22	0.57
1:A:97:PRO:HA	1:A:100:LEU:HG	1.87	0.57
1:A:461:LYS:O	1:A:463:ARG:N	2.38	0.57
1:A:543:GLY:N	2:B:284:ARG:HA	2.14	0.57
2:B:41:MET:CB	2:B:47:ILE:HG12	2.34	0.57
1:A:108:VAL:HA	1:A:187:LEU:O	2.04	0.57
2:B:325:LEU:HG	2:B:387:PRO:HB3	1.85	0.57
1:A:188:TYR:CD2	3:A:559:TBO:H122	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.39	0.57
2:B:380:ILE:HA	2:B:385:LYS:H	1.68	0.57
1:A:162:SER:O	1:A:166:LYS:HG3	2.04	0.57
1:A:199:ARG:NH1	1:A:199:ARG:HB2	2.20	0.57
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.70	0.56
2:B:342:TYR:CB	2:B:348:ASN:HA	2.33	0.56
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.35	0.56
2:B:178:ILE:O	2:B:178:ILE:HG22	2.04	0.56
1:A:329:ILE:HG22	1:A:330:GLN:N	2.20	0.56
2:B:107:THR:O	2:B:188:TYR:HA	2.06	0.56
1:A:379:SER:CB	1:A:387:PRO:HD3	2.34	0.56
1:A:492:GLU:HG3	1:A:529:GLU:OE1	2.04	0.56
2:B:382:ILE:HB	2:B:383:TRP:CZ3	2.40	0.56
2:B:62:ALA:HB1	2:B:71:TRP:CE3	2.41	0.56
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.06	0.56
2:B:333:GLY:N	2:B:336:GLN:HB2	2.20	0.56
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.71	0.56
1:A:233:GLU:N	1:A:240:THR:O	2.35	0.56
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.41	0.56
2:B:393:ILE:HG12	2:B:394:GLN:H	1.69	0.56
1:A:472:THR:OG1	1:A:477:THR:HG23	2.05	0.56
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.87	0.56
2:B:169:GLU:O	2:B:173:LYS:HG3	2.06	0.56
2:B:128:THR:HB	2:B:146:TYR:HB2	1.87	0.56
1:A:255:ASN:HA	1:A:258:GLN:OE1	2.05	0.56
2:B:210:LEU:HD13	2:B:216:THR:HA	1.87	0.56
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.74	0.55
2:B:41:MET:HB2	2:B:47:ILE:HG12	1.88	0.55
2:B:38:CYS:O	2:B:47:ILE:HD11	2.06	0.55
1:A:97:PRO:HD2	1:A:232:TYR:CZ	2.41	0.55
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.40	0.55
1:A:438:GLU:HG2	1:A:459:THR:HB	1.88	0.55
2:B:296:THR:HG22	2:B:299:ALA:H	1.71	0.55
2:B:421:PRO:HG2	2:B:424:LYS:HB2	1.88	0.55
2:B:253:THR:HA	2:B:291:GLU:O	2.07	0.55
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.42	0.55
1:A:68:SER:HB2	1:A:70:LYS:CE	2.37	0.55
2:B:115:TYR:H	2:B:115:TYR:HD1	1.50	0.55
1:A:442:VAL:HA	1:A:457:TYR:HB3	1.88	0.55
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.41	0.55
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HB3	3:A:559:TBO:N1	2.22	0.55
2:B:177:ASP:O	2:B:179:VAL:HG23	2.07	0.55
2:B:198:HIS:O	2:B:201:LYS:HB3	2.06	0.55
1:A:31:ILE:HD13	1:A:133:PRO:O	2.07	0.55
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.42	0.55
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.88	0.54
2:B:380:ILE:HA	2:B:385:LYS:N	2.23	0.54
1:A:49:LYS:O	1:A:49:LYS:HG3	2.08	0.54
1:A:271:TYR:HE1	1:A:314:VAL:H	1.55	0.54
2:B:12:LEU:HD23	2:B:83:ARG:O	2.07	0.54
2:B:59:PRO:HB2	2:B:76:ASP:CB	2.33	0.54
2:B:131:THR:HG23	2:B:143:ARG:HG3	1.90	0.54
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.07	0.54
1:A:162:SER:O	1:A:165:THR:HB	2.08	0.54
1:A:383:TRP:O	1:A:385:LYS:HG2	2.08	0.54
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.42	0.54
2:B:378:GLU:O	2:B:382:ILE:HD12	2.07	0.54
2:B:78:ARG:NH1	2:B:412:PRO:O	2.41	0.54
1:A:19:PRO:HA	1:A:83:ARG:HH12	1.73	0.54
1:A:101:LYS:NZ	1:A:321:PRO:HG2	2.23	0.54
2:B:299:ALA:O	2:B:302:GLU:HB2	2.08	0.54
1:A:46:LYS:HG3	1:A:148:VAL:HG11	1.90	0.54
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.28	0.54
1:A:537:PRO:HB2	1:A:540:LYS:HB2	1.89	0.54
2:B:393:ILE:O	2:B:416:PHE:HB3	2.08	0.54
1:A:377:THR:O	1:A:381:VAL:HG23	2.07	0.54
1:A:466:VAL:CG1	1:A:467:VAL:N	2.71	0.53
1:A:372:VAL:O	1:A:375:ILE:HB	2.08	0.53
2:B:338:THR:HG22	2:B:339:TYR:N	2.23	0.53
1:A:372:VAL:HG13	1:A:389:PHE:CE2	2.43	0.53
2:B:127:TYR:C	2:B:129:ALA:H	2.12	0.53
1:A:320:ASP:O	1:A:343:GLN:NE2	2.41	0.53
1:A:441:TYR:HA	1:A:496:VAL:HB	1.90	0.53
1:A:469:LEU:HB2	1:A:472:THR:HG21	1.91	0.53
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.90	0.53
2:B:167:ILE:O	2:B:208:HIS:NE2	2.41	0.53
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.92	0.53
1:A:111:VAL:HG22	1:A:187:LEU:HD12	1.90	0.53
1:A:426:TRP:CE3	1:A:426:TRP:HA	2.43	0.53
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.89	0.53
2:B:332:GLN:HB3	2:B:336:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ILE:HD11	2:B:375:ILE:CD1	2.38	0.53
1:A:56:TYR:O	1:A:143:ARG:NH2	2.42	0.53
1:A:268:SER:HA	1:A:274:ILE:HD12	1.89	0.53
2:B:59:PRO:O	2:B:75:VAL:HG13	2.08	0.53
1:A:23:GLN:HE22	1:A:26:LEU:HD23	1.73	0.52
1:A:473:THR:HG22	1:A:475:GLN:H	1.73	0.52
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.74	0.52
2:B:325:LEU:H	2:B:325:LEU:HD23	1.73	0.52
2:B:330:GLN:HB2	2:B:332:GLN:NE2	2.24	0.52
1:A:486:LEU:HD11	1:A:521:ILE:HG23	1.90	0.52
1:A:340:GLN:HA	1:A:350:LYS:O	2.08	0.52
2:B:234:LEU:HD13	2:B:377:THR:HG21	1.91	0.52
1:A:207:GLN:O	1:A:210:LEU:HB3	2.10	0.52
2:B:324:ASP:O	2:B:343:GLN:HG2	2.09	0.52
1:A:420:PRO:CB	1:A:421:PRO:HD3	2.40	0.52
2:B:244:ILE:HG12	2:B:427:TYR:HB2	1.90	0.52
2:B:253:THR:HG23	2:B:289:LEU:O	2.10	0.52
2:B:253:THR:HG23	2:B:291:GLU:H	1.75	0.52
1:A:325:LEU:HD12	1:A:385:LYS:HB2	1.92	0.52
1:A:408:ALA:O	2:B:393:ILE:HG13	2.09	0.52
2:B:400:THR:HG22	2:B:400:THR:O	2.10	0.52
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.74	0.52
2:B:368:LEU:O	2:B:372:VAL:HG23	2.09	0.52
1:A:328:GLU:O	1:A:339:TYR:HA	2.10	0.52
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.39	0.52
1:A:116:PHE:O	1:A:148:VAL:HB	2.10	0.52
1:A:170:PRO:O	1:A:173:LYS:HB3	2.10	0.52
2:B:115:TYR:HB3	2:B:149:LEU:HB3	1.92	0.51
1:A:81:ASN:O	1:A:84:THR:HB	2.10	0.51
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.45	0.51
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.08	0.51
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.26	0.51
2:B:344:GLU:HB2	2:B:347:LYS:CB	2.38	0.51
1:A:101:LYS:HG2	1:A:319:TYR:HB3	1.92	0.51
1:A:408:ALA:HB1	2:B:364:ASP:CB	2.41	0.51
1:A:40:GLU:O	1:A:44:GLU:N	2.44	0.51
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.45	0.51
1:A:458:VAL:HA	1:A:463:ARG:O	2.09	0.51
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.46	0.51
2:B:111:VAL:N	2:B:185:ASP:O	2.43	0.50
1:A:365:VAL:HG22	1:A:423:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:GLY:HA3	2:B:287:LYS:HD2	1.92	0.50
1:A:362:THR:HG22	1:A:363:ASN:H	1.75	0.50
1:A:317:VAL:HG23	1:A:349:LEU:CD1	2.37	0.50
1:A:195:ILE:HG23	1:A:199:ARG:HH12	1.76	0.50
1:A:500:GLN:O	1:A:503:LEU:HB3	2.11	0.50
1:A:211:ARG:NH1	1:A:211:ARG:HG3	2.27	0.50
1:A:505:ILE:HG22	1:A:506:ILE:N	2.26	0.50
2:B:229:TRP:C	2:B:231:GLY:H	2.13	0.50
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.94	0.50
1:A:103:LYS:O	1:A:236:PRO:HB2	2.10	0.50
2:B:69:THR:HG22	2:B:70:LYS:N	2.27	0.50
1:A:245:VAL:O	1:A:247:PRO:HD3	2.11	0.50
1:A:188:TYR:HB3	3:A:559:TBO:H122	1.92	0.50
1:A:452:LEU:HD22	1:A:470:THR:HA	1.93	0.50
2:B:99:GLY:O	2:B:102:LYS:HB2	2.11	0.50
2:B:65:LYS:HB2	2:B:72:ARG:HG3	1.93	0.50
1:A:153:TRP:CE3	1:A:156:SER:N	2.80	0.50
1:A:427:TYR:CZ	1:A:509:GLN:HA	2.47	0.50
2:B:338:THR:HG22	2:B:339:TYR:H	1.76	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.26	0.50
2:B:260:LEU:HD23	2:B:279:LEU:HD21	1.94	0.49
1:A:542:ILE:HG12	1:A:544:GLY:N	2.27	0.49
1:A:394:GLN:HB3	1:A:397:THR:OG1	2.12	0.49
1:A:153:TRP:HB3	1:A:156:SER:OG	2.12	0.49
2:B:21:VAL:HG23	2:B:57:ASN:O	2.12	0.49
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.27	0.49
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.94	0.49
2:B:210:LEU:HD13	2:B:216:THR:CA	2.42	0.49
1:A:12:LEU:HD22	1:A:83:ARG:C	2.32	0.49
1:A:164:MET:SD	1:A:168:LEU:CD2	2.98	0.49
1:A:479:LEU:HA	1:A:482:ILE:CD1	2.40	0.49
2:B:239:TRP:HE3	2:B:350:LYS:HG3	1.78	0.49
2:B:320:ASP:H	2:B:343:GLN:HE22	1.60	0.49
2:B:253:THR:HB	2:B:256:ASP:CG	2.32	0.49
2:B:319:TYR:CE2	2:B:383:TRP:HD1	2.31	0.49
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.49
1:A:387:PRO:HG2	1:A:389:PHE:CE1	2.47	0.49
2:B:246:LEU:HD11	2:B:307:ARG:HA	1.94	0.49
1:A:314:VAL:HG12	1:A:315:HIS:N	2.28	0.49
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.27	0.49
2:B:47:ILE:HB	2:B:145:GLN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:CG2	1:A:485:ALA:HB2	2.43	0.49
1:A:328:GLU:HA	1:A:390:LYS:HB2	1.95	0.49
1:A:131:THR:HG1	1:A:143:ARG:NH1	2.10	0.49
2:B:50:ILE:HD12	2:B:143:ARG:HB3	1.94	0.49
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.48	0.49
2:B:308:GLU:HG3	2:B:311:LYS:HD2	1.94	0.49
2:B:179:VAL:O	2:B:189:VAL:HA	2.12	0.49
2:B:178:ILE:CD1	2:B:191:SER:HB3	2.43	0.49
2:B:255:ASN:O	2:B:258:GLN:HB2	2.12	0.49
1:A:33:ALA:O	1:A:37:ILE:HG13	2.13	0.49
1:A:59:PRO:O	1:A:75:VAL:HG13	2.12	0.49
2:B:263:LYS:HE2	2:B:425:LEU:CD1	2.35	0.49
2:B:268:SER:HA	2:B:274:ILE:CG2	2.43	0.49
1:A:257:ILE:O	1:A:261:VAL:HG23	2.13	0.49
2:B:398:TRP:C	2:B:400:THR:H	2.15	0.49
2:B:320:ASP:O	2:B:343:GLN:OE1	2.31	0.49
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.94	0.49
2:B:397:THR:O	2:B:401:TRP:HD1	1.95	0.48
1:A:495:ILE:HB	1:A:533:LEU:HD13	1.94	0.48
1:A:459:THR:CG2	1:A:463:ARG:HD2	2.44	0.48
2:B:115:TYR:C	2:B:117:SER:H	2.16	0.48
2:B:128:THR:HG21	2:B:146:TYR:HB2	1.94	0.48
1:A:19:PRO:HA	1:A:83:ARG:NH1	2.28	0.48
2:B:193:LEU:HD22	2:B:197:GLN:CB	2.43	0.48
2:B:30:LYS:HG2	2:B:71:TRP:CZ3	2.48	0.48
1:A:105:SER:HB3	1:A:198:HIS:CG	2.48	0.48
2:B:391:LEU:HB2	2:B:416:PHE:CD2	2.47	0.48
2:B:340:GLN:HA	2:B:351:THR:HA	1.96	0.48
1:A:272:PRO:CA	1:A:351:THR:HG21	2.29	0.48
2:B:254:VAL:HG23	2:B:291:GLU:HB3	1.96	0.48
2:B:35:VAL:CG2	2:B:36:GLU:N	2.76	0.48
2:B:325:LEU:CD2	2:B:387:PRO:HA	2.44	0.48
2:B:86:ASP:O	2:B:89:GLU:HG2	2.13	0.48
1:A:12:LEU:HD23	1:A:124:PHE:HZ	1.78	0.48
1:A:60:VAL:HA	1:A:75:VAL:CG2	2.29	0.48
1:A:468:PRO:O	1:A:469:LEU:HD23	2.14	0.48
1:A:474:ASN:ND2	1:A:474:ASN:H	2.11	0.48
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.79	0.48
1:A:486:LEU:HB3	1:A:524:GLN:OE1	2.13	0.48
1:A:553:SER:HA	1:A:556:ILE:O	2.13	0.48
2:B:88:TRP:CZ3	2:B:92:LEU:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.49	0.48
2:B:253:THR:CG2	2:B:289:LEU:O	2.62	0.48
1:A:274:ILE:HA	1:A:306:ASN:OD1	2.14	0.47
1:A:341:ILE:HD12	1:A:350:LYS:O	2.14	0.47
1:A:441:TYR:CD1	1:A:441:TYR:N	2.82	0.47
1:A:519:ASN:O	1:A:522:ILE:HB	2.13	0.47
2:B:206:ARG:O	2:B:209:LEU:HB2	2.14	0.47
1:A:23:GLN:HG2	1:A:24:TRP:N	2.28	0.47
2:B:62:ALA:HB1	2:B:71:TRP:HE3	1.78	0.47
2:B:27:THR:CG2	2:B:30:LYS:HG3	2.45	0.47
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.44	0.47
2:B:178:ILE:HD12	2:B:189:VAL:HG12	1.95	0.47
1:A:246:LEU:HD21	1:A:310:LEU:HD13	1.97	0.47
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.96	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.47
2:B:104:LYS:O	2:B:235:HIS:HA	2.14	0.47
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.15	0.47
2:B:164:MET:SD	2:B:168:LEU:CD1	3.01	0.47
1:A:34:LEU:HB3	1:A:132:ILE:HD13	1.97	0.47
2:B:425:LEU:CD1	2:B:427:TYR:HB3	2.42	0.47
1:A:433:PRO:HG2	2:B:290:THR:HG23	1.97	0.47
2:B:342:TYR:HB3	2:B:348:ASN:HB3	1.96	0.47
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.97	0.46
2:B:271:TYR:O	2:B:273:GLY:N	2.48	0.46
2:B:296:THR:HB	2:B:299:ALA:CB	2.45	0.46
2:B:246:LEU:N	2:B:246:LEU:HD23	2.30	0.46
1:A:378:GLU:O	1:A:382:ILE:HG13	2.15	0.46
1:A:474:ASN:H	1:A:474:ASN:HD22	1.63	0.46
2:B:5:ILE:HG22	2:B:6:GLU:N	2.29	0.46
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.33	0.46
2:B:64:LYS:HE3	2:B:71:TRP:CZ2	2.50	0.46
2:B:320:ASP:N	2:B:343:GLN:HE22	2.13	0.46
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.97	0.46
1:A:199:ARG:CZ	1:A:199:ARG:HB2	2.46	0.46
1:A:13:LYS:HG3	1:A:83:ARG:O	2.16	0.46
2:B:304:ALA:O	2:B:307:ARG:HB3	2.16	0.46
1:A:77:PHE:CB	1:A:80:LEU:HD23	2.45	0.46
2:B:10:VAL:HG12	2:B:11:LYS:N	2.31	0.46
1:A:47:ILE:HG22	1:A:48:SER:N	2.29	0.46
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.97	0.46
1:A:241:VAL:HG21	1:A:266:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:414:TRP:HD1	1.99	0.46
2:B:65:LYS:HE3	2:B:407:GLN:HE21	1.81	0.46
2:B:116:PHE:HA	2:B:148:VAL:CG2	2.45	0.46
2:B:12:LEU:HD23	2:B:84:THR:HG23	1.98	0.46
2:B:303:LEU:HD11	2:B:307:ARG:NH2	2.30	0.46
1:A:373:GLN:HE22	2:B:397:THR:HA	1.76	0.46
1:A:442:VAL:HG12	1:A:481:ALA:HB1	1.98	0.46
1:A:12:LEU:HD22	1:A:83:ARG:O	2.15	0.46
1:A:406:TRP:CH2	2:B:417:VAL:O	2.69	0.46
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.51	0.46
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.98	0.46
1:A:420:PRO:HG2	1:A:421:PRO:HD3	1.98	0.46
1:A:329:ILE:HG23	1:A:338:THR:O	2.16	0.46
1:A:153:TRP:CH2	1:A:155:GLY:HA3	2.51	0.46
1:A:87:PHE:O	2:B:55:PRO:HB3	2.16	0.46
2:B:379:SER:O	2:B:383:TRP:HE3	1.98	0.45
1:A:194:GLU:HB2	1:A:197:GLN:HB3	1.98	0.45
1:A:547:GLN:HA	1:A:550:LYS:HB2	1.97	0.45
2:B:163:SER:C	2:B:167:ILE:HG12	2.36	0.45
1:A:375:ILE:HG21	1:A:389:PHE:CE2	2.50	0.45
2:B:296:THR:HG22	2:B:299:ALA:N	2.31	0.45
1:A:545:ASN:HA	1:A:548:VAL:CG2	2.47	0.45
1:A:65:LYS:HD2	1:A:66:LYS:N	2.30	0.45
2:B:178:ILE:HG23	2:B:189:VAL:CG1	2.46	0.45
2:B:377:THR:HG22	2:B:381:VAL:CG2	2.46	0.45
1:A:207:GLN:OE1	1:A:210:LEU:HD23	2.17	0.45
2:B:314:VAL:HG23	2:B:316:GLY:H	1.80	0.45
1:A:244:ILE:HG22	1:A:310:LEU:HD11	1.97	0.45
1:A:341:ILE:HD12	1:A:341:ILE:N	2.32	0.45
2:B:375:ILE:HD12	2:B:389:PHE:HE1	1.81	0.45
1:A:365:VAL:O	1:A:368:LEU:HB3	2.17	0.45
1:A:283:LEU:O	1:A:285:GLY:N	2.50	0.45
1:A:317:VAL:O	1:A:349:LEU:HD12	2.17	0.45
1:A:318:TYR:CZ	3:A:559:TBO:H10	2.49	0.45
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.30	0.45
2:B:373:GLN:NE2	2:B:406:TRP:CD2	2.84	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.45
1:A:459:THR:HG21	1:A:463:ARG:HD2	1.98	0.45
1:A:168:LEU:HD23	1:A:209:LEU:HD21	1.99	0.45
1:A:106:VAL:O	1:A:107:THR:HB	2.17	0.45
2:B:128:THR:CG2	2:B:146:TYR:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:O	1:A:419:THR:HG23	2.17	0.45
1:A:376:THR:O	1:A:380:ILE:HG12	2.16	0.45
2:B:253:THR:O	2:B:257:ILE:HG22	2.17	0.45
1:A:479:LEU:HD13	1:A:517:LEU:HG	1.97	0.45
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.82	0.45
2:B:132:ILE:HG23	2:B:142:ILE:CB	2.42	0.45
1:A:195:ILE:HG22	1:A:199:ARG:HH12	1.81	0.45
2:B:74:LEU:C	2:B:74:LEU:HD23	2.37	0.45
1:A:341:ILE:CD1	1:A:350:LYS:HB3	2.42	0.45
2:B:354:TYR:HE1	2:B:356:ARG:HD3	1.82	0.45
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.45
2:B:326:ILE:CD1	2:B:388:LYS:HE2	2.42	0.45
1:A:438:GLU:CD	1:A:461:LYS:HD2	2.38	0.45
1:A:178:ILE:HG23	1:A:190:GLY:O	2.16	0.45
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.30	0.45
1:A:419:THR:CB	1:A:420:PRO:HD2	2.46	0.45
1:A:296:THR:O	1:A:299:ALA:HB3	2.17	0.45
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.20	0.44
2:B:234:LEU:CD1	2:B:377:THR:HG21	2.47	0.44
2:B:380:ILE:O	2:B:384:GLY:CA	2.65	0.44
2:B:170:PRO:HG2	2:B:171:PHE:H	1.82	0.44
1:A:105:SER:HB3	1:A:198:HIS:ND1	2.32	0.44
1:A:174:GLN:O	1:A:176:PRO:HD3	2.17	0.44
1:A:142:ILE:HG13	1:A:142:ILE:O	2.18	0.44
1:A:532:TYR:CE2	2:B:289:LEU:HD13	2.52	0.44
1:A:260:LEU:HD23	1:A:279:LEU:HD13	1.98	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.44
2:B:303:LEU:O	2:B:307:ARG:HB2	2.17	0.44
2:B:191:SER:OG	2:B:198:HIS:ND1	2.50	0.44
2:B:257:ILE:CD1	2:B:282:LEU:HB3	2.47	0.44
2:B:126:LYS:HA	2:B:145:GLN:HE21	1.81	0.44
1:A:183:TYR:O	1:A:186:ASP:HB2	2.17	0.44
2:B:96:HIS:CE1	2:B:382:ILE:O	2.71	0.44
1:A:479:LEU:CD1	1:A:517:LEU:HG	2.46	0.44
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.99	0.44
2:B:2:ILE:HG22	2:B:2:ILE:O	2.16	0.44
1:A:188:TYR:HD2	3:A:559:TBO:H71	1.82	0.44
2:B:410:TRP:O	2:B:410:TRP:CE3	2.70	0.44
1:A:224:GLU:C	1:A:226:PRO:HD2	2.37	0.44
1:A:511:ASP:HA	1:A:522:ILE:HD13	1.99	0.44
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LEU:O	2:B:215:THR:OG1	2.36	0.44
2:B:103:LYS:HD2	2:B:191:SER:CA	2.48	0.44
2:B:406:TRP:HH2	2:B:412:PRO:HD2	1.83	0.44
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.99	0.44
2:B:21:VAL:CB	2:B:59:PRO:HD3	2.44	0.44
1:A:47:ILE:HG23	1:A:145:GLN:O	2.17	0.44
1:A:202:ILE:HG21	1:A:221:HIS:CB	2.47	0.44
2:B:241:VAL:O	2:B:241:VAL:HG12	2.18	0.44
1:A:450:THR:O	1:A:452:LEU:HG	2.18	0.44
1:A:264:LEU:HD11	1:A:279:LEU:CD1	2.48	0.44
1:A:51:GLY:HA2	1:A:143:ARG:HD3	1.99	0.44
2:B:109:LEU:O	2:B:187:LEU:N	2.47	0.44
1:A:2:ILE:O	1:A:213:GLY:HA3	2.18	0.44
1:A:240:THR:HG22	1:A:315:HIS:HA	1.98	0.43
2:B:376:THR:HG22	2:B:380:ILE:HD11	2.00	0.43
1:A:373:GLN:O	1:A:376:THR:N	2.51	0.43
2:B:401:TRP:O	2:B:404:GLU:HB3	2.18	0.43
2:B:246:LEU:CD1	2:B:307:ARG:HA	2.48	0.43
2:B:371:ALA:O	2:B:372:VAL:C	2.57	0.43
1:A:259:LYS:O	1:A:263:LYS:HG3	2.18	0.43
1:A:149:LEU:HD22	1:A:156:SER:HA	1.99	0.43
2:B:125:ARG:NE	2:B:147:ASN:HA	2.30	0.43
2:B:188:TYR:CD1	2:B:188:TYR:N	2.86	0.43
2:B:63:ILE:O	2:B:72:ARG:N	2.51	0.43
2:B:171:PHE:CE2	2:B:205:LEU:CA	3.00	0.43
1:A:465:LYS:O	1:A:466:VAL:HG23	2.17	0.43
2:B:329:ILE:CG2	2:B:330:GLN:N	2.82	0.43
1:A:483:TYR:O	1:A:486:LEU:HB2	2.17	0.43
2:B:363:ASN:O	2:B:364:ASP:C	2.56	0.43
2:B:60:VAL:HA	2:B:74:LEU:O	2.18	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.66	0.43
1:A:523:GLU:HA	1:A:526:ILE:HD12	1.99	0.43
1:A:532:TYR:HE2	2:B:289:LEU:HD13	1.83	0.43
1:A:521:ILE:HG22	1:A:525:LEU:HD11	1.99	0.43
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.19	0.43
1:A:410:TRP:CE3	1:A:410:TRP:HA	2.53	0.43
2:B:349:LEU:H	2:B:349:LEU:HG	1.54	0.43
1:A:380:ILE:O	1:A:384:GLY:HA2	2.18	0.43
2:B:81:ASN:HD22	2:B:154:LYS:HG3	1.82	0.43
1:A:473:THR:HG22	1:A:474:ASN:N	2.34	0.43
2:B:31:ILE:O	2:B:35:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLN:O	1:A:483:TYR:HB3	2.18	0.43
2:B:206:ARG:HA	2:B:209:LEU:HD12	2.00	0.43
2:B:342:TYR:HB3	2:B:348:ASN:CB	2.49	0.43
2:B:354:TYR:CE1	2:B:356:ARG:HD3	2.53	0.43
1:A:178:ILE:CG2	1:A:189:VAL:HG12	2.49	0.43
2:B:108:VAL:CG1	2:B:186:ASP:HB3	2.49	0.43
1:A:368:LEU:O	1:A:372:VAL:HG23	2.18	0.43
1:A:426:TRP:HE3	1:A:426:TRP:HA	1.84	0.43
1:A:23:GLN:HG2	1:A:24:TRP:O	2.19	0.42
1:A:393:ILE:HG12	1:A:394:GLN:N	2.33	0.42
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.82	0.42
1:A:73:LYS:HG2	1:A:74:LEU:N	2.34	0.42
1:A:242:GLN:N	1:A:243:PRO:HD2	2.34	0.42
1:A:543:GLY:HA2	1:A:546:GLU:CB	2.42	0.42
2:B:377:THR:O	2:B:381:VAL:HG23	2.19	0.42
1:A:68:SER:HB2	1:A:70:LYS:HE2	2.02	0.42
1:A:206:ARG:NH1	1:A:219:LYS:O	2.50	0.42
1:A:433:PRO:HA	1:A:532:TYR:CE2	2.54	0.42
2:B:255:ASN:O	2:B:259:LYS:HG3	2.19	0.42
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.84	0.42
2:B:100:LEU:HD11	2:B:190:GLY:HA3	2.01	0.42
2:B:377:THR:HA	2:B:380:ILE:HD12	2.02	0.42
1:A:210:LEU:O	1:A:210:LEU:HD12	2.19	0.42
2:B:373:GLN:HA	2:B:376:THR:OG1	2.19	0.42
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.02	0.42
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.79	0.42
2:B:195:ILE:H	2:B:195:ILE:HD12	1.85	0.42
1:A:30:LYS:HD3	1:A:62:ALA:O	2.20	0.42
2:B:200:THR:C	2:B:202:ILE:N	2.73	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.75	0.42
2:B:153:TRP:HE3	2:B:156:SER:OG	2.03	0.42
2:B:132:ILE:HA	2:B:133:PRO:HD3	1.56	0.42
1:A:477:THR:O	1:A:480:GLN:HB3	2.20	0.42
2:B:65:LYS:HD2	2:B:65:LYS:HA	1.80	0.42
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.33	0.42
1:A:46:LYS:HE2	1:A:116:PHE:HB3	2.00	0.42
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.19	0.42
1:A:23:GLN:HB2	1:A:59:PRO:HB3	2.01	0.42
1:A:229:TRP:O	1:A:232:TYR:N	2.52	0.42
2:B:329:ILE:CG2	2:B:337:TRP:HE3	2.32	0.42
2:B:375:ILE:O	2:B:376:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:CD1	1:A:205:LEU:HD13	2.54	0.42
2:B:325:LEU:HG	2:B:387:PRO:HA	2.02	0.42
1:A:69:THR:H	1:A:70:LYS:HD3	1.84	0.42
2:B:297:GLU:O	2:B:301:LEU:HD13	2.20	0.42
1:A:543:GLY:CA	2:B:284:ARG:O	2.63	0.42
2:B:337:TRP:O	2:B:353:LYS:HG3	2.20	0.42
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.96	0.42
1:A:92:LEU:HD21	2:B:22:LYS:HD3	2.02	0.42
2:B:5:ILE:HD12	2:B:118:VAL:HG22	2.00	0.42
2:B:325:LEU:HG	2:B:387:PRO:CB	2.50	0.42
1:A:200:THR:O	1:A:204:GLU:HG3	2.20	0.42
1:A:97:PRO:HG2	1:A:232:TYR:CG	2.54	0.42
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.55	0.42
2:B:27:THR:HG22	2:B:30:LYS:HG3	2.01	0.42
1:A:510:PRO:O	1:A:511:ASP:HB3	2.20	0.42
2:B:398:TRP:O	2:B:400:THR:N	2.53	0.42
1:A:235:HIS:O	1:A:237:ASP:N	2.53	0.42
2:B:377:THR:O	2:B:378:GLU:C	2.58	0.42
2:B:253:THR:H	2:B:256:ASP:HB2	1.85	0.42
2:B:65:LYS:CD	2:B:407:GLN:HG2	2.47	0.42
2:B:111:VAL:O	2:B:115:TYR:HE1	2.02	0.41
2:B:48:SER:O	2:B:145:GLN:N	2.52	0.41
1:A:68:SER:HB2	1:A:70:LYS:NZ	2.35	0.41
1:A:391:LEU:HB2	1:A:414:TRP:CE3	2.54	0.41
1:A:276:VAL:O	1:A:276:VAL:HG12	2.20	0.41
1:A:191:SER:OG	1:A:198:HIS:CE1	2.73	0.41
2:B:20:LYS:HG3	2:B:56:TYR:HA	2.02	0.41
2:B:110:ASP:HA	2:B:185:ASP:O	2.20	0.41
2:B:23:GLN:CG	2:B:133:PRO:HG3	2.47	0.41
1:A:483:TYR:O	1:A:487:GLN:HG3	2.20	0.41
2:B:410:TRP:HE3	2:B:410:TRP:O	2.03	0.41
1:A:329:ILE:O	1:A:392:PRO:HG3	2.20	0.41
2:B:27:THR:O	2:B:31:ILE:HG13	2.20	0.41
1:A:443:ASP:HB3	1:A:548:VAL:HB	2.00	0.41
1:A:524:GLN:O	1:A:528:LYS:HG3	2.21	0.41
1:A:149:LEU:HD13	1:A:156:SER:O	2.21	0.41
1:A:69:THR:N	1:A:70:LYS:HD3	2.36	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.81	0.41
2:B:162:SER:O	2:B:165:THR:HB	2.21	0.41
2:B:380:ILE:O	2:B:381:VAL:C	2.59	0.41
1:A:518:VAL:HA	1:A:521:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:HA3	1:A:382:ILE:CG2	2.51	0.41
1:A:90:VAL:CG2	1:A:91:GLN:N	2.84	0.41
2:B:330:GLN:O	2:B:338:THR:N	2.53	0.41
2:B:329:ILE:HA	2:B:338:THR:O	2.20	0.41
1:A:440:PHE:CE2	1:A:459:THR:HG22	2.55	0.41
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.56	0.41
2:B:264:LEU:HB3	2:B:274:ILE:HD11	2.03	0.41
1:A:545:ASN:HA	1:A:548:VAL:HG22	2.03	0.41
1:A:205:LEU:O	1:A:208:HIS:HB3	2.21	0.41
2:B:125:ARG:O	2:B:128:THR:N	2.54	0.41
2:B:239:TRP:CE3	2:B:350:LYS:HG3	2.54	0.41
2:B:216:THR:HA	2:B:217:PRO:HD3	1.80	0.41
1:A:70:LYS:N	1:A:70:LYS:HD3	2.36	0.41
2:B:308:GLU:C	2:B:310:LEU:N	2.75	0.41
1:A:77:PHE:O	1:A:80:LEU:N	2.53	0.41
2:B:269:GLN:OE1	2:B:269:GLN:HA	2.21	0.41
1:A:515:SER:O	1:A:516:GLU:C	2.59	0.41
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.44	0.41
2:B:369:THR:CG2	2:B:370:GLU:N	2.83	0.41
2:B:77:PHE:CD2	2:B:152:GLY:HA3	2.51	0.41
2:B:100:LEU:CD1	2:B:190:GLY:HA3	2.51	0.41
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.51	0.41
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.81	0.41
2:B:181:CYS:N	2:B:188:TYR:O	2.53	0.41
1:A:132:ILE:O	1:A:142:ILE:HG12	2.20	0.40
2:B:103:LYS:HD2	2:B:191:SER:C	2.42	0.40
2:B:368:LEU:HA	2:B:368:LEU:HD12	1.90	0.40
2:B:33:ALA:O	2:B:36:GLU:HB2	2.20	0.40
1:A:99:GLY:HA3	1:A:382:ILE:HG22	2.03	0.40
1:A:393:ILE:O	1:A:416:PHE:HB2	2.21	0.40
1:A:420:PRO:CG	1:A:421:PRO:HD3	2.51	0.40
1:A:40:GLU:C	1:A:44:GLU:HG2	2.41	0.40
2:B:210:LEU:HD12	2:B:214:LEU:HA	2.03	0.40
2:B:342:TYR:C	2:B:342:TYR:CD1	2.95	0.40
2:B:96:HIS:CD2	2:B:384:GLY:HA3	2.56	0.40
1:A:484:LEU:O	1:A:485:ALA:C	2.59	0.40
2:B:166:LYS:O	2:B:170:PRO:CD	2.66	0.40
2:B:193:LEU:HD23	2:B:193:LEU:HA	1.73	0.40
1:A:350:LYS:HG2	1:A:351:THR:N	2.37	0.40
1:A:81:ASN:OD1	1:A:153:TRP:HA	2.22	0.40
1:A:90:VAL:CG2	1:A:91:GLN:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.88	0.40
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.90	0.40
1:A:225:PRO:N	1:A:226:PRO:HD2	2.37	0.40
2:B:395:LYS:O	2:B:399:GLU:HG3	2.21	0.40
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.22	0.40
1:A:127:TYR:C	1:A:129:ALA:H	2.25	0.40
1:A:434:ILE:HG13	1:A:532:TYR:HB2	2.03	0.40
2:B:98:ALA:O	2:B:100:LEU:N	2.55	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	556/558 (100%)	415 (75%)	114 (20%)	27 (5%)	3	22
2	B	425/427 (100%)	309 (73%)	76 (18%)	40 (9%)	1	5
All	All	981/985 (100%)	724 (74%)	190 (19%)	67 (7%)	1	11

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	287	LYS
1	A	420	PRO
1	A	556	ILE
2	B	71	TRP
2	B	116	PHE
2	B	195	ILE
2	B	226	PRO
2	B	295	LEU
2	B	316	GLY

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Mol	Chain	Res	Type
1	A	52	PRO
1	A	63	ILE
1	A	67	ASP
1	A	90	VAL
1	A	274	ILE
1	A	284	ARG
1	A	462	GLY
2	B	2	ILE
2	B	4	PRO
2	B	45	GLY
2	B	93	GLY
2	B	99	GLY
2	B	162	SER
2	B	244	ILE
2	B	296	THR
2	B	372	VAL
1	A	134	SER
1	A	429	LEU
1	A	501	TYR
2	B	68	SER
2	B	213	GLY
2	B	273	GLY
2	B	317	VAL
2	B	359	GLY
1	A	114	ALA
1	A	135	ILE
1	A	169	GLU
1	A	236	PRO
2	B	122	GLU
2	B	128	THR
2	B	178	ILE
2	B	345	PRO
2	B	381	VAL
1	A	111	VAL
1	A	138	GLU
1	A	295	LEU
2	B	92	LEU
2	B	115	TYR
2	B	356	ARG
1	A	510	PRO
2	B	225	PRO
2	B	357	MET

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Mol	Chain	Res	Type
2	B	358	ARG
2	B	363	ASN
2	B	399	GLU
2	B	55	PRO
2	B	148	VAL
2	B	176	PRO
2	B	243	PRO
1	A	142	ILE
1	A	156	SER
1	A	294	PRO
2	B	314	VAL
2	B	421	PRO
1	A	276	VAL
2	B	217	PRO
1	A	505	ILE

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	453/498 (91%)	424 (94%)	29 (6%)	22	62
2	B	367/389 (94%)	323 (88%)	44 (12%)	6	28
All	All	820/887 (92%)	747 (91%)	73 (9%)	12	44

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	70	LYS
1	A	73	LYS
1	A	77	PHE
1	A	78	ARG
1	A	94	ILE
1	A	97	PRO
1	A	109	LEU

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Mol	Chain	Res	Type
1	A	124	PHE
1	A	172	LYS
1	A	199	ARG
1	A	242	GLN
1	A	296	THR
1	A	310	LEU
1	A	338	THR
1	A	340	GLN
1	A	341	ILE
1	A	344	GLU
1	A	351	THR
1	A	362	THR
1	A	405	TYR
1	A	411	ILE
1	A	426	TRP
1	A	454	LYS
1	A	505	ILE
1	A	514	GLU
1	A	529	GLU
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	20	LYS
2	B	21	VAL
2	B	46	LYS
2	B	49	LYS
2	B	50	ILE
2	B	60	VAL
2	B	63	ILE
2	B	70	LYS
2	B	88	TRP
2	B	91	GLN
2	B	101	LYS
2	B	132	ILE
2	B	139	THR
2	B	164	MET
2	B	178	ILE
2	B	185	ASP
2	B	194	GLU
2	B	205	LEU
2	B	218	ASP
2	B	250	ASP

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Mol	Chain	Res	Type
2	B	266	TRP
2	B	269	GLN
2	B	283	LEU
2	B	287	LYS
2	B	290	THR
2	B	293	ILE
2	B	297	GLU
2	B	315	HIS
2	B	318	TYR
2	B	325	LEU
2	B	330	GLN
2	B	340	GLN
2	B	345	PRO
2	B	356	ARG
2	B	369	THR
2	B	378	GLU
2	B	386	THR
2	B	405	TYR
2	B	407	GLN
2	B	410	TRP
2	B	414	TRP
2	B	425	LEU
2	B	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	255	ASN
1	A	336	GLN
1	A	373	GLN
1	A	407	GLN
1	A	471	ASN
1	A	474	ASN
1	A	480	GLN
2	B	96	HIS
2	B	137	ASN
2	B	145	GLN
2	B	161	GLN
2	B	207	GLN
2	B	255	ASN
2	B	332	GLN

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Mol	Chain	Res	Type
2	B	340	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 ⓘ

1 ligand is 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	$\# Z > 2$
3	TBO	A	559	-	19,23,23	2.40	7 (36%)	15,34,34	2.44	2 (13%)

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
3	TBO	A	559	-	-	0/4/17/17	0/2/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	559	TBO	C4-N3	-6.46	1.44	1.49
3	A	559	TBO	C7-N6	-2.81	1.43	1.47
3	A	559	TBO	C7A-C3A	-2.59	1.40	1.43
3	A	559	TBO	C3A-C1A	-2.59	1.34	1.43
3	A	559	TBO	C8-C7A	2.12	1.43	1.39
3	A	559	TBO	C12-N6	2.82	1.51	1.47
3	A	559	TBO	C10-C9	4.18	1.45	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	559	TBO	C15-C14-C13	-5.11	106.17	122.61
3	A	559	TBO	C16-C14-C15	6.71	131.14	114.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	559	TBO	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 ⓘ

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	558/558 (100%)	-0.45	5 (0%) 85 78	22, 71, 97, 100	0
2	B	427/427 (100%)	-0.46	6 (1%) 78 65	18, 59, 97, 100	0
All	All	985/985 (100%)	-0.45	11 (1%) 82 72	18, 68, 97, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	3.0
2	B	225	PRO	2.7
1	A	557	ARG	2.7
1	A	24	TRP	2.6
1	A	66	LYS	2.6
1	A	67	ASP	2.4
2	B	2	ILE	2.4
1	A	65	LYS	2.3
2	B	316	GLY	2.3
2	B	3	SER	2.3
2	B	224	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [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
3	TBO	A	559	21/21	0.96	0.17	-0.40	59,67,70,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.