



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:28 am GMT

PDB ID : 2Q2E
Title : Crystal structure of the topoisomerase VI holoenzyme from *Methanosarcina mazei*
Authors : Corbett, K.D.; Benedetti, P.; Berger, J.M.
Deposited on : 2007-05-28
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

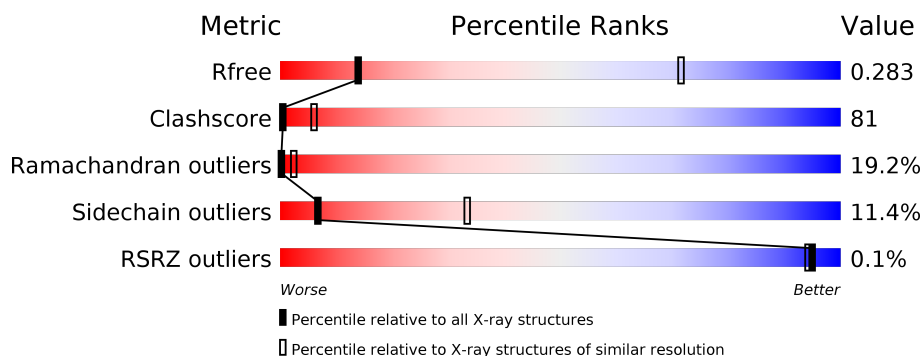
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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	369	
2	B	621	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7039 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 Type II DNA topoisomerase VI subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2532	1610	423	490	9			

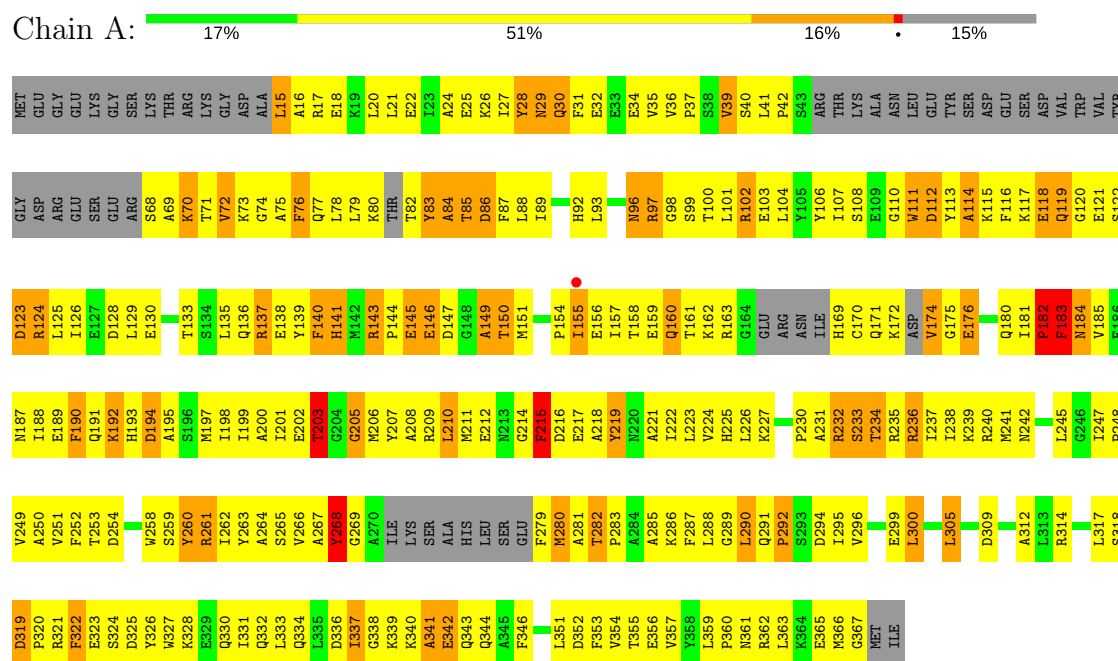
- Molecule 2 is a protein called Type 2 DNA topoisomerase 6 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	582	Total	C	N	O	S	0	0	1
			4507	2878	768	843	18			

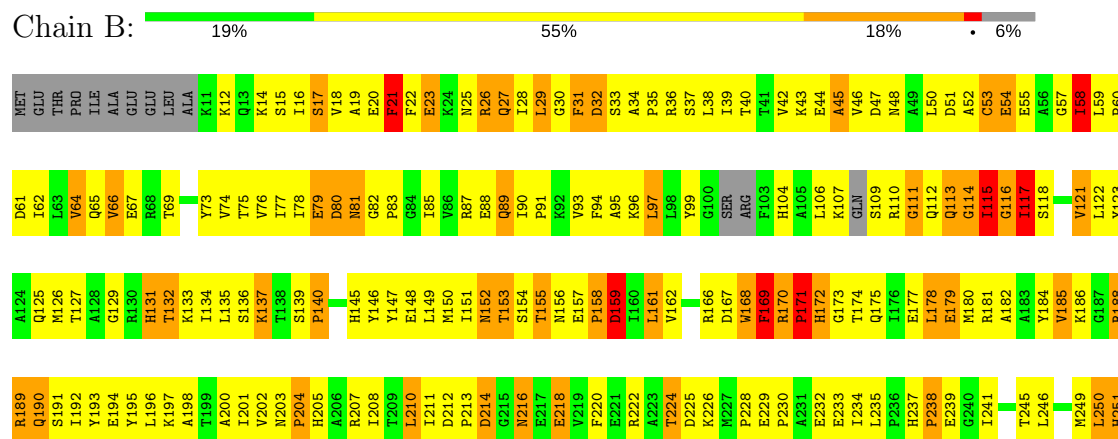
3 Residue-property plots

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

• Molecule 1: Type II DNA topoisomerase VI subunit A



• Molecule 2: Type 2 DNA topoisomerase 6 subunit B



V561		D500	D440	V380	I320	Y252
	M564	I501	I441	P381	G321	T253
		N502	P442	L382	E322	E254
		P503	V443	L383	D323	ARG
	D567	V504	I444	Y384	L324	GLN
	Y568	V505	K445	Q385	I325	LYS
	D569	A506	E446	Q386	Y326	LEU
	Y570	K507	E447	G387	R327	ALA
	V571	I508	I448	G388	G260	
		N509	D449	C389	L329	F261
		O510	L450	V390	E330	L262
	S575	N511	A451	T391	K331	R263
	A576	L512	I452	T392	E332	
	S577	L513	K453	H393	T333	C267
		V514	E454	A394	T394	K269
	S580	H515	V455	V395	V335	ILE
	S581	K582	A456	E396	D336	GLY
	V583	R516	R457	D397	F337	L271
	L584	V517	K458	T398	I338	L272
	S585	I518	L459	K399	A339	T273
			K460	W400	T340	A274
	Y586	N521	H461	K401	S341	
	K587	O522	Y462	Q402	T342	T277
	I588	D523	L463	Y403	R343	C278
	E589	O524	S464	G404	K344	
	S590	T525	K465	L405	P345	A281
	A591	V526	Q466	N406	A346	G282
	S592	D527	S467	Q407	V347	L283
	E593	V528	N468	P408	Y348	D284
	E594	A529	L469	G409	S349	P285
	E595	I530	K470	G410	G350	E286
	L596	K531	K471	Q411	N351	T287
	Q597	V532	K472	I412	P352	D288
	K598	K533	R473	P413	F353	P289
	L599	N534	E474	V414	V354	H290
	P600	PHE	K475	G415	V355	A291
	Q601	GLY	E476	P416	E356	L292
	L602	THR	I477	V417	V357	
	I603	SER	I478	I418	G358	A297
	V604	A539	I479	L419	M359	
	E605	Y540	T480	L420	A360	L300
	GLY	S541	K481	I421	Y361	L301
	ILE	F542	V482	H422	G362	E302
	GLU	R543	L483	V423	G363	A303
	GLU	V544	P484	A424	N364	F304
	GLU	H545	K485	S425	L365	E305
	LEU	E546	L486	I426	P366	K306
	VAL	N547	A487	N427	K367	V307
	T613	L548	A488	V428	E368	K308
	G614	P549	K489	P429	E369	I309
	A615	C550	V490	F430	K370	K310
	K616	K551	A491	T431	I371	A311
	ALA	V552	H492	S432	S372	P312
	PHE	SER	V493	E433	I373	P313
	LYS	GLY	L494	S434	M374	T314
	GLY	ALA	E495	K435	R375	D315
	VAL	K556	K496	D436	F376	C316
		P557	D497	A437	A377	L317
		E558	V498	I438	N378	S318
		P559	P499	A439	R379	P319
		K560				

4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	227.81Å 227.81Å 208.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.00 92.23 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-4.00) 94.1 (92.23-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.306 , 0.349 0.302 , 0.283	Depositor DCC
R_{free} test set	1298 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	153.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 210.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2579	0.71	0/3471
2	B	0.51	1/4591 (0.0%)	0.83	5/6215 (0.1%)
All	All	0.47	1/7170 (0.0%)	0.79	5/9686 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	CYS	CB-SG	-6.66	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	GLY	N-CA-C	5.88	127.79	113.10
2	B	408	PRO	N-CA-CB	5.82	110.29	103.30
2	B	522	GLY	N-CA-C	-5.75	98.72	113.10
2	B	58	ILE	N-CA-C	5.66	126.29	111.00
2	B	362	GLY	N-CA-C	5.42	126.64	113.10

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	2532	0	2476	393	0
2	B	4507	0	4565	779	0
All	All	7039	0	7041	1140	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 81.

All (1140) 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)
2:B:599:LEU:H	2:B:599:LEU:HD23	1.09	1.13
2:B:516:ARG:HH12	2:B:597:GLN:HB2	0.93	1.09
2:B:371:ILE:HG22	2:B:414:VAL:HG12	1.13	1.09
2:B:66:VAL:HG23	2:B:213:PRO:HD3	1.35	1.08
2:B:222:ARG:HH21	2:B:332:GLU:HB2	1.12	1.06
2:B:238:PRO:HA	2:B:241:ILE:HD12	1.35	1.05
1:A:31:PHE:HB2	2:B:489:LYS:HD3	1.39	1.05
1:A:15:LEU:HD12	1:A:96:ASN:HA	1.38	1.05
2:B:137:LYS:HG3	2:B:171:PRO:HA	1.34	1.05
1:A:87:PHE:HA	2:B:492:HIS:NE2	1.73	1.03
2:B:201:ILE:HD11	2:B:329:LEU:HG	1.38	1.03
2:B:77:ILE:C	2:B:78:ILE:HD12	1.78	1.01
2:B:365:LEU:HB3	2:B:366:PRO:HD2	1.41	1.01
2:B:516:ARG:NH1	2:B:597:GLN:HB2	1.75	0.99
2:B:588:ILE:HG12	2:B:589:GLU:H	1.27	0.99
2:B:497:ASP:O	2:B:499:PRO:HD3	1.62	0.99
1:A:305:LEU:HD12	1:A:305:LEU:H	1.23	0.98
2:B:168:TRP:CE3	2:B:169:PHE:HA	1.97	0.97
2:B:190:GLN:HG2	2:B:383:LEU:HD21	1.45	0.97
2:B:222:ARG:NH2	2:B:332:GLU:HB2	1.80	0.97
2:B:232:GLU:CD	2:B:316:CYS:HA	1.84	0.96
2:B:359:MET:HE1	2:B:455:VAL:HG23	1.47	0.96
1:A:83:TYR:CD1	2:B:488:ALA:HB1	2.01	0.95
2:B:246:LEU:HD23	2:B:297:ALA:HB1	1.48	0.95
2:B:307:VAL:HG22	2:B:309:ILE:HD11	1.48	0.94
2:B:335:VAL:HG22	2:B:336:ASP:H	1.33	0.94
2:B:335:VAL:HG11	2:B:338:ILE:HD11	1.50	0.93
2:B:114:GLY:O	2:B:116:GLY:N	2.01	0.93
1:A:324:SER:HB3	1:A:327:TRP:HD1	1.34	0.92
2:B:390:VAL:HG23	2:B:438:ILE:O	1.70	0.92
1:A:203:THR:OG1	1:A:206:MET:HB3	1.68	0.92
2:B:210:LEU:HD12	2:B:211:ILE:N	1.85	0.91
1:A:253:THR:HB	1:A:259:SER:HB3	1.54	0.89
1:A:20:LEU:HD12	1:A:21:LEU:N	1.88	0.89
1:A:239:LYS:NZ	1:A:279:PHE:HA	1.88	0.89
1:A:31:PHE:HB2	2:B:489:LYS:CD	2.03	0.89
2:B:411:GLY:O	2:B:412:ILE:HG13	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:HD11	1:A:207:TYR:HD1	1.37	0.88
1:A:28:TYR:HE1	2:B:489:LYS:HG2	1.38	0.87
2:B:552:VAL:HB	2:B:587:LYS:HB2	1.56	0.87
2:B:58:ILE:HG22	2:B:59:LEU:H	1.40	0.87
1:A:156:GLU:O	1:A:157:ILE:HG13	1.73	0.87
2:B:64:VAL:HG22	2:B:78:ILE:HG13	1.55	0.87
1:A:206:MET:H	1:A:344:GLN:HE21	1.23	0.87
2:B:546:GLU:HG3	2:B:548:LEU:HD11	1.57	0.86
2:B:61:ASP:HB2	2:B:207:ARG:HH11	1.38	0.86
2:B:367:LYS:HE2	2:B:367:LYS:HA	1.55	0.86
2:B:507:LYS:HG3	2:B:533:LYS:NZ	1.89	0.85
1:A:239:LYS:HD3	1:A:279:PHE:HD2	1.40	0.85
2:B:381:PRO:O	2:B:382:LEU:HB2	1.75	0.85
2:B:125:GLN:HE22	2:B:151:ILE:HB	1.42	0.85
2:B:65:GLN:HG3	2:B:211:ILE:HG13	1.59	0.85
1:A:185:VAL:HG21	1:A:236:ARG:HB3	1.56	0.84
2:B:490:VAL:C	2:B:492:HIS:H	1.79	0.84
1:A:28:TYR:CE1	2:B:489:LYS:HG2	2.13	0.83
1:A:69:ALA:HB2	1:A:78:LEU:HD11	1.60	0.83
2:B:569:ASP:OD2	2:B:571:VAL:HG23	1.78	0.83
1:A:188:ILE:HG12	1:A:240:ARG:NH2	1.93	0.83
1:A:188:ILE:HG21	1:A:240:ARG:CZ	2.08	0.82
2:B:335:VAL:HG22	2:B:336:ASP:N	1.94	0.82
2:B:497:ASP:CG	2:B:498:VAL:H	1.81	0.82
2:B:241:ILE:HG23	2:B:245:THR:HG21	1.60	0.82
2:B:96:LYS:HE2	2:B:114:GLY:HA3	1.60	0.82
1:A:197:MET:O	1:A:221:ALA:HA	1.79	0.82
1:A:252:PHE:HD1	1:A:289:GLY:HA2	1.41	0.81
1:A:338:GLY:O	1:A:339:LYS:HG3	1.80	0.81
2:B:371:ILE:CG2	2:B:414:VAL:HG12	2.04	0.81
2:B:401:LYS:HZ3	2:B:406:ASN:HD21	1.26	0.81
2:B:127:THR:CG2	2:B:181:ARG:HB3	2.09	0.81
1:A:324:SER:HB3	1:A:327:TRP:CD1	2.16	0.81
2:B:168:TRP:O	2:B:169:PHE:HB2	1.80	0.81
2:B:137:LYS:CG	2:B:172:HIS:H	1.95	0.81
1:A:31:PHE:CB	2:B:489:LYS:HD3	2.11	0.80
2:B:453:LYS:HE2	2:B:457:ARG:NH2	1.95	0.80
1:A:342:GLU:HG3	1:A:343:GLN:H	1.47	0.80
1:A:252:PHE:CD1	1:A:289:GLY:HA2	2.15	0.80
1:A:188:ILE:HG21	1:A:240:ARG:NE	1.95	0.80
1:A:237:ILE:HG22	1:A:241:MET:HE2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HB2	1:A:140:PHE:CE1	2.16	0.80
1:A:69:ALA:CB	1:A:78:LEU:HD11	2.11	0.80
1:A:161:THR:HG23	1:A:162:LYS:HG3	1.64	0.80
1:A:202:GLU:O	1:A:203:THR:HG23	1.82	0.80
1:A:101:LEU:HD22	1:A:122:SER:HB3	1.64	0.80
1:A:198:ILE:HB	1:A:249:VAL:HG22	1.64	0.80
2:B:107:LYS:HZ2	2:B:378:ASN:CG	1.84	0.80
1:A:169:HIS:O	1:A:174:VAL:HG13	1.82	0.79
2:B:27:GLN:HG2	2:B:32:ASP:HB2	1.62	0.79
2:B:501:ILE:O	2:B:505:VAL:HG23	1.82	0.79
2:B:557:PRO:HG3	2:B:584:LEU:HA	1.63	0.79
2:B:595:GLU:O	2:B:596:LEU:HG	1.82	0.79
2:B:599:LEU:HD23	2:B:599:LEU:N	1.94	0.78
1:A:239:LYS:HZ3	1:A:279:PHE:HA	1.46	0.78
1:A:70:LYS:HG2	1:A:71:THR:HG23	1.64	0.78
2:B:375:ARG:NH1	2:B:382:LEU:HD23	1.99	0.78
1:A:363:LEU:HD23	1:A:363:LEU:O	1.83	0.78
1:A:88:LEU:O	1:A:92:HIS:HB2	1.83	0.78
2:B:365:LEU:HB3	2:B:366:PRO:CD	2.12	0.78
2:B:65:GLN:O	2:B:66:VAL:HG13	1.83	0.78
2:B:127:THR:HG21	2:B:181:ARG:HB3	1.64	0.77
1:A:31:PHE:CE1	1:A:32:GLU:HG3	2.20	0.77
2:B:597:GLN:O	2:B:598:LYS:HB3	1.82	0.77
1:A:133:THR:HG1	1:A:140:PHE:HZ	1.29	0.77
2:B:80:ASP:OD1	2:B:174:THR:HG23	1.85	0.77
1:A:133:THR:O	1:A:135:LEU:HG	1.84	0.77
2:B:375:ARG:HG3	2:B:375:ARG:HH11	1.49	0.77
1:A:242:ASN:OD1	1:A:282:THR:HG23	1.84	0.76
1:A:290:LEU:HD21	1:A:341:ALA:HB1	1.68	0.76
1:A:200:ALA:HB3	1:A:251:VAL:HA	1.68	0.76
2:B:465:LYS:O	2:B:468:ASN:HB3	1.86	0.76
2:B:335:VAL:HG11	2:B:338:ILE:CD1	2.15	0.75
1:A:154:PRO:HG2	1:A:195:ALA:HB2	1.69	0.75
2:B:73:TYR:CE1	2:B:181:ARG:HB2	2.22	0.75
2:B:60:PRO:HA	2:B:81:ASN:ND2	2.00	0.75
2:B:145:HIS:HB3	2:B:147:TYR:CE1	2.22	0.75
1:A:20:LEU:HB2	1:A:135:LEU:HD13	1.68	0.75
2:B:551:LYS:HG2	2:B:552:VAL:N	2.01	0.75
2:B:353:PHE:HA	2:B:424:ALA:O	1.86	0.75
2:B:77:ILE:N	2:B:77:ILE:HD12	2.02	0.75
2:B:106:LEU:HB2	2:B:232:GLU:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LYS:HG3	2:B:172:HIS:H	1.52	0.74
1:A:328:LYS:O	1:A:332:GLN:HG3	1.88	0.74
1:A:31:PHE:O	1:A:35:VAL:HG23	1.86	0.74
2:B:107:LYS:HZ2	2:B:378:ASN:ND2	1.86	0.74
1:A:15:LEU:HD13	1:A:93:LEU:O	1.87	0.74
2:B:184:TYR:HE1	2:B:192:ILE:HG12	1.51	0.74
2:B:171:PRO:O	2:B:172:HIS:HB2	1.88	0.74
2:B:561:VAL:HG22	2:B:570:TYR:CD1	2.22	0.74
2:B:188:ARG:O	2:B:190:GLN:N	2.21	0.74
2:B:125:GLN:O	2:B:129:GLY:HA2	1.88	0.73
2:B:210:LEU:HD12	2:B:210:LEU:C	2.08	0.73
2:B:453:LYS:HE2	2:B:457:ARG:HH21	1.53	0.73
2:B:37:SER:HB2	2:B:182:ALA:HB1	1.70	0.73
2:B:507:LYS:HG3	2:B:533:LYS:HZ2	1.51	0.73
2:B:551:LYS:HE3	2:B:552:VAL:C	2.09	0.73
2:B:473:ARG:HG3	2:B:473:ARG:HH11	1.53	0.73
1:A:35:VAL:HG11	2:B:486:LEU:HD13	1.70	0.73
1:A:72:VAL:H	2:B:478:ILE:HD11	1.53	0.73
2:B:390:VAL:HG22	2:B:440:ASP:HA	1.70	0.73
1:A:225:HIS:O	1:A:226:LEU:HD23	1.89	0.73
2:B:222:ARG:HH21	2:B:332:GLU:CB	1.97	0.73
2:B:532:VAL:HG22	2:B:533:LYS:N	2.04	0.73
2:B:528:VAL:HG12	2:B:584:LEU:HD12	1.71	0.73
2:B:599:LEU:H	2:B:599:LEU:CD2	1.91	0.72
2:B:322:GLU:O	2:B:340:THR:HG21	1.89	0.72
2:B:411:GLY:C	2:B:412:ILE:HG13	2.08	0.72
1:A:264:ALA:HA	1:A:267:ALA:HB3	1.70	0.72
2:B:133:LYS:HB3	2:B:177:GLU:HB3	1.72	0.72
2:B:202:VAL:C	2:B:204:PRO:HD3	2.09	0.72
2:B:232:GLU:OE1	2:B:316:CYS:HA	1.87	0.72
2:B:74:VAL:O	2:B:179:GLU:HA	1.89	0.72
1:A:135:LEU:HB2	1:A:140:PHE:HE1	1.54	0.72
2:B:76:VAL:HG12	2:B:78:ILE:HD11	1.70	0.72
1:A:356:GLU:O	1:A:360:PRO:HG3	1.90	0.71
2:B:588:ILE:HG12	2:B:589:GLU:N	2.02	0.71
2:B:222:ARG:HH12	2:B:331:LYS:HB2	1.54	0.71
1:A:342:GLU:HG3	1:A:343:GLN:N	2.05	0.71
2:B:149:LEU:HD12	2:B:150:MET:H	1.54	0.71
2:B:237:HIS:CD2	2:B:312:PRO:HG3	2.26	0.71
2:B:401:LYS:NZ	2:B:406:ASN:HD21	1.88	0.71
2:B:490:VAL:O	2:B:492:HIS:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:C	1:A:31:PHE:H	1.92	0.71
1:A:279:PHE:O	1:A:280:MET:HG3	1.90	0.70
2:B:561:VAL:HG22	2:B:570:TYR:HD1	1.54	0.70
2:B:335:VAL:HG21	2:B:360:ALA:HB1	1.73	0.70
1:A:78:LEU:HB3	2:B:485:LYS:NZ	2.07	0.70
2:B:184:TYR:CE1	2:B:192:ILE:HG21	2.27	0.70
2:B:114:GLY:C	2:B:116:GLY:H	1.94	0.70
1:A:234:THR:O	1:A:237:ILE:HB	1.92	0.70
2:B:78:ILE:HD12	2:B:78:ILE:N	2.06	0.70
2:B:238:PRO:HG2	2:B:239:GLU:OE1	1.90	0.69
2:B:241:ILE:HG23	2:B:245:THR:CG2	2.22	0.69
1:A:235:ARG:HD3	1:A:265:SER:O	1.92	0.69
2:B:113:GLN:O	2:B:115:ILE:HG13	1.92	0.69
2:B:137:LYS:HE3	2:B:173:GLY:H	1.55	0.69
2:B:235:LEU:HD12	2:B:267:CYS:HB3	1.74	0.69
2:B:348:TYR:O	2:B:350:GLY:N	2.25	0.69
2:B:112:GLN:HB2	2:B:435:LYS:HD3	1.74	0.69
2:B:508:ILE:CG2	2:B:509:MET:N	2.55	0.69
1:A:154:PRO:O	1:A:155:ILE:HG23	1.92	0.69
2:B:65:GLN:HG2	2:B:66:VAL:H	1.56	0.69
2:B:237:HIS:CG	2:B:312:PRO:HG3	2.27	0.69
2:B:232:GLU:OE2	2:B:316:CYS:HA	1.91	0.69
2:B:170:ARG:HG2	2:B:170:ARG:HH11	1.57	0.69
1:A:20:LEU:HB2	1:A:135:LEU:CD1	2.22	0.69
1:A:15:LEU:CD1	1:A:96:ASN:HA	2.18	0.69
2:B:557:PRO:HD3	2:B:585:SER:H	1.57	0.69
2:B:90:ILE:HG22	2:B:91:PRO:N	2.08	0.69
2:B:212:ASP:HB2	2:B:213:PRO:HD2	1.75	0.69
2:B:360:ALA:HB3	2:B:418:ILE:CG2	2.22	0.69
2:B:396:GLU:HG2	2:B:412:ILE:HG23	1.75	0.69
2:B:139:SER:HB2	2:B:140:PRO:HD2	1.74	0.68
2:B:400:TRP:HZ3	2:B:408:PRO:HA	1.58	0.68
2:B:334:THR:HB	2:B:364:ASN:HB2	1.75	0.68
1:A:253:THR:CB	1:A:259:SER:HB3	2.24	0.68
2:B:107:LYS:HG3	2:B:378:ASN:HD21	1.59	0.68
1:A:157:ILE:HG22	1:A:158:THR:N	2.08	0.68
2:B:355:VAL:HG22	2:B:423:VAL:HG12	1.76	0.68
1:A:236:ARG:HG3	1:A:280:MET:HG3	1.74	0.68
1:A:214:GLY:O	1:A:215:PHE:HB2	1.92	0.68
1:A:79:LEU:O	1:A:79:LEU:HD23	1.93	0.68
2:B:38:LEU:HD13	2:B:184:TYR:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:PRO:HA	2:B:354:VAL:HG12	1.75	0.68
2:B:531:LYS:HE2	2:B:581:SER:HB2	1.76	0.68
2:B:324:LEU:H	2:B:324:LEU:HD12	1.60	0.67
2:B:66:VAL:O	2:B:213:PRO:HD3	1.94	0.67
1:A:117:LYS:NZ	1:A:117:LYS:HB2	2.10	0.67
1:A:27:ILE:HD11	1:A:133:THR:HG21	1.76	0.67
2:B:425:SER:OG	2:B:428:VAL:HG22	1.94	0.67
1:A:239:LYS:HD3	1:A:279:PHE:CD2	2.27	0.67
2:B:137:LYS:HE3	2:B:173:GLY:CA	2.25	0.67
2:B:38:LEU:HA	2:B:180:MET:CE	2.25	0.67
2:B:516:ARG:HH12	2:B:597:GLN:CB	1.89	0.67
2:B:335:VAL:CG2	2:B:336:ASP:H	2.07	0.67
2:B:531:LYS:CD	2:B:581:SER:HB2	2.25	0.67
2:B:137:LYS:HE3	2:B:173:GLY:N	2.10	0.67
2:B:320:ILE:CD1	2:B:379:ARG:HH11	2.08	0.67
2:B:343:ARG:HH11	2:B:343:ARG:HG3	1.59	0.67
2:B:342:THR:HG23	2:B:356:GLU:HG2	1.77	0.67
2:B:518:ILE:HG22	2:B:526:VAL:HG13	1.77	0.67
1:A:112:ASP:O	1:A:114:ALA:N	2.28	0.66
1:A:39:VAL:HG12	1:A:40:SER:H	1.61	0.66
2:B:366:PRO:O	2:B:416:PRO:HG3	1.95	0.66
1:A:201:ILE:HD11	1:A:207:TYR:CD1	2.26	0.66
2:B:576:ALA:HB1	2:B:580:SER:HB3	1.78	0.66
2:B:36:ARG:HA	2:B:39:ILE:HG22	1.77	0.66
1:A:181:ILE:O	1:A:181:ILE:HG13	1.94	0.66
2:B:48:ASN:HD21	2:B:117:ILE:HG12	1.61	0.66
2:B:66:VAL:HG12	2:B:76:VAL:HG22	1.75	0.66
1:A:230:PRO:HD3	1:A:262:ILE:HG23	1.77	0.66
2:B:27:GLN:CG	2:B:32:ASP:HB2	2.26	0.66
1:A:282:THR:O	1:A:282:THR:HG22	1.94	0.65
1:A:35:VAL:HG21	2:B:486:LEU:HD22	1.77	0.65
2:B:514:VAL:HG12	2:B:530:ILE:HG12	1.77	0.65
2:B:66:VAL:HA	2:B:75:THR:O	1.96	0.65
2:B:192:ILE:HG23	2:B:193:TYR:H	1.61	0.65
2:B:307:VAL:HG13	2:B:307:VAL:O	1.96	0.65
1:A:326:TYR:O	1:A:330:GLN:HG2	1.96	0.65
2:B:205:HIS:CD2	2:B:228:PRO:HD3	2.32	0.65
2:B:290:HIS:CG	2:B:291:ALA:N	2.64	0.65
1:A:266:VAL:O	1:A:281:ALA:HA	1.97	0.65
1:A:282:THR:HG22	1:A:285:ALA:HB2	1.79	0.65
2:B:190:GLN:CG	2:B:383:LEU:HD11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HD23	2:B:297:ALA:CB	2.26	0.65
2:B:96:LYS:C	2:B:97:LEU:HD23	2.17	0.65
1:A:233:SER:O	1:A:237:ILE:HG12	1.97	0.65
2:B:490:VAL:C	2:B:492:HIS:N	2.50	0.65
2:B:586:TYR:C	2:B:587:LYS:HD3	2.17	0.65
2:B:66:VAL:CG1	2:B:76:VAL:HG13	2.27	0.65
2:B:112:GLN:OE1	2:B:112:GLN:HA	1.96	0.65
2:B:284:ASP:HB2	2:B:287:ILE:HG23	1.78	0.65
1:A:83:TYR:O	1:A:85:THR:N	2.29	0.64
2:B:94:PHE:CD1	2:B:134:ILE:HD11	2.32	0.64
2:B:399:LYS:HG2	2:B:403:TYR:CD1	2.33	0.64
2:B:60:PRO:HA	2:B:81:ASN:HD22	1.60	0.64
1:A:159:GLU:O	1:A:160:GLN:HB2	1.97	0.64
1:A:154:PRO:CG	1:A:195:ALA:HB2	2.25	0.64
1:A:206:MET:N	1:A:344:GLN:HE21	1.94	0.64
2:B:576:ALA:HB2	2:B:582:LYS:HE3	1.80	0.64
1:A:133:THR:OG1	1:A:140:PHE:HZ	1.79	0.64
1:A:157:ILE:HG12	1:A:190:PHE:HA	1.79	0.64
2:B:229:GLU:HG3	2:B:230:PRO:HD2	1.79	0.64
2:B:371:ILE:HG21	2:B:413:PRO:O	1.97	0.64
2:B:523:ASP:O	2:B:588:ILE:HD12	1.97	0.64
1:A:200:ALA:HB3	1:A:250:ALA:O	1.98	0.64
1:A:181:ILE:CD1	1:A:237:ILE:HG13	2.28	0.64
1:A:31:PHE:CG	1:A:32:GLU:N	2.66	0.64
1:A:268:TYR:HB2	1:A:322:PHE:HE2	1.62	0.64
2:B:375:ARG:HD2	2:B:382:LEU:HD23	1.79	0.64
2:B:189:ARG:O	2:B:190:GLN:CB	2.46	0.64
2:B:495:GLU:O	2:B:497:ASP:N	2.31	0.64
2:B:151:ILE:O	2:B:152:ASN:C	2.35	0.64
2:B:309:ILE:HG22	2:B:310:MET:N	2.13	0.64
2:B:412:ILE:HD12	2:B:412:ILE:O	1.98	0.64
1:A:104:LEU:HD23	1:A:122:SER:OG	1.98	0.64
2:B:151:ILE:HG22	2:B:151:ILE:O	1.97	0.64
2:B:400:TRP:HZ2	2:B:411:GLY:N	1.96	0.64
2:B:531:LYS:CE	2:B:581:SER:HB2	2.28	0.64
2:B:367:LYS:O	2:B:416:PRO:HG3	1.98	0.63
2:B:373:ILE:O	2:B:373:ILE:HG12	1.99	0.63
1:A:137:ARG:HD3	1:A:232:ARG:HE	1.63	0.63
2:B:325:ILE:O	2:B:329:LEU:HD12	1.98	0.63
2:B:50:LEU:HB3	2:B:54:GLU:OE2	1.98	0.63
1:A:155:ILE:O	1:A:170:CYS:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:ILE:HG22	2:B:310:MET:H	1.61	0.63
2:B:34:ALA:N	2:B:35:PRO:HD2	2.14	0.63
2:B:36:ARG:HG3	2:B:384:TYR:OH	1.99	0.63
2:B:376:PHE:O	2:B:422:HIS:HA	1.99	0.63
1:A:24:ALA:O	1:A:27:ILE:HD12	1.98	0.63
1:A:28:TYR:O	1:A:31:PHE:N	2.31	0.63
2:B:233:GLU:HG2	2:B:234:ILE:N	2.14	0.63
2:B:290:HIS:CG	2:B:291:ALA:H	2.16	0.63
2:B:601:GLN:N	2:B:601:GLN:OE1	2.31	0.63
2:B:107:LYS:NZ	2:B:378:ASN:ND2	2.46	0.63
1:A:149:ALA:CA	1:A:180:GLN:HG3	2.29	0.63
2:B:135:LEU:HD23	2:B:169:PHE:CE2	2.34	0.63
2:B:127:THR:HG22	2:B:181:ARG:HB3	1.81	0.63
2:B:527:ASP:OD2	2:B:585:SER:HB3	1.99	0.63
1:A:203:THR:C	1:A:205:GLY:H	2.00	0.63
2:B:302:GLU:HA	2:B:305:GLU:CG	2.29	0.63
2:B:507:LYS:HE3	2:B:533:LYS:HZ3	1.64	0.63
2:B:399:LYS:O	2:B:400:TRP:CD1	2.52	0.62
1:A:346:PHE:HD1	1:A:354:VAL:HG22	1.64	0.62
2:B:168:TRP:CE3	2:B:169:PHE:CA	2.78	0.62
2:B:239:GLU:O	2:B:350:GLY:HA3	1.99	0.62
2:B:549:PRO:HG3	2:B:567:ASP:OD1	2.00	0.62
2:B:543:ARG:O	2:B:601:GLN:HB3	1.99	0.62
1:A:84:ALA:HB1	1:A:111:TRP:CE2	2.34	0.62
2:B:399:LYS:O	2:B:400:TRP:HB2	2.00	0.62
2:B:58:ILE:HG22	2:B:59:LEU:N	2.11	0.62
2:B:64:VAL:CG2	2:B:78:ILE:HG13	2.27	0.62
2:B:548:LEU:N	2:B:548:LEU:HD12	2.15	0.62
1:A:31:PHE:CD1	1:A:32:GLU:N	2.67	0.62
1:A:98:GLY:HA3	1:A:141:HIS:CE1	2.35	0.62
2:B:233:GLU:O	2:B:234:ILE:HG23	1.99	0.62
2:B:400:TRP:HH2	2:B:410:GLY:H	1.42	0.62
2:B:508:ILE:HG22	2:B:509:MET:H	1.64	0.62
2:B:66:VAL:HG13	2:B:76:VAL:HG13	1.82	0.62
1:A:198:ILE:O	1:A:199:ILE:HD13	1.99	0.62
2:B:125:GLN:NE2	2:B:151:ILE:HB	2.14	0.62
2:B:196:LEU:O	2:B:200:ALA:N	2.25	0.62
1:A:108:SER:HA	1:A:111:TRP:NE1	2.15	0.61
2:B:114:GLY:C	2:B:116:GLY:N	2.51	0.61
1:A:150:THR:CB	1:A:225:HIS:HB3	2.29	0.61
2:B:116:GLY:O	2:B:118:SER:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:PRO:HA	2:B:241:ILE:CD1	2.20	0.61
2:B:400:TRP:CZ3	2:B:407:GLN:O	2.53	0.61
2:B:507:LYS:HG3	2:B:533:LYS:HZ3	1.63	0.61
2:B:512:LEU:HD11	2:B:542:PHE:CE2	2.35	0.61
1:A:157:ILE:HG23	1:A:189:GLU:HB3	1.82	0.61
1:A:205:GLY:HA3	1:A:344:GLN:HE22	1.66	0.61
2:B:417:VAL:HG12	2:B:418:ILE:H	1.63	0.61
2:B:591:ALA:O	2:B:593:GLU:HG2	1.99	0.61
1:A:208:ALA:O	1:A:211:MET:HB3	2.01	0.61
1:A:28:TYR:O	1:A:31:PHE:HB3	2.00	0.61
2:B:222:ARG:HH22	2:B:332:GLU:N	1.98	0.61
2:B:36:ARG:NE	2:B:384:TYR:CE2	2.68	0.61
2:B:61:ASP:HB2	2:B:207:ARG:NH1	2.12	0.61
1:A:80:LYS:HD2	1:A:116:PHE:HE1	1.66	0.61
1:A:124:ARG:O	1:A:128:ASP:N	2.33	0.61
1:A:183:PHE:O	1:A:184:ASN:HB2	2.01	0.61
2:B:307:VAL:HG22	2:B:309:ILE:CD1	2.28	0.61
2:B:598:LYS:HE2	2:B:613:THR:CB	2.31	0.61
1:A:157:ILE:CG2	1:A:158:THR:N	2.64	0.61
2:B:360:ALA:O	2:B:418:ILE:HG22	2.00	0.61
2:B:66:VAL:HG23	2:B:213:PRO:CD	2.21	0.61
2:B:96:LYS:O	2:B:97:LEU:HD23	2.00	0.61
2:B:137:LYS:HG2	2:B:172:HIS:H	1.66	0.61
2:B:478:ILE:HG22	2:B:478:ILE:O	2.01	0.61
2:B:482:VAL:HG11	2:B:505:VAL:HG22	1.82	0.61
2:B:545:HIS:CG	2:B:571:VAL:HG22	2.35	0.61
2:B:169:PHE:O	2:B:169:PHE:HD1	1.84	0.60
2:B:73:TYR:HA	2:B:181:ARG:HA	1.83	0.60
2:B:399:LYS:HG2	2:B:403:TYR:CG	2.36	0.60
1:A:28:TYR:O	1:A:30:GLN:N	2.34	0.60
2:B:430:PHE:CD1	2:B:435:LYS:HA	2.36	0.60
1:A:287:PHE:CE1	1:A:289:GLY:HA3	2.36	0.60
1:A:28:TYR:C	1:A:31:PHE:HD2	2.05	0.60
1:A:351:LEU:HD12	1:A:351:LEU:N	2.15	0.60
2:B:250:LEU:O	2:B:252:TYR:N	2.33	0.60
2:B:241:ILE:HG23	2:B:245:THR:CB	2.31	0.60
2:B:399:LYS:O	2:B:400:TRP:CB	2.49	0.60
2:B:532:VAL:HG22	2:B:533:LYS:H	1.65	0.60
1:A:17:ARG:HH12	1:A:141:HIS:CB	2.14	0.60
2:B:125:GLN:HE22	2:B:151:ILE:CB	2.13	0.60
2:B:464:SER:O	2:B:468:ASN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:CD2	1:A:114:ALA:HB2	2.31	0.60
2:B:189:ARG:O	2:B:190:GLN:HB3	2.02	0.60
2:B:514:VAL:HG23	2:B:514:VAL:O	1.99	0.60
2:B:550:CYS:O	2:B:551:LYS:HB3	2.00	0.60
1:A:17:ARG:HD2	1:A:139:TYR:O	2.02	0.60
1:A:263:TYR:O	1:A:267:ALA:N	2.35	0.60
1:A:69:ALA:O	1:A:70:LYS:HB3	2.02	0.60
2:B:320:ILE:HD13	2:B:379:ARG:HH11	1.64	0.60
2:B:106:LEU:HD23	2:B:106:LEU:H	1.67	0.59
2:B:135:LEU:HD12	2:B:145:HIS:O	2.01	0.59
1:A:78:LEU:HB3	2:B:485:LYS:HZ2	1.65	0.59
2:B:125:GLN:OE1	2:B:150:MET:HA	2.01	0.59
2:B:220:PHE:HD2	2:B:332:GLU:CD	2.05	0.59
2:B:430:PHE:CZ	2:B:435:LYS:HG2	2.37	0.59
2:B:497:ASP:CG	2:B:498:VAL:N	2.54	0.59
2:B:137:LYS:HE3	2:B:173:GLY:C	2.21	0.59
2:B:375:ARG:HG3	2:B:375:ARG:NH1	2.17	0.59
2:B:75:THR:HG23	2:B:179:GLU:OE1	2.02	0.59
1:A:360:PRO:HG2	1:A:361:ASN:H	1.67	0.59
1:A:123:ASP:O	1:A:124:ARG:C	2.40	0.59
2:B:500:ASP:O	2:B:503:PRO:HD2	2.02	0.59
1:A:102:ARG:HD3	1:A:119:GLN:NE2	2.17	0.59
2:B:33:SER:HB3	2:B:35:PRO:HD2	1.84	0.59
2:B:507:LYS:HE3	2:B:533:LYS:NZ	2.18	0.59
1:A:150:THR:OG1	1:A:225:HIS:HB3	2.03	0.59
2:B:448:ILE:O	2:B:451:ALA:HB3	2.02	0.59
1:A:206:MET:HG2	1:A:343:GLN:HE21	1.68	0.59
1:A:231:ALA:HA	1:A:235:ARG:NH2	2.18	0.59
2:B:192:ILE:HG23	2:B:193:TYR:N	2.17	0.59
2:B:263:ARG:HD2	2:B:271:LEU:HG	1.84	0.59
1:A:69:ALA:HA	1:A:74:GLY:O	2.02	0.59
2:B:197:LYS:HA	2:B:220:PHE:CE2	2.37	0.59
2:B:53:CYS:O	2:B:55:GLU:N	2.35	0.59
2:B:73:TYR:CD1	2:B:181:ARG:HB2	2.38	0.59
2:B:110:ARG:HG3	2:B:380:VAL:HG22	1.84	0.58
1:A:20:LEU:HD22	1:A:139:TYR:HB3	1.85	0.58
2:B:150:MET:HE3	2:B:152:ASN:HB2	1.84	0.58
2:B:531:LYS:HG2	2:B:581:SER:HA	1.86	0.58
1:A:201:ILE:HD12	1:A:207:TYR:HA	1.86	0.58
1:A:21:LEU:O	1:A:25:GLU:HG3	2.02	0.58
2:B:115:ILE:N	2:B:115:ILE:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:GLN:OE1	2:B:613:THR:O	2.21	0.58
2:B:205:HIS:NE2	2:B:228:PRO:HD3	2.18	0.58
2:B:263:ARG:NH1	2:B:271:LEU:HD11	2.18	0.58
2:B:455:VAL:O	2:B:457:ARG:N	2.37	0.58
1:A:31:PHE:O	1:A:35:VAL:N	2.36	0.58
2:B:90:ILE:HG12	2:B:147:TYR:CD2	2.39	0.58
2:B:588:ILE:CG1	2:B:589:GLU:H	2.10	0.58
2:B:64:VAL:O	2:B:64:VAL:HG12	2.03	0.58
1:A:230:PRO:CD	1:A:262:ILE:HG23	2.34	0.58
1:A:31:PHE:HB2	2:B:489:LYS:NZ	2.19	0.58
2:B:407:GLN:CB	2:B:414:VAL:H	2.17	0.58
1:A:156:GLU:HG2	1:A:157:ILE:N	2.18	0.57
2:B:239:GLU:N	2:B:239:GLU:OE1	2.35	0.57
2:B:357:VAL:HG11	2:B:452:ILE:HA	1.85	0.57
1:A:17:ARG:HH12	1:A:141:HIS:CG	2.22	0.57
1:A:326:TYR:O	1:A:330:GLN:NE2	2.30	0.57
1:A:87:PHE:HD1	2:B:492:HIS:CD2	2.22	0.57
1:A:35:VAL:CG1	2:B:486:LEU:HD13	2.34	0.57
2:B:237:HIS:CG	2:B:238:PRO:HD2	2.39	0.57
2:B:69:THR:HG21	2:B:75:THR:HG23	1.87	0.57
1:A:28:TYR:CZ	2:B:489:LYS:HA	2.39	0.57
1:A:201:ILE:HG22	1:A:252:PHE:HB3	1.87	0.57
2:B:430:PHE:CE2	2:B:435:LYS:HG2	2.39	0.57
2:B:345:PRO:CA	2:B:354:VAL:HG12	2.35	0.57
2:B:514:VAL:HG12	2:B:530:ILE:CG1	2.34	0.57
2:B:549:PRO:HB2	2:B:589:GLU:OE2	2.05	0.57
1:A:118:GLU:C	1:A:120:GLY:H	2.07	0.57
1:A:21:LEU:HD23	1:A:21:LEU:O	2.05	0.57
1:A:237:ILE:HG22	1:A:241:MET:CE	2.32	0.57
1:A:112:ASP:C	1:A:114:ALA:N	2.56	0.57
1:A:191:GLN:O	1:A:192:LYS:HB2	2.03	0.57
2:B:213:PRO:O	2:B:214:ASP:OD1	2.23	0.57
2:B:374:MET:CE	2:B:418:ILE:HD11	2.35	0.57
1:A:79:LEU:HD22	1:A:114:ALA:HB2	1.87	0.57
1:A:206:MET:CE	1:A:354:VAL:HG11	2.35	0.57
1:A:102:ARG:HD3	1:A:119:GLN:HE22	1.68	0.57
1:A:232:ARG:O	1:A:233:SER:C	2.44	0.57
2:B:211:ILE:O	2:B:211:ILE:HG13	2.05	0.57
2:B:384:TYR:HB2	2:B:436:ASP:OD1	2.05	0.57
2:B:38:LEU:HA	2:B:180:MET:HE3	1.86	0.57
2:B:455:VAL:C	2:B:457:ARG:N	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:ILE:HG22	2:B:452:ILE:HD11	1.87	0.56
1:A:121:GLU:O	1:A:122:SER:C	2.43	0.56
1:A:159:GLU:O	1:A:160:GLN:CB	2.54	0.56
1:A:282:THR:N	1:A:283:PRO:CD	2.69	0.56
2:B:149:LEU:HD12	2:B:150:MET:N	2.19	0.56
2:B:253:THR:HG22	2:B:254:GLU:N	2.21	0.56
2:B:80:ASP:O	2:B:81:ASN:CB	2.52	0.56
1:A:18:GLU:C	1:A:20:LEU:H	2.09	0.56
2:B:135:LEU:HD23	2:B:169:PHE:HE2	1.70	0.56
2:B:401:LYS:NZ	2:B:406:ASN:ND2	2.53	0.56
2:B:473:ARG:NH1	2:B:473:ARG:HG3	2.20	0.56
2:B:597:GLN:O	2:B:598:LYS:CB	2.50	0.56
2:B:278:CYS:HB2	2:B:285:PRO:HG3	1.87	0.56
2:B:557:PRO:CD	2:B:585:SER:H	2.19	0.56
2:B:188:ARG:HG3	2:B:189:ARG:H	1.70	0.56
2:B:320:ILE:HD13	2:B:379:ARG:NH1	2.21	0.56
1:A:282:THR:H	1:A:283:PRO:CD	2.18	0.56
2:B:26:ARG:HH11	2:B:26:ARG:HG2	1.70	0.56
2:B:400:TRP:CZ2	2:B:411:GLY:N	2.74	0.56
1:A:300:LEU:HD11	1:A:346:PHE:CE2	2.40	0.56
1:A:209:ARG:O	1:A:209:ARG:HG2	2.05	0.56
1:A:203:THR:N	1:A:225:HIS:NE2	2.44	0.56
2:B:399:LYS:HA	2:B:399:LYS:HE3	1.88	0.56
2:B:485:LYS:C	2:B:487:ALA:H	2.09	0.56
2:B:77:ILE:O	2:B:78:ILE:HD12	2.05	0.56
1:A:162:LYS:NZ	1:A:182:PRO:HG2	2.20	0.56
1:A:249:VAL:O	1:A:285:ALA:HB1	2.06	0.56
2:B:21:PHE:HD1	2:B:21:PHE:O	1.88	0.56
2:B:394:ALA:HA	2:B:445:LYS:HE3	1.86	0.56
1:A:290:LEU:HD21	1:A:341:ALA:CB	2.35	0.56
2:B:148:GLU:HB2	2:B:162:VAL:HG23	1.85	0.56
2:B:375:ARG:CD	2:B:382:LEU:HD23	2.36	0.56
1:A:242:ASN:CG	1:A:282:THR:HG23	2.26	0.55
2:B:300:LEU:O	2:B:303:ALA:HB3	2.07	0.55
2:B:372:SER:O	2:B:418:ILE:HA	2.06	0.55
2:B:371:ILE:HB	2:B:414:VAL:HA	1.88	0.55
1:A:176:GLU:CD	1:A:176:GLU:H	2.09	0.55
1:A:205:GLY:HA3	1:A:344:GLN:NE2	2.21	0.55
1:A:346:PHE:CD1	1:A:354:VAL:HG22	2.41	0.55
2:B:334:THR:CB	2:B:364:ASN:HB2	2.36	0.55
1:A:149:ALA:HA	1:A:180:GLN:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:TRP:CE3	2:B:169:PHE:N	2.75	0.55
2:B:245:THR:O	2:B:249:MET:HG2	2.06	0.55
2:B:212:ASP:OD1	2:B:216:ASN:OD1	2.25	0.55
2:B:375:ARG:CZ	2:B:382:LEU:HD23	2.37	0.55
2:B:382:LEU:HD11	2:B:436:ASP:HA	1.87	0.55
1:A:100:THR:N	1:A:103:GLU:OE1	2.31	0.55
2:B:137:LYS:HG3	2:B:172:HIS:N	2.20	0.55
2:B:16:ILE:HG22	2:B:16:ILE:O	2.05	0.55
1:A:181:ILE:HD12	1:A:237:ILE:HG13	1.89	0.55
1:A:41:LEU:HA	1:A:69:ALA:HB3	1.87	0.55
1:A:288:LEU:HD12	1:A:288:LEU:C	2.27	0.55
1:A:203:THR:H	1:A:225:HIS:CD2	2.25	0.54
2:B:66:VAL:O	2:B:213:PRO:HB3	2.06	0.54
2:B:27:GLN:C	2:B:29:LEU:N	2.61	0.54
2:B:343:ARG:HG3	2:B:343:ARG:NH1	2.22	0.54
1:A:314:ARG:O	1:A:318:SER:HB2	2.08	0.54
2:B:283:LEU:HD22	2:B:287:ILE:HD11	1.88	0.54
1:A:31:PHE:CG	2:B:489:LYS:HD3	2.41	0.54
2:B:90:ILE:CD1	2:B:147:TYR:HE2	2.20	0.54
1:A:239:LYS:HZ2	1:A:279:PHE:HA	1.69	0.54
1:A:80:LYS:HD2	1:A:116:PHE:CE1	2.43	0.54
2:B:112:GLN:O	2:B:115:ILE:HD11	2.07	0.54
1:A:200:ALA:O	1:A:252:PHE:N	2.37	0.54
1:A:82:THR:N	1:A:85:THR:HG1	2.06	0.54
2:B:107:LYS:HZ3	2:B:424:ALA:HB1	1.72	0.54
2:B:170:ARG:NH1	2:B:170:ARG:HG2	2.21	0.54
1:A:32:GLU:C	1:A:34:GLU:N	2.61	0.54
2:B:25:ASN:C	2:B:27:GLN:H	2.10	0.54
2:B:598:LYS:HE2	2:B:613:THR:N	2.23	0.54
2:B:96:LYS:HB2	2:B:118:SER:OG	2.08	0.54
1:A:252:PHE:HA	1:A:289:GLY:CA	2.38	0.54
2:B:136:SER:CB	2:B:174:THR:HB	2.38	0.54
2:B:448:ILE:HG22	2:B:452:ILE:CD1	2.37	0.54
2:B:470:LYS:C	2:B:472:ARG:H	2.10	0.54
2:B:76:VAL:N	2:B:178:LEU:O	2.38	0.54
2:B:532:VAL:CG2	2:B:533:LYS:N	2.70	0.54
1:A:75:ALA:O	1:A:78:LEU:HB2	2.08	0.54
2:B:137:LYS:N	2:B:137:LYS:HD3	2.23	0.54
2:B:90:ILE:HG12	2:B:147:TYR:HD2	1.73	0.54
2:B:170:ARG:N	2:B:171:PRO:HD3	2.23	0.54
2:B:25:ASN:HB3	2:B:28:ILE:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:ILE:HG22	2:B:526:VAL:HG22	1.90	0.54
1:A:156:GLU:C	1:A:157:ILE:HG13	2.28	0.54
1:A:181:ILE:HD13	1:A:237:ILE:HG13	1.89	0.54
2:B:184:TYR:O	2:B:186:LYS:N	2.41	0.54
2:B:167:ASP:O	2:B:168:TRP:HB3	2.08	0.54
2:B:26:ARG:HG2	2:B:26:ARG:O	2.07	0.53
2:B:375:ARG:HH11	2:B:382:LEU:HD23	1.68	0.53
1:A:158:THR:O	1:A:189:GLU:HB3	2.08	0.53
2:B:373:ILE:O	2:B:373:ILE:CG1	2.55	0.53
2:B:400:TRP:CE3	2:B:407:GLN:O	2.61	0.53
2:B:398:ILE:HG13	2:B:449:ASP:OD1	2.09	0.53
2:B:539:ALA:HA	2:B:577:SER:HB2	1.90	0.53
1:A:18:GLU:C	1:A:20:LEU:N	2.61	0.53
1:A:305:LEU:HD21	1:A:339:LYS:N	2.23	0.53
2:B:168:TRP:O	2:B:169:PHE:CB	2.53	0.53
2:B:511:ASN:O	2:B:512:LEU:HB3	2.09	0.53
2:B:544:VAL:HG22	2:B:601:GLN:HG3	1.91	0.53
2:B:528:VAL:CG1	2:B:584:LEU:HD12	2.37	0.53
1:A:149:ALA:HA	1:A:180:GLN:HG3	1.89	0.53
2:B:184:TYR:CE1	2:B:192:ILE:HG12	2.39	0.53
1:A:28:TYR:CE2	2:B:492:HIS:HB3	2.43	0.53
1:A:87:PHE:HD2	1:A:111:TRP:HZ3	1.56	0.53
1:A:248:PRO:O	1:A:249:VAL:HG23	2.08	0.53
2:B:78:ILE:HG22	2:B:78:ILE:O	2.07	0.53
2:B:139:SER:CB	2:B:140:PRO:HD2	2.36	0.53
2:B:302:GLU:HA	2:B:305:GLU:HG2	1.91	0.53
2:B:360:ALA:HB3	2:B:418:ILE:HG21	1.88	0.53
2:B:77:ILE:N	2:B:77:ILE:CD1	2.72	0.53
1:A:181:ILE:HD11	1:A:234:THR:HA	1.91	0.53
1:A:100:THR:HG22	1:A:143:ARG:O	2.09	0.53
1:A:140:PHE:O	1:A:141:HIS:CB	2.57	0.53
1:A:251:VAL:HG21	1:A:263:TYR:HD1	1.74	0.53
2:B:263:ARG:HD2	2:B:271:LEU:CD2	2.39	0.53
2:B:44:GLU:HA	2:B:44:GLU:OE2	2.09	0.53
2:B:593:GLU:O	2:B:596:LEU:HD12	2.09	0.53
1:A:145:GLU:O	1:A:146:GLU:CB	2.57	0.53
1:A:185:VAL:HG11	1:A:236:ARG:HB2	1.90	0.53
1:A:281:ALA:HB1	1:A:283:PRO:HD3	1.91	0.53
1:A:31:PHE:HB2	2:B:489:LYS:CE	2.38	0.53
1:A:83:TYR:C	1:A:85:THR:N	2.61	0.53
2:B:289:PRO:O	2:B:292:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:CE1	2:B:529:ALA:HB3	2.44	0.53
2:B:151:ILE:O	2:B:152:ASN:O	2.27	0.53
2:B:448:ILE:O	2:B:452:ILE:HG13	2.09	0.53
1:A:112:ASP:C	1:A:114:ALA:H	2.11	0.52
2:B:150:MET:CE	2:B:152:ASN:HB2	2.39	0.52
2:B:61:ASP:HA	2:B:207:ARG:O	2.09	0.52
2:B:27:GLN:OE1	2:B:32:ASP:HB2	2.09	0.52
2:B:381:PRO:O	2:B:382:LEU:CB	2.49	0.52
2:B:550:CYS:O	2:B:551:LYS:CB	2.57	0.52
2:B:65:GLN:HE21	2:B:67:GLU:CG	2.22	0.52
1:A:69:ALA:O	1:A:70:LYS:CB	2.56	0.52
2:B:513:LEU:HD12	2:B:513:LEU:O	2.09	0.52
2:B:557:PRO:O	2:B:558:GLU:HB2	2.09	0.52
1:A:108:SER:C	1:A:110:GLY:H	2.12	0.52
2:B:90:ILE:HD13	2:B:147:TYR:HE2	1.74	0.52
2:B:16:ILE:O	2:B:17:SER:HB2	2.09	0.52
2:B:25:ASN:O	2:B:27:GLN:N	2.41	0.52
2:B:348:TYR:CZ	2:B:351:ASN:HB2	2.44	0.52
2:B:428:VAL:HB	2:B:430:PHE:HE2	1.73	0.52
2:B:65:GLN:HE21	2:B:67:GLU:HG2	1.75	0.52
1:A:206:MET:O	1:A:210:LEU:HB2	2.10	0.52
1:A:149:ALA:HB2	1:A:180:GLN:CD	2.30	0.52
2:B:152:ASN:O	2:B:153:THR:O	2.28	0.52
2:B:156:ASN:O	2:B:157:GLU:C	2.47	0.52
2:B:418:ILE:O	2:B:418:ILE:HG23	2.09	0.52
2:B:534:ASN:O	2:B:534:ASN:CG	2.47	0.52
2:B:322:GLU:HG3	2:B:342:THR:HB	1.92	0.52
1:A:183:PHE:N	1:A:183:PHE:CD1	2.75	0.52
1:A:323:GLU:OE2	1:A:328:LYS:HD2	2.09	0.52
2:B:392:THR:O	2:B:395:VAL:HB	2.10	0.52
2:B:337:PHE:HB2	2:B:462:TYR:CE1	2.45	0.52
1:A:83:TYR:CG	2:B:488:ALA:HB1	2.44	0.52
1:A:359:LEU:HB2	1:A:360:PRO:CD	2.40	0.52
2:B:190:GLN:HG2	2:B:383:LEU:CD2	2.30	0.52
2:B:453:LYS:HA	2:B:456:ALA:HB3	1.92	0.52
2:B:493:VAL:O	2:B:495:GLU:N	2.39	0.52
2:B:222:ARG:NH2	2:B:332:GLU:N	2.58	0.51
2:B:559:PRO:O	2:B:560:LYS:HB2	2.10	0.51
1:A:188:ILE:CG1	1:A:240:ARG:NH2	2.70	0.51
2:B:36:ARG:HA	2:B:39:ILE:CG2	2.39	0.51
1:A:79:LEU:C	1:A:79:LEU:HD23	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:O	1:A:84:ALA:C	2.48	0.51
2:B:235:LEU:HB2	2:B:267:CYS:SG	2.50	0.51
2:B:423:VAL:HG21	2:B:438:ILE:CD1	2.40	0.51
1:A:149:ALA:HB2	1:A:180:GLN:OE1	2.11	0.51
2:B:133:LYS:HE3	2:B:146:TYR:HE1	1.74	0.51
2:B:391:THR:O	2:B:395:VAL:HG23	2.10	0.51
2:B:496:LYS:O	2:B:497:ASP:HB2	2.09	0.51
2:B:539:ALA:HA	2:B:577:SER:CB	2.41	0.51
1:A:31:PHE:CB	2:B:489:LYS:NZ	2.74	0.51
2:B:190:GLN:O	2:B:383:LEU:HD21	2.11	0.51
2:B:112:GLN:HB2	2:B:435:LYS:CD	2.40	0.51
1:A:305:LEU:CD1	1:A:305:LEU:H	1.96	0.51
2:B:405:LEU:HD11	2:B:415:GLY:HA3	1.91	0.51
2:B:78:ILE:N	2:B:78:ILE:CD1	2.74	0.51
2:B:154:SER:O	2:B:156:ASN:N	2.44	0.51
2:B:90:ILE:HG22	2:B:91:PRO:CD	2.40	0.51
1:A:362:ARG:HH11	1:A:362:ARG:HG3	1.75	0.51
1:A:75:ALA:HB1	2:B:481:LYS:HD2	1.92	0.51
2:B:36:ARG:CG	2:B:384:TYR:OH	2.59	0.51
2:B:417:VAL:O	2:B:418:ILE:HB	2.11	0.51
2:B:359:MET:CE	2:B:455:VAL:HG23	2.32	0.51
2:B:548:LEU:O	2:B:568:TYR:N	2.45	0.51
2:B:233:GLU:HG2	2:B:234:ILE:H	1.75	0.50
2:B:396:GLU:HG2	2:B:412:ILE:N	2.26	0.50
2:B:477:ILE:C	2:B:479:ILE:H	2.14	0.50
2:B:543:ARG:O	2:B:601:GLN:HA	2.11	0.50
1:A:138:GLU:HG3	1:A:236:ARG:HH12	1.76	0.50
1:A:156:GLU:O	1:A:157:ILE:CG1	2.53	0.50
2:B:451:ALA:O	2:B:454:GLU:HB2	2.11	0.50
2:B:528:VAL:HG12	2:B:528:VAL:O	2.11	0.50
2:B:402:GLN:O	2:B:403:TYR:HD1	1.94	0.50
2:B:423:VAL:HG21	2:B:438:ILE:HD11	1.93	0.50
2:B:532:VAL:CG2	2:B:533:LYS:H	2.25	0.50
1:A:147:ASP:OD2	1:A:147:ASP:O	2.29	0.50
1:A:235:ARG:C	1:A:237:ILE:H	2.13	0.50
1:A:31:PHE:HB2	2:B:489:LYS:HZ2	1.77	0.50
2:B:354:VAL:HG22	2:B:424:ALA:HB3	1.93	0.50
2:B:374:MET:HE2	2:B:418:ILE:HD11	1.93	0.50
2:B:65:GLN:CG	2:B:211:ILE:HG13	2.37	0.50
2:B:251:HIS:HA	2:B:290:HIS:CE1	2.47	0.50
2:B:27:GLN:O	2:B:29:LEU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ILE:O	2:B:60:PRO:N	2.44	0.50
1:A:98:GLY:HA3	1:A:141:HIS:ND1	2.26	0.50
2:B:171:PRO:O	2:B:172:HIS:CB	2.58	0.50
2:B:115:ILE:O	2:B:116:GLY:O	2.29	0.50
2:B:253:THR:CG2	2:B:254:GLU:N	2.75	0.50
2:B:508:ILE:HG23	2:B:509:MET:N	2.25	0.50
2:B:547:MET:C	2:B:548:LEU:HD12	2.32	0.50
1:A:106:TYR:C	1:A:108:SER:H	2.15	0.50
1:A:154:PRO:HD2	1:A:221:ALA:O	2.12	0.50
1:A:346:PHE:HB2	1:A:354:VAL:HG22	1.94	0.50
2:B:145:HIS:HB3	2:B:147:TYR:HE1	1.73	0.49
2:B:198:ALA:HB1	2:B:376:PHE:CZ	2.46	0.49
2:B:235:LEU:O	2:B:267:CYS:SG	2.70	0.49
2:B:335:VAL:CG2	2:B:360:ALA:HB1	2.39	0.49
2:B:383:LEU:C	2:B:384:TYR:HD1	2.15	0.49
2:B:66:VAL:O	2:B:213:PRO:CD	2.61	0.49
1:A:150:THR:HB	1:A:225:HIS:HB3	1.93	0.49
1:A:225:HIS:C	1:A:226:LEU:HD23	2.32	0.49
1:A:72:VAL:HG21	2:B:474:GLU:HG2	1.94	0.49
2:B:428:VAL:HB	2:B:430:PHE:CE2	2.47	0.49
2:B:43:LYS:O	2:B:47:ASP:OD2	2.30	0.49
2:B:445:LYS:HA	2:B:448:ILE:HD12	1.94	0.49
1:A:96:ASN:O	1:A:97:ARG:O	2.31	0.49
2:B:112:GLN:C	2:B:115:ILE:HD11	2.32	0.49
2:B:399:LYS:O	2:B:400:TRP:CG	2.66	0.49
2:B:401:LYS:O	2:B:403:TYR:N	2.46	0.49
2:B:430:PHE:CE1	2:B:435:LYS:HG2	2.47	0.49
2:B:550:CYS:N	2:B:589:GLU:OE2	2.46	0.49
1:A:125:LEU:O	1:A:128:ASP:HB2	2.12	0.49
2:B:338:ILE:CG2	2:B:339:ALA:N	2.75	0.49
2:B:346:ALA:HB3	2:B:353:PHE:CE1	2.47	0.49
1:A:117:LYS:HB2	1:A:117:LYS:HZ3	1.75	0.49
1:A:149:ALA:HB2	1:A:180:GLN:HG3	1.94	0.49
1:A:292:PRO:C	1:A:333:LEU:HD23	2.32	0.49
2:B:132:THR:HG23	2:B:178:LEU:HD11	1.95	0.49
2:B:61:ASP:CB	2:B:207:ARG:HH11	2.16	0.49
2:B:342:THR:HG23	2:B:356:GLU:CG	2.41	0.49
1:A:154:PRO:O	1:A:155:ILE:CG2	2.59	0.49
2:B:337:PHE:CE2	2:B:459:LEU:HA	2.47	0.49
2:B:107:LYS:NZ	2:B:424:ALA:HB1	2.28	0.49
2:B:212:ASP:CG	2:B:216:ASN:OD1	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:VAL:HG12	2:B:418:ILE:N	2.27	0.49
2:B:508:ILE:HG22	2:B:509:MET:N	2.24	0.49
1:A:145:GLU:O	1:A:146:GLU:HB2	2.13	0.49
1:A:223:LEU:O	1:A:224:VAL:HG13	2.13	0.49
1:A:359:LEU:O	1:A:363:LEU:HB2	2.12	0.49
2:B:348:TYR:OH	2:B:429:PRO:HD3	2.13	0.49
2:B:594:GLU:O	2:B:596:LEU:N	2.45	0.49
2:B:273:THR:O	2:B:277:ILE:HG13	2.12	0.49
2:B:284:ASP:HB2	2:B:287:ILE:CG2	2.43	0.49
2:B:369:GLU:HG2	2:B:414:VAL:HG23	1.95	0.49
2:B:444:ILE:HG22	2:B:445:LYS:N	2.27	0.49
1:A:137:ARG:HB2	1:A:137:ARG:HH11	1.78	0.49
1:A:203:THR:C	1:A:205:GLY:N	2.67	0.49
2:B:224:THR:O	2:B:226:LYS:N	2.46	0.49
2:B:550:CYS:HB2	2:B:589:GLU:OE2	2.13	0.49
1:A:28:TYR:O	1:A:29:ASN:C	2.51	0.48
2:B:396:GLU:CG	2:B:412:ILE:HG23	2.42	0.48
2:B:400:TRP:HZ3	2:B:408:PRO:CA	2.25	0.48
2:B:560:LYS:HB3	2:B:571:VAL:O	2.12	0.48
1:A:198:ILE:HD12	1:A:249:VAL:CG2	2.44	0.48
1:A:28:TYR:CE1	2:B:489:LYS:HA	2.48	0.48
1:A:331:ILE:O	1:A:334:GLN:N	2.41	0.48
1:A:21:LEU:HD12	1:A:93:LEU:HD13	1.94	0.48
2:B:180:MET:CG	2:B:180:MET:O	2.59	0.48
2:B:398:ILE:CG2	2:B:399:LYS:N	2.76	0.48
2:B:425:SER:O	2:B:427:ASN:N	2.46	0.48
1:A:85:THR:C	1:A:87:PHE:H	2.16	0.48
2:B:75:THR:HA	2:B:178:LEU:O	2.14	0.48
2:B:193:TYR:CE1	2:B:218:GLU:HG2	2.48	0.48
1:A:156:GLU:HA	1:A:170:CYS:HB3	1.95	0.48
1:A:288:LEU:HD12	1:A:288:LEU:O	2.13	0.48
1:A:305:LEU:HD12	1:A:305:LEU:N	2.05	0.48
2:B:551:LYS:HG2	2:B:552:VAL:H	1.74	0.48
1:A:151:MET:HG3	1:A:224:VAL:CG1	2.44	0.48
2:B:20:GLU:O	2:B:22:PHE:N	2.47	0.48
2:B:361:TYR:CD2	2:B:362:GLY:N	2.82	0.48
2:B:449:ASP:C	2:B:451:ALA:N	2.66	0.48
2:B:137:LYS:CE	2:B:173:GLY:H	2.26	0.48
1:A:151:MET:HG3	1:A:224:VAL:HG12	1.95	0.48
1:A:296:VAL:HG22	1:A:337:ILE:HD11	1.94	0.48
1:A:365:GLU:HG2	1:A:367:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:VAL:C	2:B:457:ARG:H	2.17	0.48
2:B:85:ILE:HG13	2:B:90:ILE:CD1	2.44	0.48
2:B:46:VAL:O	2:B:50:LEU:HG	2.14	0.48
2:B:91:PRO:O	2:B:95:ALA:HB3	2.14	0.48
1:A:317:LEU:C	1:A:319:ASP:H	2.17	0.48
1:A:30:GLN:O	1:A:34:GLU:HB2	2.13	0.48
2:B:237:HIS:ND1	2:B:239:GLU:OE1	2.42	0.48
2:B:591:ALA:O	2:B:593:GLU:N	2.47	0.48
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.73	0.47
2:B:122:LEU:HD22	2:B:126:MET:CE	2.43	0.47
2:B:23:GLU:OE1	2:B:26:ARG:HD2	2.14	0.47
2:B:345:PRO:HB3	2:B:354:VAL:HG12	1.95	0.47
2:B:402:GLN:O	2:B:403:TYR:CD1	2.67	0.47
2:B:505:VAL:O	2:B:508:ILE:HG22	2.14	0.47
2:B:80:ASP:HB3	2:B:81:ASN:H	1.57	0.47
1:A:122:SER:O	1:A:123:ASP:O	2.32	0.47
2:B:169:PHE:CD1	2:B:169:PHE:O	2.67	0.47
2:B:65:GLN:HA	2:B:211:ILE:O	2.14	0.47
2:B:338:ILE:HG22	2:B:339:ALA:N	2.30	0.47
2:B:534:ASN:ND2	2:B:539:ALA:HB3	2.29	0.47
2:B:53:CYS:C	2:B:55:GLU:N	2.66	0.47
2:B:168:TRP:CZ3	2:B:169:PHE:HA	2.46	0.47
2:B:44:GLU:O	2:B:45:ALA:C	2.52	0.47
1:A:149:ALA:HB2	1:A:180:GLN:CG	2.44	0.47
1:A:155:ILE:HD13	1:A:222:ILE:CD1	2.45	0.47
1:A:98:GLY:CA	1:A:141:HIS:CE1	2.97	0.47
2:B:190:GLN:HG3	2:B:194:GLU:HG2	1.95	0.47
2:B:191:SER:OG	2:B:192:ILE:N	2.45	0.47
2:B:430:PHE:CD2	2:B:435:LYS:HG2	2.49	0.47
1:A:237:ILE:O	1:A:241:MET:HE2	2.14	0.47
1:A:84:ALA:HB1	1:A:111:TRP:CZ2	2.50	0.47
2:B:311:ALA:O	2:B:312:PRO:O	2.33	0.47
2:B:359:MET:HB2	2:B:419:LEU:CD2	2.44	0.47
2:B:449:ASP:C	2:B:451:ALA:H	2.16	0.47
1:A:99:SER:HB3	1:A:103:GLU:OE1	2.15	0.47
1:A:159:GLU:HG3	1:A:160:GLN:N	2.29	0.47
2:B:375:ARG:NH1	2:B:382:LEU:CD2	2.76	0.47
2:B:543:ARG:O	2:B:601:GLN:CA	2.63	0.47
1:A:264:ALA:HA	1:A:267:ALA:CB	2.42	0.47
1:A:338:GLY:C	1:A:339:LYS:HG3	2.35	0.47
2:B:263:ARG:O	2:B:263:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HD13	1:A:129:LEU:HD12	1.95	0.47
2:B:136:SER:HB2	2:B:174:THR:HB	1.97	0.47
2:B:308:LYS:HD2	2:B:308:LYS:O	2.15	0.47
2:B:355:VAL:HA	2:B:422:HIS:O	2.14	0.47
2:B:58:ILE:O	2:B:60:PRO:HD3	2.15	0.47
2:B:91:PRO:HB3	2:B:158:PRO:HG3	1.97	0.47
2:B:229:GLU:CG	2:B:230:PRO:HD2	2.45	0.47
1:A:279:PHE:O	1:A:280:MET:CG	2.61	0.47
1:A:260:TYR:HE1	1:A:287:PHE:CE2	2.33	0.47
2:B:281:ALA:HB2	2:B:300:LEU:HA	1.96	0.47
2:B:53:CYS:C	2:B:55:GLU:H	2.19	0.47
2:B:561:VAL:HG21	2:B:570:TYR:HE1	1.79	0.47
2:B:62:ILE:HG23	2:B:79:GLU:O	2.15	0.47
1:A:362:ARG:NH1	1:A:362:ARG:HG3	2.29	0.46
2:B:180:MET:HG2	2:B:180:MET:O	2.15	0.46
2:B:197:LYS:O	2:B:201:ILE:HG22	2.14	0.46
2:B:277:ILE:HG22	2:B:300:LEU:HD11	1.97	0.46
2:B:31:PHE:O	2:B:32:ASP:C	2.52	0.46
2:B:430:PHE:CZ	2:B:435:LYS:HE3	2.49	0.46
2:B:439:ALA:O	2:B:441:ILE:N	2.48	0.46
2:B:534:ASN:HD21	2:B:539:ALA:HB3	1.81	0.46
2:B:135:LEU:CD1	2:B:146:TYR:HB2	2.45	0.46
1:A:76:PHE:CD2	2:B:481:LYS:HE2	2.50	0.46
1:A:231:ALA:HA	1:A:235:ARG:HH21	1.80	0.46
2:B:106:LEU:HB3	2:B:233:GLU:HA	1.97	0.46
2:B:318:SER:OG	2:B:379:ARG:NH2	2.48	0.46
2:B:325:ILE:O	2:B:326:TYR:C	2.53	0.46
2:B:201:ILE:HG13	2:B:328:GLY:C	2.35	0.46
2:B:205:HIS:CG	2:B:205:HIS:O	2.68	0.46
2:B:27:GLN:C	2:B:29:LEU:H	2.17	0.46
2:B:448:ILE:CG2	2:B:452:ILE:HD11	2.45	0.46
1:A:138:GLU:CG	1:A:236:ARG:HH12	2.29	0.46
2:B:390:VAL:CG2	2:B:440:ASP:HA	2.43	0.46
2:B:457:ARG:HG3	2:B:458:LYS:N	2.30	0.46
2:B:50:LEU:O	2:B:54:GLU:HB2	2.15	0.46
1:A:235:ARG:CD	1:A:265:SER:O	2.63	0.46
2:B:348:TYR:O	2:B:349:SER:C	2.54	0.46
1:A:157:ILE:HD11	1:A:190:PHE:CD1	2.50	0.46
2:B:46:VAL:O	2:B:46:VAL:CG1	2.64	0.46
1:A:305:LEU:HD11	1:A:338:GLY:C	2.36	0.46
1:A:73:LYS:O	1:A:77:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ASN:N	2:B:216:ASN:OD1	2.47	0.46
2:B:36:ARG:HG2	2:B:36:ARG:O	2.16	0.46
2:B:523:ASP:O	2:B:588:ILE:CD1	2.63	0.46
2:B:58:ILE:CG2	2:B:59:LEU:H	2.22	0.46
2:B:167:ASP:O	2:B:168:TRP:CB	2.64	0.46
2:B:168:TRP:HE3	2:B:169:PHE:HA	1.72	0.46
2:B:510:GLY:O	2:B:533:LYS:O	2.34	0.46
1:A:263:TYR:CE2	1:A:327:TRP:CH2	3.03	0.46
1:A:32:GLU:C	1:A:34:GLU:H	2.20	0.46
2:B:19:ALA:O	2:B:22:PHE:HB3	2.15	0.46
2:B:561:VAL:CG2	2:B:570:TYR:CE1	2.99	0.46
1:A:291:GLN:HB2	1:A:330:GLN:OE1	2.16	0.45
2:B:65:GLN:NE2	2:B:67:GLU:HG2	2.30	0.45
1:A:252:PHE:HA	1:A:289:GLY:HA3	1.98	0.45
1:A:360:PRO:O	1:A:363:LEU:N	2.48	0.45
1:A:35:VAL:O	1:A:36:VAL:C	2.55	0.45
2:B:94:PHE:O	2:B:121:VAL:HG21	2.16	0.45
2:B:203:ASN:O	2:B:205:HIS:N	2.50	0.45
2:B:382:LEU:HD11	2:B:436:ASP:C	2.36	0.45
1:A:76:PHE:CD2	2:B:481:LYS:NZ	2.83	0.45
2:B:48:ASN:O	2:B:51:ASP:HB2	2.16	0.45
2:B:512:LEU:HD11	2:B:542:PHE:CZ	2.50	0.45
2:B:361:TYR:O	2:B:362:GLY:O	2.35	0.45
2:B:396:GLU:HG2	2:B:412:ILE:H	1.82	0.45
2:B:518:ILE:HG22	2:B:526:VAL:CG1	2.44	0.45
2:B:58:ILE:O	2:B:59:LEU:C	2.55	0.45
1:A:29:ASN:O	1:A:31:PHE:N	2.48	0.45
1:A:356:GLU:O	1:A:360:PRO:CG	2.63	0.45
1:A:353:PHE:CE1	1:A:357:VAL:HG21	2.51	0.45
2:B:18:VAL:HG23	2:B:19:ALA:H	1.81	0.45
2:B:450:LEU:O	2:B:454:GLU:HG2	2.16	0.45
1:A:291:GLN:OE1	1:A:294:ASP:OD2	2.35	0.45
2:B:21:PHE:CD1	2:B:21:PHE:O	2.68	0.45
2:B:431:THR:O	2:B:432:SER:C	2.55	0.45
1:A:136:GLN:O	1:A:137:ARG:C	2.55	0.45
1:A:17:ARG:HH12	1:A:141:HIS:CD2	2.34	0.45
1:A:155:ILE:HG22	1:A:192:LYS:O	2.17	0.45
1:A:238:ILE:HG22	1:A:282:THR:OG1	2.17	0.45
2:B:148:GLU:HB2	2:B:162:VAL:CG2	2.47	0.45
2:B:36:ARG:NH1	2:B:40:THR:OG1	2.49	0.45
2:B:468:ASN:O	2:B:471:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:VAL:HB	2:B:587:LYS:CB	2.36	0.45
2:B:110:ARG:O	2:B:111:GLY:C	2.55	0.45
2:B:170:ARG:N	2:B:171:PRO:CD	2.79	0.45
2:B:222:ARG:HB2	2:B:222:ARG:NH1	2.31	0.45
2:B:38:LEU:HA	2:B:180:MET:HE1	1.97	0.45
1:A:86:ASP:O	2:B:492:HIS:CE1	2.69	0.45
2:B:551:LYS:HZ3	2:B:586:TYR:HB3	1.81	0.45
2:B:234:ILE:O	2:B:234:ILE:HD12	2.17	0.45
2:B:27:GLN:HG2	2:B:32:ASP:CB	2.41	0.45
2:B:309:ILE:CG2	2:B:310:MET:H	2.29	0.45
2:B:543:ARG:O	2:B:601:GLN:CB	2.65	0.45
1:A:101:LEU:O	1:A:104:LEU:HB3	2.17	0.45
2:B:212:ASP:CB	2:B:213:PRO:HD2	2.46	0.45
2:B:22:PHE:O	2:B:26:ARG:N	2.50	0.45
2:B:443:VAL:HG12	2:B:443:VAL:O	2.17	0.45
2:B:545:HIS:ND1	2:B:571:VAL:HG22	2.32	0.44
1:A:155:ILE:HD13	1:A:222:ILE:HD11	1.99	0.44
1:A:32:GLU:O	1:A:34:GLU:N	2.50	0.44
2:B:361:TYR:CD2	2:B:361:TYR:C	2.90	0.44
1:A:202:GLU:HA	1:A:225:HIS:CD2	2.52	0.44
1:A:231:ALA:C	1:A:235:ARG:HE	2.20	0.44
1:A:251:VAL:CG2	1:A:263:TYR:HD1	2.30	0.44
2:B:378:ASN:O	2:B:379:ARG:HB2	2.16	0.44
2:B:194:GLU:HG2	2:B:383:LEU:HD11	1.99	0.44
2:B:531:LYS:HG2	2:B:581:SER:CA	2.48	0.44
1:A:207:TYR:HE1	1:A:223:LEU:HB3	1.83	0.44
1:A:268:TYR:HB2	1:A:322:PHE:CE2	2.47	0.44
1:A:29:ASN:C	1:A:31:PHE:N	2.61	0.44
2:B:152:ASN:ND2	2:B:155:THR:OG1	2.50	0.44
2:B:327:ARG:O	2:B:328:GLY:C	2.55	0.44
2:B:329:LEU:H	2:B:329:LEU:HD12	1.82	0.44
2:B:459:LEU:O	2:B:462:TYR:N	2.51	0.44
2:B:531:LYS:HG2	2:B:581:SER:HB2	1.99	0.44
2:B:61:ASP:OD2	2:B:61:ASP:O	2.35	0.44
2:B:89:GLN:O	2:B:93:VAL:HG23	2.17	0.44
1:A:138:GLU:O	1:A:139:TYR:C	2.55	0.44
2:B:320:ILE:HD11	2:B:379:ARG:HH11	1.80	0.44
1:A:176:GLU:CD	1:A:176:GLU:N	2.71	0.44
1:A:351:LEU:H	1:A:351:LEU:HD12	1.79	0.44
1:A:76:PHE:C	1:A:78:LEU:N	2.71	0.44
2:B:302:GLU:C	2:B:304:PHE:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:PRO:HA	2:B:487:ALA:HB3	1.99	0.44
2:B:531:LYS:HD3	2:B:581:SER:HB2	2.00	0.44
2:B:87:ARG:HG3	2:B:88:GLU:HG3	1.98	0.44
1:A:149:ALA:CB	1:A:180:GLN:HG3	2.48	0.44
1:A:216:ASP:N	1:A:216:ASP:OD2	2.50	0.44
2:B:198:ALA:HB1	2:B:376:PHE:HZ	1.81	0.44
2:B:37:SER:HB2	2:B:182:ALA:CB	2.45	0.44
2:B:195:TYR:HE1	2:B:381:PRO:HD2	1.82	0.44
2:B:440:ASP:O	2:B:440:ASP:OD1	2.35	0.44
2:B:444:ILE:O	2:B:447:GLU:HB3	2.18	0.44
2:B:521:ASN:HB2	2:B:522:GLY:H	1.50	0.44
2:B:53:CYS:SG	2:B:60:PRO:HB3	2.57	0.44
1:A:231:ALA:O	1:A:235:ARG:HB2	2.18	0.44
1:A:30:GLN:O	1:A:34:GLU:CD	2.56	0.44
2:B:150:MET:HG2	2:B:151:ILE:N	2.33	0.44
2:B:345:PRO:CB	2:B:354:VAL:HG12	2.48	0.44
1:A:233:SER:OG	1:A:234:THR:N	2.49	0.44
1:A:263:TYR:CZ	1:A:327:TRP:CH2	3.06	0.44
1:A:330:GLN:O	1:A:333:LEU:HB3	2.18	0.44
2:B:137:LYS:HG2	2:B:173:GLY:H	1.81	0.44
2:B:386:GLN:O	2:B:387:GLY:C	2.56	0.44
2:B:90:ILE:CG2	2:B:91:PRO:N	2.76	0.44
1:A:117:LYS:HB2	1:A:117:LYS:HZ2	1.82	0.43
1:A:78:LEU:HB3	2:B:485:LYS:HZ1	1.80	0.43
2:B:234:ILE:C	2:B:234:ILE:HD12	2.39	0.43
2:B:374:MET:HE3	2:B:418:ILE:HD11	1.99	0.43
2:B:514:VAL:HA	2:B:530:ILE:HG12	2.00	0.43
2:B:603:ILE:O	2:B:604:VAL:CB	2.66	0.43
1:A:106:TYR:C	1:A:108:SER:N	2.70	0.43
1:A:201:ILE:HA	1:A:252:PHE:O	2.18	0.43
2:B:30:GLY:O	2:B:31:PHE:CG	2.71	0.43
2:B:337:PHE:HE2	2:B:459:LEU:HA	1.83	0.43
2:B:42:VAL:C	2:B:44:GLU:N	2.71	0.43
2:B:473:ARG:HE	2:B:477:ILE:HD11	1.83	0.43
1:A:125:LEU:O	1:A:128:ASP:N	2.51	0.43
1:A:155:ILE:O	1:A:170:CYS:CB	2.66	0.43
1:A:217:GLU:C	1:A:219:TYR:H	2.21	0.43
2:B:153:THR:O	2:B:154:SER:OG	2.33	0.43
2:B:195:TYR:CE1	2:B:381:PRO:HG2	2.54	0.43
2:B:82:GLY:O	2:B:172:HIS:O	2.36	0.43
2:B:239:GLU:CD	2:B:239:GLU:H	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:TRP:HZ2	2:B:411:GLY:CA	2.31	0.43
2:B:355:VAL:CG2	2:B:423:VAL:HG12	2.47	0.43
2:B:64:VAL:HA	2:B:77:ILE:O	2.19	0.43
1:A:84:ALA:CB	1:A:111:TRP:CE2	3.00	0.43
1:A:235:ARG:C	1:A:237:ILE:N	2.71	0.43
1:A:24:ALA:HA	1:A:27:ILE:CD1	2.48	0.43
2:B:20:GLU:O	2:B:21:PHE:C	2.56	0.43
2:B:485:LYS:C	2:B:487:ALA:N	2.72	0.43
2:B:65:GLN:OE1	2:B:211:ILE:HD12	2.19	0.43
1:A:96:ASN:O	1:A:141:HIS:NE2	2.52	0.43
1:A:161:THR:O	1:A:162:LYS:HB2	2.19	0.43
1:A:214:GLY:O	1:A:215:PHE:CB	2.65	0.43
2:B:158:PRO:HB2	2:B:159:ASP:H	1.58	0.43
2:B:36:ARG:HG2	2:B:36:ARG:HH11	1.84	0.43
2:B:80:ASP:O	2:B:81:ASN:HB2	2.19	0.43
1:A:79:LEU:HD22	1:A:114:ALA:CB	2.48	0.43
2:B:135:LEU:HD12	2:B:135:LEU:HA	1.87	0.43
2:B:284:ASP:O	2:B:286:GLU:N	2.48	0.43
2:B:394:ALA:CA	2:B:445:LYS:HE3	2.49	0.43
1:A:101:LEU:C	1:A:103:GLU:H	2.22	0.43
1:A:130:GLU:CD	1:A:136:GLN:HE22	2.22	0.43
1:A:15:LEU:HD11	1:A:141:HIS:CD2	2.53	0.43
1:A:206:MET:N	1:A:344:GLN:NE2	2.66	0.43
2:B:90:ILE:CD1	2:B:147:TYR:CE2	3.02	0.43
2:B:222:ARG:NH2	2:B:332:GLU:CB	2.67	0.43
2:B:302:GLU:HA	2:B:305:GLU:HG3	2.00	0.43
2:B:502:ASN:HB3	2:B:503:PRO:HD3	2.00	0.43
2:B:541:SER:HA	2:B:575:SER:OG	2.19	0.43
2:B:551:LYS:HB3	2:B:570:TYR:OH	2.19	0.43
1:A:107:ILE:HG22	1:A:107:ILE:O	2.19	0.43
1:A:145:GLU:O	1:A:146:GLU:HG3	2.18	0.43
2:B:203:ASN:O	2:B:204:PRO:C	2.57	0.43
2:B:411:GLY:O	2:B:412:ILE:CG1	2.57	0.43
2:B:500:ASP:HB3	2:B:503:PRO:HD3	2.01	0.43
1:A:32:GLU:O	1:A:35:VAL:N	2.52	0.43
1:A:85:THR:C	1:A:87:PHE:N	2.72	0.43
1:A:96:ASN:O	1:A:97:ARG:C	2.57	0.43
2:B:235:LEU:HB2	2:B:267:CYS:H	1.84	0.43
2:B:314:THR:O	2:B:316:CYS:N	2.51	0.43
2:B:375:ARG:HD2	2:B:382:LEU:CD2	2.45	0.43
2:B:357:VAL:CG2	2:B:421:ILE:HG12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:LEU:HD11	2:B:436:ASP:O	2.19	0.43
2:B:204:PRO:HA	2:B:222:ARG:HD3	2.01	0.42
2:B:337:PHE:HB2	2:B:462:TYR:CD1	2.54	0.42
2:B:61:ASP:OD1	2:B:207:ARG:NH1	2.52	0.42
1:A:79:LEU:HD21	1:A:114:ALA:HB2	1.98	0.42
1:A:118:GLU:C	1:A:120:GLY:N	2.73	0.42
2:B:122:LEU:HD22	2:B:126:MET:HE1	2.00	0.42
2:B:300:LEU:HD12	2:B:303:ALA:HB3	2.01	0.42
1:A:268:TYR:HB3	1:A:269:GLY:H	1.61	0.42
2:B:48:ASN:ND2	2:B:117:ILE:HG12	2.32	0.42
2:B:117:ILE:O	2:B:121:VAL:HG23	2.20	0.42
2:B:263:ARG:HD2	2:B:271:LEU:CG	2.47	0.42
2:B:376:PHE:CD2	2:B:381:PRO:HA	2.54	0.42
2:B:389:CYS:O	2:B:390:VAL:C	2.56	0.42
2:B:475:LYS:O	2:B:479:ILE:HG13	2.18	0.42
2:B:479:ILE:HG23	2:B:505:VAL:HG11	2.01	0.42
2:B:576:ALA:HB2	2:B:582:LYS:CE	2.49	0.42
1:A:135:LEU:CB	1:A:140:PHE:HE1	2.30	0.42
1:A:155:ILE:O	1:A:155:ILE:HG13	2.20	0.42
2:B:353:PHE:CA	2:B:424:ALA:O	2.61	0.42
2:B:479:ILE:HG22	2:B:479:ILE:O	2.19	0.42
2:B:576:ALA:CB	2:B:582:LYS:HE3	2.48	0.42
2:B:81:ASN:O	2:B:81:ASN:CG	2.56	0.42
1:A:102:ARG:O	1:A:106:TYR:HD1	2.01	0.42
2:B:382:LEU:HD11	2:B:436:ASP:CA	2.49	0.42
1:A:169:HIS:HD2	1:A:172:LYS:H	1.68	0.42
1:A:300:LEU:HD11	1:A:346:PHE:HE2	1.84	0.42
2:B:184:TYR:CE2	2:B:212:ASP:HB2	2.54	0.42
2:B:507:LYS:HA	2:B:533:LYS:HD2	2.01	0.42
2:B:65:GLN:OE1	2:B:211:ILE:CD1	2.68	0.42
1:A:20:LEU:C	1:A:22:GLU:N	2.73	0.42
2:B:232:GLU:CD	2:B:316:CYS:CA	2.73	0.42
2:B:342:THR:HA	2:B:356:GLU:HG2	2.02	0.42
1:A:155:ILE:C	1:A:170:CYS:HB3	2.40	0.42
1:A:169:HIS:O	1:A:174:VAL:N	2.53	0.42
1:A:194:ASP:N	1:A:194:ASP:OD1	2.53	0.42
2:B:18:VAL:CG1	2:B:156:ASN:OD1	2.68	0.42
2:B:222:ARG:HB2	2:B:222:ARG:HH11	1.85	0.42
2:B:455:VAL:O	2:B:456:ALA:C	2.58	0.42
2:B:455:VAL:HG23	2:B:456:ALA:N	2.35	0.42
2:B:453:LYS:CE	2:B:457:ARG:HH21	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:VAL:O	2:B:46:VAL:HG12	2.20	0.42
2:B:490:VAL:HG21	2:B:498:VAL:HG22	2.02	0.42
1:A:78:LEU:O	1:A:79:LEU:C	2.57	0.42
2:B:190:GLN:NE2	2:B:383:LEU:HD11	2.35	0.42
2:B:405:LEU:HD22	2:B:417:VAL:HG21	2.02	0.42
2:B:65:GLN:HG2	2:B:66:VAL:N	2.30	0.42
1:A:206:MET:HG2	1:A:343:GLN:NE2	2.34	0.42
1:A:26:LYS:HB2	1:A:26:LYS:HE3	1.78	0.42
2:B:21:PHE:CD1	2:B:21:PHE:C	2.92	0.42
2:B:232:GLU:OE2	2:B:316:CYS:CA	2.65	0.42
2:B:500:ASP:HB3	2:B:503:PRO:CD	2.50	0.42
2:B:359:MET:HE1	2:B:455:VAL:CG2	2.34	0.41
2:B:445:LYS:C	2:B:447:GLU:N	2.73	0.41
2:B:480:THR:O	2:B:480:THR:HG22	2.20	0.41
1:A:180:GLN:O	1:A:182:PRO:HD3	2.19	0.41
1:A:71:THR:HA	2:B:478:ILE:HD13	2.02	0.41
2:B:323:ASP:O	2:B:326:TYR:HB3	2.19	0.41
2:B:34:ALA:N	2:B:35:PRO:CD	2.83	0.41
2:B:531:LYS:CG	2:B:581:SER:HB2	2.49	0.41
1:A:118:GLU:O	1:A:120:GLY:N	2.54	0.41
1:A:309:ASP:O	1:A:312:ALA:HB3	2.20	0.41
2:B:263:ARG:HH11	2:B:271:LEU:HD11	1.83	0.41
2:B:307:VAL:CG1	2:B:307:VAL:O	2.67	0.41
2:B:309:ILE:O	2:B:310:MET:O	2.37	0.41
2:B:329:LEU:O	2:B:330:GLU:C	2.59	0.41
2:B:39:ILE:HG23	2:B:40:THR:N	2.35	0.41
2:B:434:SER:O	2:B:435:LYS:C	2.59	0.41
1:A:159:GLU:HG3	1:A:160:GLN:H	1.83	0.41
1:A:185:VAL:HG21	1:A:236:ARG:CB	2.40	0.41
1:A:41:LEU:HD22	1:A:68:SER:O	2.20	0.41
2:B:131:HIS:HB2	2:B:132:THR:H	1.74	0.41
2:B:417:VAL:O	2:B:418:ILE:CB	2.68	0.41
2:B:478:ILE:C	2:B:479:ILE:HG13	2.41	0.41
2:B:543:ARG:HB2	2:B:602:LEU:HB2	2.03	0.41
1:A:135:LEU:O	1:A:140:PHE:HE1	2.03	0.41
2:B:110:ARG:HB3	2:B:111:GLY:H	1.51	0.41
2:B:178:LEU:HA	2:B:178:LEU:HD12	1.83	0.41
2:B:30:GLY:O	2:B:31:PHE:CD1	2.73	0.41
2:B:343:ARG:NH1	2:B:447:GLU:OE2	2.54	0.41
1:A:138:GLU:HB2	1:A:236:ARG:HH12	1.86	0.41
1:A:158:THR:H	1:A:189:GLU:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LYS:O	1:A:163:ARG:C	2.58	0.41
1:A:154:PRO:HA	1:A:171:GLN:HA	2.02	0.41
1:A:180:GLN:O	1:A:181:ILE:C	2.58	0.41
1:A:215:PHE:CE2	1:A:219:TYR:HD2	2.38	0.41
1:A:321:ARG:HA	1:A:321:ARG:HD3	1.89	0.41
2:B:118:SER:O	2:B:121:VAL:HG23	2.21	0.41
2:B:483:LEU:HB3	2:B:484:PRO:CD	2.51	0.41
2:B:556:LYS:N	2:B:556:LYS:HD3	2.36	0.41
2:B:167:ASP:O	2:B:168:TRP:CD1	2.73	0.41
2:B:381:PRO:HB2	2:B:382:LEU:H	1.61	0.41
2:B:44:GLU:O	2:B:47:ASP:N	2.42	0.41
1:A:240:ARG:HG2	1:A:240:ARG:O	2.20	0.41
1:A:31:PHE:HE1	1:A:32:GLU:HG3	1.77	0.41
2:B:153:THR:O	2:B:155:THR:N	2.54	0.41
2:B:188:ARG:CG	2:B:189:ARG:H	2.32	0.41
2:B:309:ILE:CG2	2:B:310:MET:N	2.81	0.41
2:B:365:LEU:CD1	2:B:417:VAL:O	2.69	0.41
2:B:615:ALA:O	2:B:616:LYS:CB	2.68	0.41
1:A:193:HIS:CG	1:A:193:HIS:O	2.73	0.41
1:A:346:PHE:CB	1:A:354:VAL:HG22	2.50	0.41
2:B:161:LEU:O	2:B:162:VAL:HG22	2.20	0.41
2:B:262:LEU:HD13	2:B:274:ALA:HA	2.02	0.41
2:B:267:CYS:O	2:B:268:LYS:C	2.59	0.41
2:B:27:GLN:HE21	2:B:27:GLN:C	2.24	0.41
2:B:462:TYR:O	2:B:466:GLN:N	2.28	0.41
2:B:544:VAL:HG12	2:B:544:VAL:O	2.19	0.41
1:A:20:LEU:HB2	1:A:135:LEU:HD11	2.01	0.41
1:A:245:LEU:HD13	1:A:247:ILE:HD12	2.02	0.41
1:A:300:LEU:HD11	1:A:346:PHE:CD2	2.56	0.41
1:A:340:LYS:O	1:A:341:ALA:HB2	2.21	0.41
2:B:307:VAL:CG2	2:B:309:ILE:HD11	2.34	0.41
2:B:345:PRO:HB3	2:B:354:VAL:CG1	2.51	0.41
2:B:470:LYS:O	2:B:472:ARG:N	2.50	0.41
2:B:512:LEU:N	2:B:512:LEU:HD23	2.36	0.41
2:B:561:VAL:HG22	2:B:570:TYR:CE1	2.56	0.41
1:A:245:LEU:HB3	1:A:247:ILE:CD1	2.51	0.41
1:A:357:VAL:O	1:A:361:ASN:HB2	2.20	0.41
1:A:68:SER:O	1:A:69:ALA:HB3	2.20	0.41
1:A:72:VAL:HA	2:B:481:LYS:HZ2	1.86	0.41
2:B:25:ASN:C	2:B:27:GLN:N	2.74	0.41
2:B:31:PHE:CE2	2:B:123:TYR:CG	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ARG:HB2	2:B:384:TYR:OH	2.21	0.41
2:B:355:VAL:HG13	2:B:422:HIS:O	2.21	0.41
2:B:390:VAL:HB	2:B:438:ILE:HB	2.02	0.41
1:A:21:LEU:HD23	1:A:21:LEU:C	2.41	0.40
1:A:258:TRP:CZ3	1:A:261:ARG:CZ	3.05	0.40
2:B:202:VAL:C	2:B:204:PRO:CD	2.85	0.40
2:B:309:ILE:O	2:B:310:MET:C	2.59	0.40
2:B:417:VAL:CG1	2:B:418:ILE:H	2.24	0.40
2:B:80:ASP:HB2	2:B:174:THR:H	1.85	0.40
1:A:17:ARG:NH1	1:A:17:ARG:HG3	2.36	0.40
1:A:231:ALA:HA	1:A:235:ARG:CZ	2.51	0.40
2:B:44:GLU:OE1	2:B:116:GLY:HA2	2.20	0.40
2:B:96:LYS:CB	2:B:118:SER:OG	2.70	0.40
2:B:425:SER:O	2:B:426:ILE:C	2.59	0.40
2:B:42:VAL:C	2:B:44:GLU:H	2.24	0.40
2:B:484:PRO:O	2:B:487:ALA:HB3	2.21	0.40
2:B:516:ARG:NH2	2:B:546:GLU:OE1	2.54	0.40
2:B:576:ALA:HB1	2:B:580:SER:CB	2.48	0.40
2:B:148:GLU:HG3	2:B:162:VAL:HG21	2.02	0.40
2:B:246:LEU:O	2:B:250:LEU:HG	2.22	0.40
2:B:58:ILE:O	2:B:60:PRO:CD	2.68	0.40
1:A:235:ARG:O	1:A:237:ILE:N	2.54	0.40
1:A:76:PHE:CE2	2:B:481:LYS:HE2	2.56	0.40
2:B:208:ILE:HB	2:B:220:PHE:HB2	2.04	0.40
2:B:224:THR:HG22	2:B:224:THR:O	2.22	0.40
2:B:284:ASP:C	2:B:286:GLU:H	2.25	0.40
2:B:320:ILE:HA	2:B:320:ILE:HD13	1.91	0.40
2:B:333:THR:HB	2:B:334:THR:H	1.47	0.40
2:B:497:ASP:O	2:B:499:PRO:CD	2.51	0.40
1:A:147:ASP:HB2	1:A:180:GLN:NE2	2.37	0.40
1:A:346:PHE:HB2	1:A:354:VAL:CG2	2.52	0.40
1:A:357:VAL:O	1:A:360:PRO:HG2	2.21	0.40
1:A:80:LYS:HG2	1:A:114:ALA:O	2.21	0.40
2:B:401:LYS:HZ2	2:B:406:ASN:CG	2.24	0.40
2:B:425:SER:OG	2:B:427:ASN:O	2.31	0.40
2:B:430:PHE:CD1	2:B:435:LYS:HG2	2.57	0.40
2:B:65:GLN:HB3	2:B:77:ILE:HD13	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	303/369 (82%)	163 (54%)	78 (26%)	62 (20%)	0	2
2	B	566/621 (91%)	339 (60%)	122 (22%)	105 (19%)	0	2
All	All	869/990 (88%)	502 (58%)	200 (23%)	167 (19%)	0	2

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	72	VAL
1	A	97	ARG
1	A	112	ASP
1	A	113	TYR
1	A	115	LYS
1	A	123	ASP
1	A	124	ARG
1	A	137	ARG
1	A	146	GLU
1	A	160	GLN
1	A	192	LYS
1	A	215	PHE
1	A	280	MET
1	A	282	THR
1	A	300	LEU
2	B	12	LYS
2	B	14	LYS
2	B	26	ARG
2	B	58	ILE
2	B	66	VAL
2	B	81	ASN
2	B	115	ILE
2	B	116	GLY
2	B	117	ILE

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Mol	Chain	Res	Type
2	B	131	HIS
2	B	132	THR
2	B	152	ASN
2	B	153	THR
2	B	158	PRO
2	B	159	ASP
2	B	168	TRP
2	B	169	PHE
2	B	171	PRO
2	B	172	HIS
2	B	185	VAL
2	B	189	ARG
2	B	190	GLN
2	B	224	THR
2	B	225	ASP
2	B	251	HIS
2	B	267	CYS
2	B	310	MET
2	B	349	SER
2	B	362	GLY
2	B	367	LYS
2	B	381	PRO
2	B	382	LEU
2	B	385	GLN
2	B	400	TRP
2	B	418	ILE
2	B	440	ASP
2	B	491	ALA
2	B	494	LEU
2	B	496	LYS
2	B	498	VAL
2	B	551	LYS
2	B	560	LYS
2	B	589	GLU
2	B	592	SER
2	B	603	ILE
1	A	16	ALA
1	A	39	VAL
1	A	70	LYS
1	A	83	TYR
1	A	84	ALA
1	A	85	THR

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Mol	Chain	Res	Type
1	A	119	GLN
1	A	141	HIS
1	A	149	ALA
1	A	150	THR
1	A	155	ILE
1	A	175	GLY
1	A	183	PHE
1	A	205	GLY
1	A	227	LYS
1	A	232	ARG
1	A	233	SER
1	A	254	ASP
1	A	290	LEU
1	A	299	GLU
1	A	366	MET
2	B	17	SER
2	B	31	PHE
2	B	52	ALA
2	B	54	GLU
2	B	104	HIS
2	B	111	GLY
2	B	114	GLY
2	B	140	PRO
2	B	155	THR
2	B	289	PRO
2	B	312	PRO
2	B	365	LEU
2	B	403	TYR
2	B	431	THR
2	B	435	LYS
2	B	456	ALA
2	B	497	ASP
2	B	500	ASP
2	B	512	LEU
2	B	524	GLY
2	B	546	GLU
2	B	593	GLU
2	B	598	LYS
2	B	604	VAL
1	A	102	ARG
1	A	144	PRO
1	A	203	THR

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Mol	Chain	Res	Type
1	A	341	ALA
1	A	342	GLU
2	B	23	GLU
2	B	32	ASP
2	B	45	ALA
2	B	238	PRO
2	B	426	ILE
2	B	432	SER
2	B	449	ASP
2	B	454	GLU
2	B	586	TYR
2	B	595	GLU
2	B	596	LEU
1	A	37	PRO
1	A	42	PRO
1	A	86	ASP
1	A	96	ASN
1	A	114	ALA
1	A	184	ASN
1	A	234	THR
1	A	236	ARG
1	A	268	TYR
2	B	21	PHE
2	B	80	ASP
2	B	113	GLN
2	B	188	ARG
2	B	250	LEU
2	B	285	PRO
2	B	333	THR
2	B	402	GLN
2	B	471	LYS
2	B	499	PRO
2	B	521	ASN
2	B	557	PRO
2	B	558	GLU
1	A	30	GLN
1	A	89	ILE
1	A	212	GLU
1	A	218	ALA
1	A	336	ASP
2	B	15	SER
2	B	204	PRO

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Mol	Chain	Res	Type
2	B	313	PRO
2	B	334	THR
2	B	433	GLU
2	B	550	CYS
2	B	588	ILE
1	A	190	PHE
1	A	320	PRO
2	B	483	LEU
2	B	412	ILE
2	B	417	VAL
1	A	182	PRO
1	A	337	ILE
2	B	559	PRO
1	A	295	ILE
1	A	292	PRO
2	B	478	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	268/315 (85%)	240 (90%)	28 (10%)	8	37
2	B	486/527 (92%)	428 (88%)	58 (12%)	6	32
All	All	754/842 (90%)	668 (89%)	86 (11%)	7	33

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	28	TYR
1	A	76	PHE
1	A	111	TRP
1	A	118	GLU
1	A	140	PHE
1	A	143	ARG

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Mol	Chain	Res	Type
1	A	145	GLU
1	A	174	VAL
1	A	176	GLU
1	A	182	PRO
1	A	183	PHE
1	A	187	ASN
1	A	194	ASP
1	A	203	THR
1	A	210	LEU
1	A	215	PHE
1	A	219	TYR
1	A	260	TYR
1	A	261	ARG
1	A	268	TYR
1	A	286	LYS
1	A	305	LEU
1	A	319	ASP
1	A	322	PHE
1	A	325	ASP
1	A	352	ASP
1	A	355	THR
2	B	21	PHE
2	B	27	GLN
2	B	29	LEU
2	B	58	ILE
2	B	64	VAL
2	B	79	GLU
2	B	83	PRO
2	B	89	GLN
2	B	97	LEU
2	B	99	TYR
2	B	109	SER
2	B	115	ILE
2	B	117	ILE
2	B	121	VAL
2	B	137	LYS
2	B	159	ASP
2	B	161	LEU
2	B	166	ARG
2	B	169	PHE
2	B	170	ARG
2	B	171	PRO

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Mol	Chain	Res	Type
2	B	175	GLN
2	B	178	LEU
2	B	179	GLU
2	B	185	VAL
2	B	210	LEU
2	B	214	ASP
2	B	216	ASN
2	B	218	GLU
2	B	261	PHE
2	B	308	LYS
2	B	310	MET
2	B	315	ASP
2	B	333	THR
2	B	334	THR
2	B	366	PRO
2	B	373	ILE
2	B	383	LEU
2	B	391	THR
2	B	397	ASP
2	B	402	GLN
2	B	403	TYR
2	B	436	ASP
2	B	461	HIS
2	B	473	ARG
2	B	492	HIS
2	B	502	ASN
2	B	513	LEU
2	B	516	ARG
2	B	521	ASN
2	B	527	ASP
2	B	540	TYR
2	B	542	PHE
2	B	548	LEU
2	B	551	LYS
2	B	556	LYS
2	B	564	MET
2	B	599	LEU

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	77	GLN

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Mol	Chain	Res	Type
1	A	90	ASN
1	A	119	GLN
1	A	187	ASN
1	A	193	HIS
1	A	332	GLN
1	A	344	GLN
2	B	25	ASN
2	B	48	ASN
2	B	81	ASN
2	B	152	ASN
2	B	175	GLN
2	B	190	GLN
2	B	378	ASN
2	B	406	ASN
2	B	502	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/369 (85%)	-0.04	1 (0%) 93 91	139, 217, 258, 265	0
2	B	582/621 (93%)	-0.06	0 100 100	93, 175, 248, 265	0
All	All	897/990 (90%)	-0.05	1 (0%) 95 94	93, 192, 254, 265	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.