



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:40 PM UTC

PDB ID : 3IKL / pdb_00003ikl
Title : Crystal structure of Pol gB delta-I4.
Authors : Lee, Y.S.; Kennedy, W.D.; Yin, Y.W.
Deposited on : 2009-08-06
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

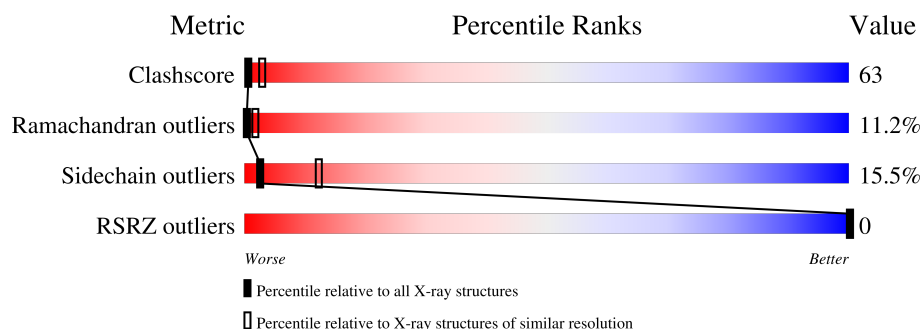
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	459	
1	B	459	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5866 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 DNA polymerase subunit gamma-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2931	1877	515	523	16			
1	B	364	Total	C	N	O	S	0	0	0
			2935	1880	517	522	16			

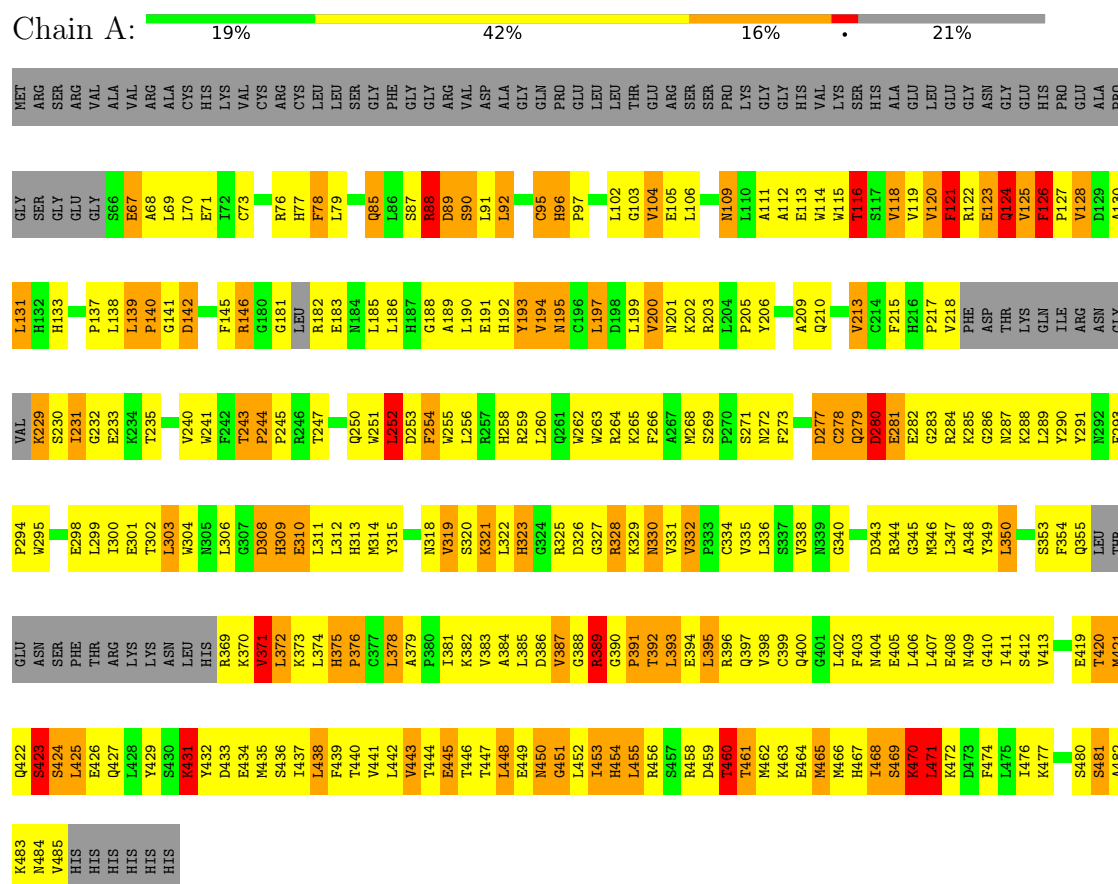
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLY	-	linker	UNP Q9UHN1
A	181	GLY	-	linker	UNP Q9UHN1
A	486	HIS	-	expression tag	UNP Q9UHN1
A	487	HIS	-	expression tag	UNP Q9UHN1
A	488	HIS	-	expression tag	UNP Q9UHN1
A	489	HIS	-	expression tag	UNP Q9UHN1
A	490	HIS	-	expression tag	UNP Q9UHN1
A	491	HIS	-	expression tag	UNP Q9UHN1
B	180	GLY	-	linker	UNP Q9UHN1
B	181	GLY	-	linker	UNP Q9UHN1
B	486	HIS	-	expression tag	UNP Q9UHN1
B	487	HIS	-	expression tag	UNP Q9UHN1
B	488	HIS	-	expression tag	UNP Q9UHN1
B	489	HIS	-	expression tag	UNP Q9UHN1
B	490	HIS	-	expression tag	UNP Q9UHN1
B	491	HIS	-	expression tag	UNP Q9UHN1

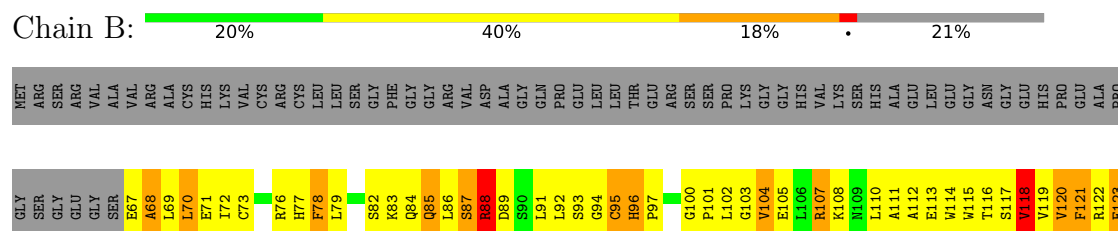
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA polymerase subunit gamma-2, mitochondrial



- Molecule 1: DNA polymerase subunit gamma-2, mitochondrial



HIS	G416	S353	L289	ARG	Q124
HIS	Y417	F354	Y290	ASN	V125
HIS	L418	Q355	Y291	GLY	F126
	E419	LEU		VAL	P127
	T420	THR	P294	K229	V128
	M421	GLU	W295	S230	D129
	Q422	ASN	G286	I231	A130
	S423	SER	K297	G232	L131
	S424	PHE	E298	E233	H132
	L425	THR	L299	K234	H133
	E426	ARG	I300		K134
	Q427	LYS	E301	V240	P135
	L428	LYS	T302	W241	G136
		ASN	L303	F242	P137
		LEU	W304	T243	L138
	K431	H368	N305	P244	L139
	Y432	R369	L306	P245	
	D433	K370	G307	R246	F145
		V371	I308	T247	R146
	L437	L372	H309	S248	G180
	L438	K373	E310	N249	G181
	L439	L374	L311	Q250	LEU
	T440	H375	L312	W251	R182
	V441		H313	L252	E183
	L442	P376	M314	D253	
	V443	G377	Y315	P254	L186
	T444	L378		W255	
	E445		N318	L256	A189
	T446	K382	V319	R257	L190
	T447	V383	S320	H258	E191
	L448	A384	K321	R259	H192
	E449	L385	L322	L260	Y193
		D386	H323	Q261	V194
	L452	V387	G324	W262	
	L453	G388	R325	W263	L197
	H454	R389	D326	R264	D198
	L455	G390	G327	K265	L199
	R456	P391	R328	F266	V200
	S457	T392	K329	A267	N201
	R458	L393	N330	M268	K202
	D459	E394	V331	S269	R203
	T460	L395	V332	P270	
	T461	R396	P333	S271	Y206
	M462	Q397	C334	N272	G207
		V398	V335	F273	L268
	M465	C399	L336	S274	A209
	M466	Q400	G401	S275	Q210
	K472	L402	V338	S276	
	D473	F403	N339	D277	V213
		M404	G340	C278	C214
	K477	E405	D341	Q279	F215
	Y478	L406		D280	H216
	L479	L407	R344	E281	P217
	S480	E408	G345	E282	V218
	S481		M346	G283	PHE
			L347	R284	ASP
			A348	K285	THR
	M484	I411		G286	LYS
	V485	S412		N287	GLN
	HIS	V413	Y351		ILE
		W414	D352		
		P415			

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	64.43Å 64.43Å 260.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.82 – 3.10 45.82 – 3.10	Depositor EDS
% Data completeness (in resolution range)	74.6 (45.82-3.10) 74.7 (45.82-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.294 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5866	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	0/3006	1.18	40/4067 (1.0%)
1	B	0.54	0/3011	1.17	37/4074 (0.9%)
All	All	0.55	0/6017	1.17	77/8141 (0.9%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	PHE	N-CA-C	-10.24	101.28	113.88
1	B	197	LEU	N-CA-C	-9.77	101.87	113.88
1	B	332	VAL	CA-C-N	9.16	129.72	119.92
1	B	332	VAL	C-N-CA	9.16	129.72	119.92
1	B	78	PHE	N-CA-C	-9.02	102.78	113.88
1	A	77	HIS	N-CA-C	8.82	121.23	110.91
1	B	282	GLU	N-CA-C	-8.51	103.40	112.93
1	B	400	GLN	N-CA-C	-8.08	103.88	114.31
1	A	431	LYS	N-CA-C	-7.93	102.57	112.72
1	B	375	HIS	CA-C-N	7.75	129.53	119.84
1	B	375	HIS	C-N-CA	7.75	129.53	119.84
1	A	281	GLU	N-CA-C	-7.57	99.51	111.02
1	A	124	GLN	N-CA-C	-7.56	94.69	110.80
1	A	215	PHE	N-CA-C	7.46	121.08	108.02
1	A	269	SER	CA-C-N	7.24	127.57	119.32
1	A	269	SER	C-N-CA	7.24	127.57	119.32
1	B	387	VAL	N-CA-C	7.20	120.47	108.81
1	B	441	VAL	N-CA-C	7.11	118.12	108.17
1	B	307	GLY	N-CA-C	-6.98	103.89	112.33
1	A	471	LEU	N-CA-C	-6.94	103.41	110.97
1	A	126	PHE	N-CA-C	6.84	119.23	108.55
1	A	139	LEU	CA-C-N	6.80	128.35	119.84
1	A	139	LEU	C-N-CA	6.80	128.35	119.84
1	A	470	LYS	N-CA-C	-6.74	105.09	113.38
1	A	282	GLU	N-CA-C	-6.68	102.33	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ARG	N-CA-C	6.34	120.12	108.58
1	B	207	GLY	N-CA-C	6.32	121.68	111.38
1	A	268	MET	N-CA-C	-6.29	105.18	112.92
1	B	333	PRO	N-CA-C	6.28	121.08	111.34
1	A	279	GLN	N-CA-C	6.18	118.17	108.96
1	A	197	LEU	N-CA-C	-6.15	105.27	112.89
1	B	397	GLN	N-CA-C	-6.15	105.91	113.41
1	A	424	SER	CB-CA-C	-6.07	108.97	117.23
1	B	425	LEU	N-CA-C	-6.05	104.61	112.23
1	A	243	THR	N-CA-C	6.02	117.94	108.55
1	B	407	LEU	N-CA-C	-5.97	104.69	111.07
1	B	231	ILE	N-CA-C	5.95	116.50	108.17
1	B	272	ASN	N-CA-C	-5.95	104.49	113.89
1	A	139	LEU	N-CA-C	5.78	117.97	110.40
1	B	376	PRO	N-CA-C	5.78	124.37	112.47
1	B	268	MET	N-CA-C	-5.77	105.83	112.92
1	A	272	ASN	N-CA-C	-5.75	106.26	113.28
1	B	124	GLN	N-CA-C	-5.74	98.57	110.80
1	B	398	VAL	N-CA-C	-5.74	103.75	111.44
1	B	243	THR	N-CA-C	5.72	117.49	108.23
1	A	183	GLU	N-CA-C	-5.68	102.87	111.56
1	A	426	GLU	N-CA-C	-5.68	105.01	111.14
1	B	216	HIS	CA-C-N	5.66	125.58	119.76
1	B	216	HIS	C-N-CA	5.66	125.58	119.76
1	A	375	HIS	CA-C-N	5.63	126.88	119.84
1	A	375	HIS	C-N-CA	5.63	126.88	119.84
1	A	252	LEU	N-CA-C	-5.59	105.09	111.07
1	A	116	THR	N-CA-C	-5.59	105.96	112.89
1	B	304	TRP	N-CA-C	5.53	117.42	108.41
1	B	313	HIS	N-CA-C	-5.52	105.34	111.36
1	A	332	VAL	CA-C-N	5.50	126.71	119.84
1	A	332	VAL	C-N-CA	5.50	126.71	119.84
1	B	458	ARG	N-CA-C	-5.48	99.13	110.80
1	A	453	ILE	N-CA-C	-5.48	102.14	108.82
1	A	319	VAL	N-CA-C	-5.46	107.03	113.42
1	A	387	VAL	N-CA-C	5.46	115.55	108.35
1	B	433	ASP	N-CA-C	-5.44	105.38	112.23
1	B	139	LEU	CA-C-N	5.41	126.60	119.84
1	B	139	LEU	C-N-CA	5.41	126.60	119.84
1	B	279	GLN	N-CA-C	5.34	116.76	109.18
1	B	253	ASP	N-CA-C	-5.29	105.60	111.36
1	B	339	ASN	N-CA-C	5.22	116.92	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	VAL	N-CA-C	5.20	120.15	109.34
1	A	465	MET	N-CA-C	-5.19	101.52	109.41
1	B	465	MET	N-CA-C	-5.16	103.11	110.59
1	A	350	LEU	N-CA-C	5.15	116.70	111.14
1	B	394	GLU	N-CA-C	-5.12	105.83	111.71
1	A	194	VAL	N-CA-C	5.12	118.30	111.44
1	A	125	VAL	N-CA-C	-5.08	100.93	108.45
1	A	244	PRO	N-CA-C	-5.08	104.50	110.70
1	A	413	VAL	N-CA-C	5.03	115.36	108.12
1	A	423	SER	N-CA-C	-5.02	104.50	111.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2931	0	2915	399	0
1	B	2935	0	2917	344	0
All	All	5866	0	5832	732	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 63.

All (732) 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:231:ILE:H	1:A:231:ILE:HD12	1.16	1.10
1:A:280:ASP:H	1:A:284:ARG:HA	1.23	1.03
1:B:392:THR:HG22	1:B:393:LEU:H	1.24	1.03
1:A:448:LEU:HD23	1:A:448:LEU:H	1.23	1.02
1:A:450:ASN:HD21	1:A:452:LEU:HB2	1.24	1.01
1:B:303:LEU:HG	1:B:338:VAL:HG22	1.43	0.99
1:B:454:HIS:HE1	1:B:465:MET:HG2	1.27	0.99
1:A:88:ARG:HA	1:A:91:LEU:HD12	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:VAL:HG12	1:A:455:LEU:HB3	1.43	0.95
1:B:395:LEU:O	1:B:398:VAL:HG12	1.66	0.94
1:A:320:SER:HA	1:A:323:HIS:NE2	1.81	0.94
1:A:197:LEU:HD11	1:A:202:LYS:HG3	1.48	0.94
1:B:438:LEU:O	1:B:458:ARG:HB2	1.68	0.93
1:A:186:LEU:HD11	1:A:306:LEU:HD11	1.51	0.91
1:A:391:PRO:HD2	1:A:395:LEU:HD21	1.51	0.91
1:A:303:LEU:HD11	1:A:338:VAL:HG13	1.52	0.89
1:A:88:ARG:HD2	1:A:88:ARG:N	1.88	0.88
1:A:201:ASN:HD22	1:A:203:ARG:NH2	1.69	0.88
1:A:369:ARG:HH21	1:A:371:VAL:HG21	1.37	0.88
1:A:388:GLY:O	1:A:390:GLY:N	2.07	0.87
1:B:445:GLU:C	1:B:447:THR:H	1.82	0.86
1:B:454:HIS:CE1	1:B:465:MET:HG2	2.10	0.86
1:A:431:LYS:HB2	1:A:431:LYS:NZ	1.92	0.85
1:A:389:ARG:HH11	1:A:444:THR:HG21	1.39	0.84
1:B:121:PHE:O	1:B:122:ARG:HG2	1.78	0.84
1:B:406:LEU:HD12	1:B:406:LEU:H	1.39	0.84
1:B:252:LEU:HB2	1:B:336:LEU:HD11	1.57	0.84
1:B:406:LEU:H	1:B:406:LEU:CD1	1.90	0.83
1:A:67:GLU:HG2	1:A:69:LEU:H	1.42	0.83
1:A:450:ASN:ND2	1:A:452:LEU:HB2	1.92	0.83
1:B:280:ASP:HA	1:B:284:ARG:HH21	1.43	0.83
1:A:393:LEU:HD23	1:A:397:GLN:HG3	1.60	0.83
1:A:256:LEU:HD22	1:A:287:ASN:ND2	1.94	0.82
1:A:421:MET:HG3	1:A:422:GLN:H	1.43	0.82
1:A:201:ASN:HD22	1:A:203:ARG:HH22	1.24	0.82
1:A:116:THR:HA	1:A:120:VAL:CG2	2.10	0.82
1:A:243:THR:HG23	1:A:334:CYS:HB2	1.62	0.81
1:A:394:GLU:O	1:A:397:GLN:HB2	1.81	0.81
1:B:134:LYS:H	1:B:180:GLY:HA2	1.46	0.81
1:A:381:ILE:HD11	1:A:437:ILE:HD12	1.62	0.81
1:A:448:LEU:HD23	1:A:448:LEU:N	1.96	0.80
1:B:320:SER:HA	1:B:323:HIS:CD2	2.17	0.80
1:B:122:ARG:HB3	1:B:122:ARG:NH1	1.97	0.80
1:A:450:ASN:HD22	1:A:452:LEU:HD23	1.46	0.80
1:B:128:VAL:HG13	1:B:210:GLN:HB2	1.65	0.79
1:A:385:LEU:HD23	1:A:385:LEU:H	1.45	0.79
1:A:419:GLU:HG3	1:A:420:THR:H	1.49	0.77
1:A:231:ILE:H	1:A:231:ILE:CD1	1.96	0.77
1:B:301:GLU:OE2	1:B:340:GLY:HA3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:HB3	1:B:122:ARG:HH11	1.48	0.77
1:B:445:GLU:HA	1:B:445:GLU:OE1	1.83	0.77
1:A:353:SER:HB3	1:A:374:LEU:HD23	1.67	0.77
1:B:406:LEU:HD12	1:B:406:LEU:N	1.98	0.77
1:A:396:ARG:HA	1:A:399:CYS:HB2	1.65	0.77
1:B:122:ARG:O	1:B:124:GLN:HG3	1.85	0.77
1:A:455:LEU:HD11	1:A:474:PHE:HE2	1.49	0.77
1:A:231:ILE:HD12	1:A:231:ILE:N	1.97	0.76
1:A:389:ARG:NH1	1:A:444:THR:HG21	1.98	0.76
1:B:373:LYS:HE2	1:B:459:ASP:HA	1.64	0.76
1:A:303:LEU:HG	1:A:338:VAL:HG22	1.66	0.76
1:A:421:MET:CG	1:A:422:GLN:H	1.95	0.76
1:B:249:ASN:CG	1:B:250:GLN:N	2.44	0.76
1:B:477:LYS:HA	1:B:480:SER:HB3	1.68	0.75
1:B:122:ARG:HB2	1:B:124:GLN:NE2	2.00	0.75
1:A:389:ARG:HD2	1:A:444:THR:HB	1.69	0.75
1:A:454:HIS:CD2	1:A:465:MET:HE3	2.22	0.75
1:B:310:GLU:CD	1:B:310:GLU:H	1.94	0.75
1:B:384:ALA:O	1:B:385:LEU:HB3	1.86	0.75
1:B:229:LYS:HE2	1:B:229:LYS:HA	1.70	0.74
1:B:392:THR:HG22	1:B:393:LEU:N	2.02	0.74
1:A:131:LEU:HD21	1:B:97:PRO:O	1.88	0.74
1:B:280:ASP:O	1:B:281:GLU:HB2	1.87	0.74
1:A:69:LEU:HD13	1:A:354:PHE:CD2	2.23	0.74
1:A:116:THR:HG23	1:A:120:VAL:HG21	1.71	0.73
1:A:280:ASP:N	1:A:284:ARG:HA	2.00	0.73
1:B:389:ARG:HG2	1:B:444:THR:HB	1.69	0.73
1:A:370:LYS:O	1:A:371:VAL:HG12	1.87	0.72
1:B:257:ARG:HB3	1:B:257:ARG:NH2	2.04	0.72
1:B:128:VAL:HG22	1:B:129:ASP:N	2.05	0.71
1:A:441:VAL:CG1	1:A:455:LEU:HB3	2.20	0.71
1:A:444:THR:OG1	1:A:446:THR:HG22	1.91	0.71
1:B:256:LEU:HD22	1:B:287:ASN:ND2	2.06	0.71
1:B:134:LYS:H	1:B:180:GLY:CA	2.03	0.71
1:B:289:LEU:HB2	1:B:301:GLU:HB3	1.72	0.71
1:B:257:ARG:HB3	1:B:257:ARG:HH21	1.54	0.71
1:B:325:ARG:HA	1:B:329:LYS:O	1.90	0.71
1:B:420:THR:HG23	1:B:421:MET:H	1.54	0.71
1:A:303:LEU:CD1	1:A:338:VAL:HG13	2.20	0.71
1:A:243:THR:HG22	1:A:334:CYS:O	1.91	0.71
1:A:325:ARG:HG2	1:A:325:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TYR:O	1:A:437:ILE:HG12	1.91	0.70
1:A:391:PRO:CD	1:A:395:LEU:HD21	2.21	0.70
1:A:116:THR:HA	1:A:120:VAL:HG23	1.73	0.69
1:A:133:HIS:HA	1:A:181:GLY:HA2	1.74	0.69
1:A:327:GLY:O	1:A:328:ARG:HB2	1.91	0.69
1:B:197:LEU:HD11	1:B:202:LYS:HA	1.72	0.69
1:A:393:LEU:O	1:A:397:GLN:HG2	1.92	0.69
1:A:375:HIS:ND1	1:A:376:PRO:HD2	2.07	0.69
1:B:191:GLU:HA	1:B:314:MET:HE1	1.74	0.69
1:B:291:TYR:OH	1:B:352:ASP:HB2	1.91	0.69
1:B:294:PRO:HD2	1:B:295:TRP:CZ3	2.28	0.69
1:B:91:LEU:HD13	1:B:96:HIS:HB3	1.75	0.69
1:A:318:ASN:ND2	1:A:319:VAL:H	1.91	0.69
1:B:420:THR:HG23	1:B:421:MET:N	2.08	0.69
1:A:262:TRP:O	1:A:265:LYS:HB3	1.93	0.69
1:A:231:ILE:HG22	1:A:232:GLY:H	1.59	0.68
1:A:421:MET:HG3	1:A:422:GLN:N	2.07	0.68
1:B:422:GLN:HG3	1:B:423:SER:N	2.07	0.68
1:A:251:TRP:O	1:A:254:PHE:HB3	1.93	0.68
1:A:382:LYS:N	1:A:382:LYS:HD2	2.08	0.68
1:B:260:LEU:HD13	1:B:275:SER:HB3	1.76	0.68
1:A:411:ILE:HD11	1:A:476:ILE:CD1	2.23	0.68
1:A:431:LYS:HB2	1:A:431:LYS:HZ2	1.56	0.68
1:B:416:GLY:O	1:B:418:LEU:N	2.27	0.68
1:A:468:ILE:HD12	1:A:469:SER:N	2.09	0.68
1:B:128:VAL:CG1	1:B:210:GLN:HB2	2.23	0.67
1:B:415:PRO:HB2	1:B:418:LEU:HD13	1.76	0.67
1:B:197:LEU:C	1:B:199:LEU:H	2.00	0.67
1:A:217:PRO:HB2	1:A:229:LYS:HD3	1.76	0.67
1:A:460:THR:C	1:A:462:MET:H	2.02	0.67
1:A:460:THR:O	1:A:462:MET:N	2.27	0.67
1:B:91:LEU:N	1:B:91:LEU:HD22	2.09	0.67
1:B:112:ALA:O	1:B:116:THR:HG23	1.93	0.67
1:A:393:LEU:HD23	1:A:397:GLN:CG	2.25	0.67
1:B:131:LEU:O	1:B:182:ARG:HD3	1.94	0.67
1:B:460:THR:HB	1:B:462:MET:HG2	1.77	0.67
1:B:256:LEU:HD12	1:B:256:LEU:C	2.20	0.66
1:A:92:LEU:HD22	1:A:344:ARG:CZ	2.25	0.66
1:B:405:GLU:O	1:B:408:GLU:HB2	1.96	0.66
1:A:146:ARG:HA	1:A:146:ARG:HH11	1.60	0.66
1:A:263:TRP:CZ3	1:A:300:ILE:HD12	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:HIS:HB2	1:A:331:VAL:C	2.21	0.66
1:A:450:ASN:ND2	1:A:452:LEU:HD23	2.11	0.66
1:B:193:TYR:CZ	1:B:333:PRO:HG3	2.31	0.66
1:B:402:LEU:O	1:B:406:LEU:HD13	1.96	0.66
1:A:453:ILE:HD12	1:A:454:HIS:N	2.09	0.65
1:A:477:LYS:HA	1:A:480:SER:HB3	1.77	0.65
1:B:445:GLU:O	1:B:447:THR:N	2.30	0.65
1:B:325:ARG:HG2	1:B:325:ARG:HH11	1.61	0.65
1:A:88:ARG:N	1:A:88:ARG:CD	2.53	0.65
1:B:249:ASN:CG	1:B:250:GLN:H	2.03	0.65
1:B:91:LEU:HD22	1:B:91:LEU:H	1.61	0.65
1:B:88:ARG:HD2	1:B:89:ASP:N	2.12	0.64
1:A:123:GLU:O	1:A:124:GLN:HG3	1.97	0.64
1:A:383:VAL:HG22	1:A:384:ALA:N	2.12	0.64
1:A:453:ILE:HD12	1:A:453:ILE:C	2.22	0.64
1:B:303:LEU:HG	1:B:338:VAL:CG2	2.22	0.64
1:A:96:HIS:CD2	1:A:96:HIS:H	2.15	0.64
1:A:325:ARG:NH1	1:A:330:ASN:HD21	1.94	0.64
1:B:115:TRP:CZ2	1:B:119:VAL:HG11	2.33	0.64
1:A:122:ARG:HG3	1:A:122:ARG:O	1.99	0.64
1:A:448:LEU:H	1:A:448:LEU:CD2	1.91	0.63
1:B:392:THR:CG2	1:B:393:LEU:H	2.05	0.63
1:B:128:VAL:HG12	1:B:209:ALA:O	1.98	0.63
1:A:424:SER:OG	1:A:427:GLN:HG3	1.98	0.63
1:B:376:PRO:C	1:B:378:LEU:H	2.06	0.63
1:B:424:SER:HB3	1:B:427:GLN:CG	2.28	0.63
1:A:76:ARG:HB3	1:A:435:MET:HG2	1.79	0.63
1:B:145:PHE:CZ	1:B:217:PRO:HB3	2.34	0.63
1:A:420:THR:OG1	1:A:421:MET:N	2.29	0.63
1:B:457:SER:HB2	1:B:462:MET:HG3	1.80	0.63
1:B:94:GLY:O	1:B:232:GLY:HA2	1.98	0.63
1:B:193:TYR:OH	1:B:333:PRO:HG3	1.97	0.63
1:A:299:LEU:C	1:A:299:LEU:HD23	2.24	0.62
1:A:459:ASP:C	1:A:461:THR:H	2.07	0.62
1:A:199:LEU:HD21	1:B:101:PRO:HG2	1.81	0.62
1:A:259:ARG:HH21	1:A:301:GLU:CD	2.07	0.62
1:B:453:ILE:HD12	1:B:453:ILE:C	2.23	0.62
1:A:182:ARG:HD2	1:A:213:VAL:O	1.99	0.62
1:A:303:LEU:CD1	1:A:338:VAL:HG22	2.29	0.62
1:A:290:TYR:HD1	1:A:299:LEU:HA	1.63	0.62
1:A:437:ILE:O	1:A:438:LEU:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HA	1:B:72:ILE:HD12	1.81	0.62
1:B:424:SER:HB3	1:B:427:GLN:CD	2.25	0.62
1:A:404:ASN:O	1:A:408:GLU:HG2	1.99	0.62
1:B:314:MET:HE3	1:B:315:TYR:CE2	2.33	0.62
1:B:445:GLU:C	1:B:447:THR:N	2.52	0.62
1:B:253:ASP:HB3	1:B:257:ARG:HH12	1.65	0.62
1:B:258:HIS:ND1	1:B:259:ARG:N	2.48	0.62
1:B:88:ARG:CD	1:B:89:ASP:H	2.13	0.61
1:B:180:GLY:O	1:B:181:GLY:C	2.43	0.61
1:B:302:THR:C	1:B:303:LEU:HD12	2.26	0.61
1:A:231:ILE:HB	1:B:133:HIS:NE2	2.16	0.61
1:A:69:LEU:HD13	1:A:354:PHE:CG	2.36	0.61
1:A:325:ARG:NH1	1:A:330:ASN:ND2	2.49	0.61
1:A:321:LYS:C	1:A:322:LEU:HD23	2.26	0.61
1:A:422:GLN:HG3	1:A:424:SER:H	1.66	0.61
1:B:252:LEU:HA	1:B:336:LEU:HD21	1.83	0.61
1:A:309:HIS:O	1:A:310:GLU:C	2.44	0.61
1:A:201:ASN:ND2	1:A:203:ARG:HH22	1.98	0.60
1:A:303:LEU:CG	1:A:338:VAL:HG22	2.31	0.60
1:A:405:GLU:O	1:A:408:GLU:HB2	2.00	0.60
1:A:123:GLU:C	1:A:124:GLN:HG3	2.26	0.60
1:B:301:GLU:OE2	1:B:340:GLY:CA	2.49	0.60
1:A:391:PRO:HG2	1:A:395:LEU:HD23	1.83	0.60
1:A:327:GLY:O	1:A:328:ARG:CB	2.49	0.60
1:A:385:LEU:HD23	1:A:385:LEU:N	2.16	0.60
1:A:404:ASN:O	1:A:408:GLU:CG	2.49	0.60
1:B:252:LEU:C	1:B:252:LEU:HD13	2.26	0.60
1:B:395:LEU:C	1:B:397:GLN:H	2.10	0.60
1:A:450:ASN:CG	1:A:451:GLY:H	2.09	0.60
1:A:88:ARG:CA	1:A:91:LEU:HD12	2.26	0.60
1:A:389:ARG:HD2	1:A:444:THR:CB	2.31	0.60
1:A:455:LEU:HD11	1:A:474:PHE:CE2	2.33	0.60
1:A:199:LEU:HD13	1:B:77:HIS:CD2	2.37	0.60
1:A:306:LEU:HD12	1:A:335:VAL:HG12	1.83	0.59
1:B:322:LEU:N	1:B:322:LEU:HD23	2.18	0.59
1:A:423:SER:O	1:A:427:GLN:HB2	2.03	0.59
1:B:311:LEU:O	1:B:314:MET:HB2	2.03	0.59
1:A:233:GLU:HG3	1:B:133:HIS:HE1	1.68	0.59
1:A:411:ILE:HD11	1:A:476:ILE:HD13	1.84	0.59
1:B:441:VAL:HG12	1:B:455:LEU:CB	2.32	0.59
1:A:102:LEU:HD21	1:A:435:MET:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:HA	1:A:448:LEU:HD21	1.85	0.59
1:B:190:LEU:CB	1:B:314:MET:HE2	2.33	0.59
1:A:262:TRP:O	1:A:265:LYS:CB	2.51	0.58
1:A:277:ASP:OD2	1:A:277:ASP:N	2.36	0.58
1:B:91:LEU:O	1:B:92:LEU:C	2.47	0.58
1:B:286:GLY:HA3	1:B:304:TRP:CE3	2.38	0.58
1:B:325:ARG:HG2	1:B:325:ARG:NH1	2.16	0.58
1:B:331:VAL:HG22	1:B:332:VAL:N	2.18	0.58
1:A:309:HIS:O	1:A:311:LEU:N	2.36	0.58
1:A:432:TYR:CD2	1:A:440:THR:HG23	2.39	0.58
1:B:110:LEU:HD13	1:B:378:LEU:HD11	1.85	0.58
1:B:290:TYR:CD1	1:B:299:LEU:HA	2.38	0.58
1:A:320:SER:C	1:A:322:LEU:H	2.11	0.58
1:B:447:THR:O	1:B:449:GLU:N	2.37	0.58
1:A:279:GLN:HB3	1:A:285:LYS:H	1.68	0.58
1:A:455:LEU:HD23	1:A:455:LEU:H	1.68	0.58
1:A:381:ILE:HA	1:A:412:SER:OG	2.03	0.58
1:A:395:LEU:N	1:A:395:LEU:HD22	2.18	0.58
1:B:371:VAL:HA	1:B:433:ASP:HB3	1.85	0.58
1:A:87:SER:O	1:A:89:ASP:N	2.37	0.58
1:A:243:THR:OG1	1:A:244:PRO:HD2	2.03	0.58
1:A:310:GLU:O	1:A:313:HIS:HB3	2.04	0.58
1:B:87:SER:HB2	1:B:88:ARG:CZ	2.34	0.58
1:B:95:CYS:O	1:B:96:HIS:C	2.47	0.58
1:A:466:MET:CE	1:A:471:LEU:HA	2.34	0.57
1:A:395:LEU:H	1:A:395:LEU:CD2	2.16	0.57
1:A:460:THR:C	1:A:462:MET:N	2.61	0.57
1:B:351:TYR:C	1:B:353:SER:H	2.12	0.57
1:A:139:LEU:HB2	1:A:140:PRO:HD2	1.86	0.57
1:A:197:LEU:HD12	1:A:197:LEU:O	2.05	0.57
1:B:121:PHE:C	1:B:122:ARG:HG2	2.30	0.57
1:B:391:PRO:HG2	1:B:395:LEU:HD13	1.86	0.57
1:A:431:LYS:CG	1:A:432:TYR:N	2.67	0.57
1:B:385:LEU:C	1:B:385:LEU:HD12	2.30	0.57
1:B:420:THR:CG2	1:B:421:MET:H	2.14	0.57
1:B:438:LEU:HD23	1:B:458:ARG:NH1	2.19	0.57
1:A:389:ARG:HG2	1:A:389:ARG:O	2.05	0.57
1:A:402:LEU:O	1:A:406:LEU:HD23	2.05	0.57
1:A:306:LEU:HD12	1:A:335:VAL:CG1	2.35	0.57
1:A:394:GLU:C	1:A:397:GLN:HB2	2.30	0.57
1:A:244:PRO:HG2	1:A:247:THR:OG1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD21	1:A:264:ARG:NH2	2.20	0.57
1:B:92:LEU:HD22	1:B:298:GLU:HG2	1.87	0.57
1:A:130:ALA:HB1	1:A:188:GLY:HA3	1.86	0.56
1:B:121:PHE:O	1:B:122:ARG:CG	2.52	0.56
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.70	0.56
1:A:468:ILE:O	1:A:469:SER:HB3	2.03	0.56
1:B:392:THR:O	1:B:394:GLU:N	2.38	0.56
1:A:120:VAL:O	1:A:121:PHE:C	2.48	0.56
1:B:128:VAL:CG2	1:B:129:ASP:N	2.67	0.56
1:A:231:ILE:HG22	1:A:232:GLY:N	2.20	0.56
1:A:411:ILE:HD11	1:A:476:ILE:HD11	1.86	0.56
1:A:218:VAL:C	1:A:229:LYS:HG3	2.30	0.56
1:A:320:SER:HA	1:A:323:HIS:HE2	1.65	0.56
1:A:456:ARG:HA	1:A:462:MET:O	2.06	0.56
1:B:115:TRP:CE3	1:B:119:VAL:HG21	2.41	0.56
1:B:241:TRP:CD1	1:B:243:THR:CG2	2.88	0.56
1:B:421:MET:O	1:B:422:GLN:C	2.48	0.56
1:A:265:LYS:HD2	1:A:266:PHE:CZ	2.40	0.56
1:A:381:ILE:CD1	1:A:437:ILE:HD12	2.32	0.56
1:B:116:THR:HA	1:B:120:VAL:CG2	2.35	0.56
1:B:251:TRP:O	1:B:254:PHE:HB3	2.05	0.56
1:B:120:VAL:HG12	1:B:121:PHE:N	2.20	0.56
1:B:280:ASP:HA	1:B:284:ARG:NH2	2.17	0.56
1:B:384:ALA:HB2	1:B:437:ILE:HG21	1.87	0.56
1:A:432:TYR:HD2	1:A:440:THR:HG23	1.71	0.56
1:B:122:ARG:HB2	1:B:124:GLN:HE21	1.71	0.56
1:A:460:THR:OG1	1:A:462:MET:HB2	2.06	0.56
1:B:253:ASP:C	1:B:257:ARG:NH1	2.64	0.56
1:B:382:LYS:HE3	1:B:479:ILE:HD13	1.88	0.56
1:A:445:GLU:O	1:A:448:LEU:HG	2.05	0.55
1:B:87:SER:O	1:B:88:ARG:C	2.50	0.55
1:B:428:LEU:HD12	1:B:428:LEU:N	2.22	0.55
1:A:484:ASN:O	1:A:485:VAL:C	2.50	0.55
1:B:189:ALA:CB	1:B:240:VAL:HG21	2.36	0.55
1:B:88:ARG:O	1:B:91:LEU:N	2.40	0.55
1:B:100:GLY:O	1:B:104:VAL:HG23	2.07	0.55
1:B:128:VAL:HG22	1:B:129:ASP:H	1.71	0.55
1:A:325:ARG:HH12	1:A:330:ASN:HD21	1.53	0.55
1:A:395:LEU:N	1:A:395:LEU:CD2	2.70	0.55
1:B:111:ALA:O	1:B:114:TRP:HB3	2.06	0.55
1:A:87:SER:HB3	1:A:88:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD12	1:A:102:LEU:N	2.22	0.55
1:A:326:ASP:OD1	1:A:326:ASP:C	2.49	0.55
1:A:424:SER:OG	1:A:425:LEU:N	2.39	0.55
1:B:472:LYS:HD3	1:B:473:ASP:N	2.21	0.55
1:A:113:GLU:HG2	1:A:266:PHE:CZ	2.41	0.55
1:B:86:LEU:HD22	1:B:86:LEU:N	2.22	0.55
1:B:405:GLU:HB3	1:B:406:LEU:HD12	1.89	0.55
1:A:197:LEU:HD21	1:A:202:LYS:HE3	1.89	0.54
1:B:113:GLU:OE2	1:B:266:PHE:HZ	1.90	0.54
1:A:105:GLU:O	1:A:109:ASN:HB2	2.07	0.54
1:A:320:SER:C	1:A:322:LEU:N	2.65	0.54
1:B:281:GLU:C	1:B:283:GLY:H	2.15	0.54
1:A:381:ILE:O	1:A:381:ILE:HG13	2.07	0.54
1:A:391:PRO:HG2	1:A:395:LEU:CD2	2.37	0.54
1:B:122:ARG:HH11	1:B:122:ARG:CB	2.17	0.54
1:A:273:PHE:CE1	1:A:291:TYR:HD1	2.25	0.54
1:A:419:GLU:HG3	1:A:420:THR:N	2.19	0.54
1:A:466:MET:HE1	1:A:471:LEU:HA	1.90	0.54
1:B:87:SER:HB2	1:B:88:ARG:NE	2.22	0.54
1:B:128:VAL:CG2	1:B:129:ASP:H	2.21	0.54
1:A:78:PHE:CE1	1:A:102:LEU:HB3	2.43	0.54
1:A:197:LEU:HD12	1:A:202:LYS:HA	1.89	0.54
1:A:435:MET:HB3	1:A:437:ILE:HD11	1.89	0.54
1:B:69:LEU:HD13	1:B:354:PHE:CD2	2.43	0.54
1:B:441:VAL:HG12	1:B:455:LEU:HB2	1.89	0.54
1:B:88:ARG:HD2	1:B:89:ASP:H	1.70	0.54
1:A:67:GLU:HG2	1:A:69:LEU:N	2.19	0.54
1:A:116:THR:HA	1:A:120:VAL:HG21	1.89	0.54
1:A:286:GLY:HA3	1:A:304:TRP:CE3	2.43	0.54
1:A:323:HIS:HB3	1:A:332:VAL:HG22	1.90	0.54
1:B:114:TRP:O	1:B:117:SER:HB3	2.08	0.54
1:A:127:PRO:HB2	1:B:104:VAL:HG11	1.90	0.54
1:B:303:LEU:HD12	1:B:303:LEU:N	2.22	0.54
1:A:145:PHE:HE2	1:A:229:LYS:HD2	1.73	0.53
1:A:260:LEU:HD13	1:A:289:LEU:HD12	1.90	0.53
1:A:373:LYS:HA	1:A:458:ARG:CZ	2.38	0.53
1:B:437:ILE:O	1:B:438:LEU:C	2.51	0.53
1:A:466:MET:CE	1:A:471:LEU:HD22	2.39	0.53
1:B:87:SER:OG	1:B:88:ARG:CZ	2.56	0.53
1:B:190:LEU:HB3	1:B:314:MET:HE2	1.90	0.53
1:B:255:TRP:O	1:B:256:LEU:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:O	1:A:322:LEU:HD23	2.07	0.53
1:A:431:LYS:HB2	1:A:431:LYS:HZ3	1.72	0.53
1:B:78:PHE:C	1:B:79:LEU:HD22	2.34	0.53
1:B:252:LEU:HD13	1:B:252:LEU:O	2.08	0.53
1:A:243:THR:CG2	1:A:334:CYS:HB2	2.37	0.53
1:B:192:HIS:O	1:B:194:VAL:N	2.42	0.53
1:A:454:HIS:HD2	1:A:465:MET:HE3	1.70	0.53
1:B:457:SER:OG	1:B:458:ARG:N	2.28	0.53
1:A:320:SER:O	1:A:322:LEU:N	2.42	0.53
1:A:455:LEU:O	1:A:463:LYS:HA	2.09	0.53
1:B:193:TYR:O	1:B:197:LEU:HB2	2.08	0.53
1:A:199:LEU:CD2	1:B:101:PRO:HG2	2.39	0.52
1:A:320:SER:HA	1:A:323:HIS:CE1	2.43	0.52
1:A:372:LEU:HD12	1:A:434:GLU:C	2.34	0.52
1:A:279:GLN:CB	1:A:285:LYS:H	2.22	0.52
1:B:107:ARG:HG3	1:B:108:LYS:N	2.17	0.52
1:B:102:LEU:O	1:B:103:GLY:C	2.52	0.52
1:A:87:SER:O	1:A:88:ARG:C	2.53	0.52
1:A:126:PHE:HB3	1:A:127:PRO:HD2	1.91	0.52
1:B:190:LEU:C	1:B:192:HIS:H	2.16	0.52
1:B:289:LEU:HD12	1:B:301:GLU:HG2	1.90	0.52
1:B:368:HIS:HB3	1:B:370:LYS:HE2	1.90	0.52
1:A:255:TRP:O	1:A:256:LEU:C	2.52	0.52
1:B:115:TRP:CE2	1:B:119:VAL:HG11	2.44	0.52
1:A:407:LEU:HD23	1:A:411:ILE:O	2.10	0.52
1:A:468:ILE:O	1:A:469:SER:CB	2.57	0.52
1:B:116:THR:HA	1:B:120:VAL:HG23	1.91	0.52
1:B:332:VAL:CG1	1:B:333:PRO:HD2	2.40	0.52
1:B:252:LEU:CB	1:B:336:LEU:HD11	2.35	0.52
1:B:438:LEU:HA	1:B:458:ARG:HD3	1.92	0.52
1:A:146:ARG:O	1:A:146:ARG:NH1	2.43	0.52
1:A:459:ASP:C	1:A:461:THR:N	2.67	0.52
1:A:200:VAL:C	1:A:202:LYS:N	2.67	0.51
1:A:405:GLU:OE2	1:A:472:LYS:HB2	2.10	0.51
1:B:88:ARG:O	1:B:89:ASP:C	2.53	0.51
1:A:369:ARG:HE	1:A:371:VAL:CG1	2.23	0.51
1:A:146:ARG:HH11	1:A:146:ARG:CA	2.24	0.51
1:A:369:ARG:NH2	1:A:458:ARG:O	2.40	0.51
1:B:87:SER:H	1:B:91:LEU:HD21	1.75	0.51
1:B:114:TRP:O	1:B:117:SER:N	2.40	0.51
1:B:321:LYS:O	1:B:321:LYS:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ARG:HG3	1:B:369:ARG:HH11	1.74	0.51
1:A:369:ARG:NH2	1:A:371:VAL:HG21	2.16	0.51
1:A:397:GLN:OE1	1:A:397:GLN:HA	2.09	0.51
1:B:197:LEU:C	1:B:199:LEU:N	2.69	0.51
1:B:251:TRP:HA	1:B:254:PHE:HB3	1.92	0.51
1:A:450:ASN:ND2	1:A:452:LEU:CB	2.71	0.51
1:A:471:LEU:O	1:A:474:PHE:HB3	2.10	0.51
1:B:87:SER:CB	1:B:88:ARG:CZ	2.88	0.51
1:B:287:ASN:HB2	1:B:303:LEU:HB2	1.91	0.51
1:B:389:ARG:HG2	1:B:389:ARG:O	2.10	0.51
1:B:424:SER:HB3	1:B:427:GLN:HB2	1.93	0.51
1:B:258:HIS:ND1	1:B:258:HIS:C	2.69	0.51
1:B:447:THR:O	1:B:448:LEU:C	2.53	0.51
1:A:410:GLY:O	1:A:411:ILE:HD13	2.10	0.51
1:A:470:LYS:HE2	1:A:470:LYS:HA	1.92	0.51
1:A:309:HIS:O	1:A:312:LEU:N	2.41	0.51
1:A:244:PRO:O	1:A:245:PRO:C	2.53	0.50
1:B:297:LYS:O	1:B:298:GLU:OE1	2.29	0.50
1:A:116:THR:CG2	1:A:120:VAL:HG21	2.41	0.50
1:A:392:THR:O	1:A:393:LEU:C	2.54	0.50
1:A:468:ILE:HD12	1:A:468:ILE:C	2.35	0.50
1:B:376:PRO:C	1:B:378:LEU:N	2.69	0.50
1:A:76:ARG:HG3	1:A:434:GLU:O	2.11	0.50
1:A:481:SER:O	1:A:482:ALA:C	2.54	0.50
1:B:182:ARG:NH2	1:B:213:VAL:O	2.32	0.50
1:A:120:VAL:HG12	1:A:121:PHE:N	2.24	0.50
1:A:128:VAL:HG12	1:A:209:ALA:O	2.11	0.50
1:A:302:THR:O	1:A:303:LEU:HD12	2.11	0.50
1:A:456:ARG:HG2	1:A:456:ARG:HH11	1.77	0.50
1:B:306:LEU:HB2	1:B:335:VAL:HG23	1.92	0.50
1:A:189:ALA:CB	1:A:240:VAL:HG21	2.42	0.50
1:A:456:ARG:HG2	1:A:456:ARG:NH1	2.27	0.50
1:B:345:GLY:O	1:B:348:ALA:N	2.44	0.50
1:A:197:LEU:CD1	1:A:202:LYS:HG3	2.33	0.50
1:A:419:GLU:HG3	1:A:420:THR:HG22	1.94	0.50
1:B:73:CYS:O	1:B:78:PHE:HB2	2.11	0.50
1:A:114:TRP:O	1:A:118:VAL:HG13	2.11	0.50
1:A:218:VAL:C	1:A:229:LYS:CG	2.85	0.50
1:A:325:ARG:HG2	1:A:325:ARG:NH1	2.25	0.50
1:A:89:ASP:O	1:A:90:SER:C	2.55	0.49
1:A:145:PHE:HE2	1:A:229:LYS:HZ3	1.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:C	1:A:397:GLN:H	2.20	0.49
1:A:466:MET:HG2	1:A:467:HIS:N	2.27	0.49
1:B:389:ARG:O	1:B:389:ARG:CG	2.59	0.49
1:A:306:LEU:HB2	1:A:335:VAL:HB	1.94	0.49
1:A:313:HIS:C	1:A:313:HIS:CD2	2.90	0.49
1:A:345:GLY:O	1:A:348:ALA:N	2.44	0.49
1:B:318:ASN:N	1:B:318:ASN:ND2	2.59	0.49
1:B:110:LEU:CD1	1:B:378:LEU:HD11	2.42	0.49
1:B:136:GLY:O	1:B:138:LEU:HD22	2.12	0.49
1:A:310:GLU:O	1:A:313:HIS:N	2.46	0.49
1:B:371:VAL:CA	1:B:433:ASP:HB3	2.41	0.49
1:B:460:THR:O	1:B:462:MET:N	2.45	0.49
1:B:254:PHE:CD2	1:B:255:TRP:N	2.81	0.49
1:B:386:ASP:HB3	1:B:417:TYR:N	2.28	0.49
1:A:254:PHE:O	1:A:255:TRP:C	2.56	0.49
1:B:134:LYS:N	1:B:180:GLY:HA2	2.21	0.49
1:B:277:ASP:HA	1:B:287:ASN:OD1	2.12	0.49
1:A:252:LEU:HD11	1:A:287:ASN:HD22	1.78	0.49
1:B:93:SER:O	1:B:94:GLY:C	2.54	0.49
1:B:402:LEU:O	1:B:403:PHE:C	2.55	0.49
1:B:421:MET:O	1:B:423:SER:N	2.45	0.49
1:A:383:VAL:CG2	1:A:384:ALA:N	2.76	0.49
1:B:87:SER:O	1:B:88:ARG:HD2	2.13	0.48
1:B:405:GLU:O	1:B:408:GLU:N	2.46	0.48
1:A:106:LEU:HD12	1:A:106:LEU:O	2.14	0.48
1:B:252:LEU:C	1:B:252:LEU:CD1	2.86	0.48
1:B:424:SER:O	1:B:428:LEU:CD1	2.61	0.48
1:A:195:ASN:C	1:A:197:LEU:H	2.21	0.48
1:A:252:LEU:O	1:A:253:ASP:C	2.56	0.48
1:A:254:PHE:CD2	1:A:255:TRP:N	2.81	0.48
1:A:459:ASP:O	1:A:461:THR:N	2.46	0.48
1:B:416:GLY:HA2	1:B:419:GLU:OE1	2.13	0.48
1:B:415:PRO:HB2	1:B:418:LEU:CD1	2.44	0.48
1:B:441:VAL:HG12	1:B:455:LEU:HB3	1.94	0.48
1:B:472:LYS:HD3	1:B:472:LYS:C	2.39	0.48
1:A:266:PHE:HB2	1:A:349:TYR:CE1	2.49	0.48
1:A:420:THR:HG23	1:A:421:MET:N	2.28	0.48
1:B:256:LEU:HG	1:B:257:ARG:N	2.29	0.48
1:B:415:PRO:O	1:B:418:LEU:HD13	2.14	0.48
1:A:451:GLY:O	1:A:467:HIS:HA	2.13	0.48
1:B:137:PRO:O	1:B:138:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:CA	1:B:284:ARG:HH21	2.22	0.48
1:A:103:GLY:O	1:A:104:VAL:C	2.57	0.48
1:A:314:MET:HG2	1:A:315:TYR:CE1	2.48	0.48
1:A:186:LEU:HD11	1:A:306:LEU:CD1	2.35	0.48
1:B:290:TYR:HD1	1:B:299:LEU:HA	1.77	0.48
1:B:373:LYS:HE2	1:B:459:ASP:CA	2.40	0.48
1:A:436:SER:C	1:A:437:ILE:HD13	2.38	0.47
1:B:77:HIS:O	1:B:102:LEU:HB2	2.13	0.47
1:A:189:ALA:HB3	1:A:240:VAL:HG21	1.96	0.47
1:A:393:LEU:C	1:A:397:GLN:HG2	2.38	0.47
1:B:87:SER:C	1:B:88:ARG:HD2	2.38	0.47
1:B:286:GLY:HA2	1:B:303:LEU:O	2.14	0.47
1:B:452:LEU:N	1:B:452:LEU:CD2	2.77	0.47
1:B:299:LEU:C	1:B:299:LEU:HD13	2.39	0.47
1:B:326:ASP:O	1:B:329:LYS:HB2	2.14	0.47
1:B:256:LEU:HB2	1:B:287:ASN:HD22	1.79	0.47
1:A:87:SER:C	1:A:88:ARG:HD2	2.38	0.47
1:A:382:LYS:N	1:A:412:SER:OG	2.46	0.47
1:A:306:LEU:HB2	1:A:335:VAL:O	2.14	0.47
1:A:394:GLU:OE2	1:A:394:GLU:HA	2.14	0.47
1:A:477:LYS:O	1:A:481:SER:HB3	2.14	0.47
1:A:121:PHE:N	1:A:121:PHE:CD2	2.77	0.47
1:A:130:ALA:HB3	1:A:210:GLN:HE22	1.79	0.47
1:A:192:HIS:O	1:A:194:VAL:N	2.48	0.47
1:A:288:LYS:HD3	1:A:299:LEU:HD12	1.97	0.47
1:A:308:ASP:O	1:A:309:HIS:O	2.32	0.47
1:A:371:VAL:HG23	1:A:433:ASP:HB3	1.96	0.47
1:A:390:GLY:HA2	1:A:445:GLU:HB3	1.97	0.47
1:A:437:ILE:O	1:A:439:PHE:N	2.48	0.47
1:B:332:VAL:HG13	1:B:333:PRO:HD2	1.97	0.47
1:B:145:PHE:CE1	1:B:217:PRO:HB3	2.48	0.47
1:A:322:LEU:O	1:A:323:HIS:C	2.58	0.47
1:A:385:LEU:HB3	1:A:441:VAL:HG23	1.97	0.47
1:B:234:LYS:HD3	1:B:341:ASP:OD2	2.15	0.47
1:A:88:ARG:CD	1:A:88:ARG:H	2.24	0.47
1:A:407:LEU:O	1:A:408:GLU:C	2.58	0.47
1:B:115:TRP:HH2	1:B:127:PRO:HB3	1.80	0.47
1:B:385:LEU:HD12	1:B:385:LEU:O	2.14	0.47
1:B:387:VAL:HG12	1:B:443:VAL:HG12	1.97	0.47
1:B:120:VAL:HG12	1:B:121:PHE:CD2	2.50	0.46
1:B:458:ARG:HB3	1:B:459:ASP:H	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:NH2	1:A:301:GLU:OE2	2.38	0.46
1:A:429:TYR:CE2	1:A:456:ARG:HD3	2.51	0.46
1:A:463:LYS:HD2	1:A:463:LYS:N	2.30	0.46
1:A:229:LYS:HG2	1:A:230:SER:N	2.30	0.46
1:B:370:LYS:O	1:B:371:VAL:O	2.32	0.46
1:A:89:ASP:O	1:A:91:LEU:N	2.49	0.46
1:A:266:PHE:HB2	1:A:349:TYR:HE1	1.80	0.46
1:A:291:TYR:CG	1:A:348:ALA:HB1	2.51	0.46
1:A:381:ILE:HD11	1:A:437:ILE:CD1	2.42	0.46
1:B:244:PRO:HG2	1:B:247:THR:OG1	2.16	0.46
1:A:141:GLY:O	1:A:142:ASP:O	2.34	0.46
1:A:353:SER:HB2	1:A:373:LYS:C	2.40	0.46
1:B:197:LEU:HD21	1:B:202:LYS:HG3	1.98	0.46
1:A:95:CYS:SG	1:A:218:VAL:HG21	2.56	0.46
1:B:422:GLN:CG	1:B:423:SER:N	2.77	0.46
1:A:303:LEU:HD11	1:A:338:VAL:CG1	2.36	0.46
1:B:125:VAL:HA	1:B:207:GLY:O	2.15	0.46
1:A:112:ALA:O	1:A:116:THR:OG1	2.33	0.46
1:B:369:ARG:HG3	1:B:369:ARG:NH1	2.31	0.46
1:A:392:THR:HG22	1:A:393:LEU:N	2.31	0.46
1:B:192:HIS:O	1:B:193:TYR:C	2.58	0.46
1:B:318:ASN:N	1:B:318:ASN:HD22	2.13	0.46
1:B:460:THR:HB	1:B:462:MET:CG	2.45	0.46
1:A:290:TYR:CD1	1:A:299:LEU:HA	2.49	0.45
1:A:293:PHE:O	1:A:295:TRP:N	2.50	0.45
1:A:301:GLU:OE2	1:A:340:GLY:HA3	2.16	0.45
1:A:369:ARG:HE	1:A:371:VAL:HG11	1.81	0.45
1:B:69:LEU:O	1:B:70:LEU:C	2.59	0.45
1:B:455:LEU:HD12	1:B:455:LEU:O	2.16	0.45
1:B:460:THR:HB	1:B:462:MET:SD	2.56	0.45
1:A:128:VAL:HG23	1:A:192:HIS:CD2	2.52	0.45
1:A:318:ASN:OD1	1:A:320:SER:HB2	2.16	0.45
1:B:126:PHE:HB3	1:B:127:PRO:HD2	1.97	0.45
1:A:115:TRP:CZ2	1:A:119:VAL:HG11	2.51	0.45
1:A:119:VAL:O	1:A:123:GLU:HG3	2.15	0.45
1:A:200:VAL:C	1:A:202:LYS:H	2.24	0.45
1:A:263:TRP:CH2	1:A:300:ILE:HD12	2.51	0.45
1:A:454:HIS:N	1:A:454:HIS:ND1	2.63	0.45
1:A:481:SER:OG	1:A:482:ALA:N	2.46	0.45
1:B:424:SER:O	1:B:428:LEU:HD13	2.17	0.45
1:B:437:ILE:HG22	1:B:439:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:MET:O	1:B:466:MET:HB2	2.16	0.45
1:A:255:TRP:O	1:A:258:HIS:HB3	2.17	0.45
1:A:394:GLU:O	1:A:398:VAL:HG12	2.16	0.45
1:A:403:PHE:HZ	1:B:123:GLU:HB2	1.82	0.45
1:B:314:MET:HE3	1:B:315:TYR:CZ	2.52	0.45
1:B:320:SER:HA	1:B:323:HIS:NE2	2.31	0.45
1:A:279:GLN:HB2	1:A:284:ARG:HA	1.99	0.45
1:B:305:ASN:HB2	1:B:336:LEU:HD12	1.99	0.45
1:B:420:THR:O	1:B:422:GLN:N	2.50	0.45
1:B:426:GLU:HA	1:B:426:GLU:OE1	2.17	0.45
1:A:281:GLU:OE2	1:A:304:TRP:CD1	2.70	0.45
1:A:450:ASN:CG	1:A:451:GLY:N	2.75	0.45
1:B:263:TRP:CZ3	1:B:300:ILE:HD12	2.51	0.45
1:A:323:HIS:CB	1:A:331:VAL:C	2.89	0.45
1:A:394:GLU:HA	1:A:397:GLN:HB2	1.99	0.45
1:A:205:PRO:HG3	1:A:251:TRP:CZ2	2.52	0.45
1:A:258:HIS:C	1:A:258:HIS:ND1	2.74	0.45
1:A:280:ASP:HA	1:A:283:GLY:C	2.42	0.45
1:A:326:ASP:HB3	1:A:329:LYS:O	2.16	0.45
1:A:126:PHE:CD1	1:A:126:PHE:N	2.84	0.45
1:A:402:LEU:O	1:A:403:PHE:C	2.57	0.45
1:B:115:TRP:CH2	1:B:127:PRO:HB3	2.52	0.45
1:A:87:SER:C	1:A:89:ASP:N	2.74	0.44
1:A:137:PRO:O	1:A:138:LEU:HG	2.17	0.44
1:A:145:PHE:CE2	1:A:229:LYS:HD2	2.51	0.44
1:A:318:ASN:ND2	1:A:319:VAL:N	2.60	0.44
1:A:369:ARG:HG3	1:A:370:LYS:H	1.82	0.44
1:B:264:ARG:HB3	1:B:270:PRO:HB3	1.99	0.44
1:A:299:LEU:O	1:A:344:ARG:HD2	2.17	0.44
1:B:256:LEU:HD12	1:B:256:LEU:O	2.16	0.44
1:B:392:THR:HG22	1:B:393:LEU:HD22	1.98	0.44
1:A:241:TRP:HB3	1:A:336:LEU:HD22	2.00	0.44
1:A:409:ASN:ND2	1:A:472:LYS:HD2	2.32	0.44
1:B:73:CYS:CB	1:B:79:LEU:HD23	2.48	0.44
1:B:123:GLU:C	1:B:124:GLN:HG3	2.38	0.44
1:B:398:VAL:C	1:B:400:GLN:H	2.26	0.44
1:A:85:GLN:H	1:A:85:GLN:HG2	1.49	0.44
1:A:435:MET:HE2	1:A:437:ILE:HD11	1.99	0.44
1:B:73:CYS:HB3	1:B:79:LEU:HD23	2.00	0.44
1:B:200:VAL:O	1:B:203:ARG:HG3	2.17	0.44
1:B:264:ARG:HB3	1:B:270:PRO:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PHE:HB3	1:B:378:LEU:HD22	2.00	0.44
1:B:290:TYR:HE1	1:B:299:LEU:HB2	1.83	0.44
1:B:319:VAL:O	1:B:319:VAL:HG22	2.17	0.44
1:B:396:ARG:HA	1:B:399:CYS:HB2	2.00	0.44
1:A:259:ARG:O	1:A:262:TRP:HB3	2.18	0.44
1:A:345:GLY:O	1:A:346:MET:C	2.61	0.44
1:A:306:LEU:HB3	1:A:310:GLU:OE1	2.18	0.44
1:A:369:ARG:CG	1:A:370:LYS:N	2.80	0.44
1:A:431:LYS:HA	1:A:434:GLU:HB2	2.00	0.44
1:A:76:ARG:HB3	1:A:435:MET:CG	2.46	0.44
1:A:130:ALA:CB	1:A:210:GLN:HE22	2.30	0.44
1:A:322:LEU:O	1:A:323:HIS:HD2	2.01	0.44
1:B:82:SER:OG	1:B:83:LYS:N	2.51	0.44
1:B:259:ARG:O	1:B:263:TRP:HD1	2.00	0.44
1:A:393:LEU:HD21	1:A:397:GLN:HE21	1.83	0.44
1:B:197:LEU:CD1	1:B:202:LYS:HA	2.45	0.44
1:B:424:SER:HB3	1:B:427:GLN:CB	2.48	0.44
1:A:403:PHE:CZ	1:B:123:GLU:HB2	2.53	0.43
1:B:122:ARG:O	1:B:124:GLN:N	2.51	0.43
1:A:106:LEU:HG	1:A:346:MET:HG2	1.99	0.43
1:A:433:ASP:C	1:A:435:MET:H	2.24	0.43
1:A:443:VAL:HG22	1:A:453:ILE:HG22	2.01	0.43
1:A:444:THR:O	1:A:447:THR:OG1	2.34	0.43
1:A:467:HIS:O	1:A:470:LYS:HB2	2.18	0.43
1:B:130:ALA:CB	1:B:210:GLN:HE22	2.31	0.43
1:B:259:ARG:HD2	1:B:259:ARG:HA	1.72	0.43
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.62	0.43
1:B:67:GLU:O	1:B:68:ALA:C	2.61	0.43
1:B:351:TYR:C	1:B:353:SER:N	2.76	0.43
1:B:420:THR:O	1:B:421:MET:C	2.60	0.43
1:A:231:ILE:HD13	1:B:133:HIS:CD2	2.53	0.43
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.72	0.43
1:B:130:ALA:HB3	1:B:210:GLN:HE22	1.83	0.43
1:A:200:VAL:O	1:A:202:LYS:N	2.52	0.43
1:A:432:TYR:HD2	1:A:440:THR:CG2	2.31	0.43
1:B:82:SER:C	1:B:84:GLN:H	2.27	0.43
1:B:87:SER:H	1:B:91:LEU:CD2	2.31	0.43
1:B:92:LEU:CD2	1:B:298:GLU:HG2	2.47	0.43
1:B:258:HIS:O	1:B:259:ARG:C	2.60	0.43
1:B:439:PHE:HD1	1:B:456:ARG:O	2.01	0.43
1:A:441:VAL:HG11	1:A:471:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:CYS:O	1:B:96:HIS:O	2.35	0.43
1:B:215:PHE:CD1	1:B:215:PHE:N	2.86	0.43
1:B:286:GLY:CA	1:B:303:LEU:O	2.66	0.43
1:B:373:LYS:HA	1:B:458:ARG:NH2	2.33	0.43
1:A:96:HIS:H	1:A:96:HIS:HD2	1.61	0.43
1:A:235:THR:N	1:A:343:ASP:OD2	2.38	0.43
1:A:102:LEU:N	1:A:102:LEU:CD1	2.80	0.43
1:A:241:TRP:HE1	1:A:251:TRP:CG	2.36	0.43
1:A:450:ASN:N	1:A:450:ASN:OD1	2.51	0.43
1:B:108:LYS:O	1:B:111:ALA:HB3	2.19	0.43
1:B:118:VAL:HG13	1:B:119:VAL:H	1.84	0.43
1:A:381:ILE:CG1	1:A:437:ILE:HD12	2.49	0.43
1:B:82:SER:N	1:B:85:GLN:OE1	2.42	0.43
1:A:68:ALA:O	1:A:69:LEU:C	2.62	0.42
1:A:85:GLN:C	1:A:87:SER:H	2.27	0.42
1:B:252:LEU:HD23	1:B:336:LEU:HD11	2.01	0.42
1:B:331:VAL:CG2	1:B:332:VAL:N	2.80	0.42
1:B:395:LEU:C	1:B:397:GLN:N	2.71	0.42
1:B:406:LEU:HB3	1:B:411:ILE:HB	2.00	0.42
1:A:122:ARG:O	1:A:122:ARG:CG	2.67	0.42
1:B:421:MET:C	1:B:423:SER:N	2.75	0.42
1:B:265:LYS:HB2	1:B:265:LYS:HE3	1.90	0.42
1:B:278:CYS:SG	1:B:304:TRP:CZ2	3.12	0.42
1:B:287:ASN:N	1:B:303:LEU:O	2.51	0.42
1:B:372:LEU:O	1:B:374:LEU:N	2.52	0.42
1:B:289:LEU:CB	1:B:301:GLU:HB3	2.45	0.42
1:B:281:GLU:OE1	1:B:304:TRP:CE2	2.72	0.42
1:B:397:GLN:O	1:B:397:GLN:HG2	2.13	0.42
1:A:277:ASP:C	1:A:278:CYS:SG	3.03	0.42
1:A:354:PHE:CG	1:A:355:GLN:N	2.87	0.42
1:A:378:LEU:O	1:A:379:ALA:C	2.63	0.42
1:B:87:SER:N	1:B:91:LEU:HD21	2.35	0.42
1:B:182:ARG:HH21	1:B:213:VAL:C	2.25	0.42
1:A:431:LYS:HG2	1:A:432:TYR:N	2.34	0.42
1:B:119:VAL:HG22	1:B:209:ALA:HB3	2.01	0.42
1:B:422:GLN:O	1:B:423:SER:C	2.63	0.42
1:A:188:GLY:HA2	1:A:191:GLU:OE2	2.20	0.42
1:A:372:LEU:CB	1:A:436:SER:HB2	2.49	0.42
1:A:407:LEU:HD13	1:B:120:VAL:HG12	2.01	0.42
1:B:122:ARG:C	1:B:124:GLN:HG3	2.44	0.42
1:B:258:HIS:O	1:B:261:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:C	1:A:197:LEU:N	2.77	0.42
1:B:70:LEU:O	1:B:71:GLU:C	2.61	0.42
1:B:107:ARG:HH11	1:B:107:ARG:HG2	1.85	0.42
1:B:193:TYR:O	1:B:193:TYR:CD1	2.73	0.42
1:B:269:SER:HB2	1:B:272:ASN:HD22	1.84	0.42
1:A:139:LEU:CD1	1:A:142:ASP:HB2	2.50	0.42
1:A:385:LEU:CB	1:A:441:VAL:HG23	2.49	0.42
1:A:466:MET:CG	1:A:467:HIS:N	2.82	0.42
1:A:481:SER:O	1:A:483:LYS:N	2.53	0.42
1:B:186:LEU:HD21	1:B:306:LEU:HD11	2.01	0.42
1:B:481:SER:O	1:B:484:ASN:HB2	2.20	0.42
1:A:202:LYS:O	1:A:202:LYS:HG2	2.20	0.41
1:A:389:ARG:HD2	1:A:444:THR:CG2	2.50	0.41
1:B:82:SER:HB3	1:B:85:GLN:OE1	2.20	0.41
1:B:244:PRO:HA	1:B:245:PRO:HD3	1.91	0.41
1:A:375:HIS:HA	1:A:376:PRO:HD3	1.92	0.41
1:A:399:CYS:O	1:A:400:GLN:C	2.63	0.41
1:B:76:ARG:HA	1:B:76:ARG:HD3	1.64	0.41
1:A:111:ALA:O	1:A:112:ALA:C	2.64	0.41
1:A:121:PHE:HB2	1:A:122:ARG:H	1.72	0.41
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.73	0.41
1:A:466:MET:HE1	1:A:471:LEU:HD13	2.01	0.41
1:B:416:GLY:O	1:B:417:TYR:C	2.63	0.41
1:B:385:LEU:HD23	1:B:413:VAL:CG1	2.51	0.41
1:B:115:TRP:CZ3	1:B:119:VAL:HG21	2.55	0.41
1:B:391:PRO:HG2	1:B:392:THR:H	1.84	0.41
1:B:460:THR:CB	1:B:462:MET:HG2	2.48	0.41
1:A:127:PRO:HA	1:A:209:ALA:O	2.21	0.41
1:A:385:LEU:N	1:A:385:LEU:CD2	2.83	0.41
1:A:453:ILE:C	1:A:453:ILE:CD1	2.89	0.41
1:A:96:HIS:HB2	1:A:97:PRO:HD2	2.03	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.82	0.41
1:A:448:LEU:N	1:A:448:LEU:CD2	2.65	0.41
1:B:69:LEU:O	1:B:72:ILE:HB	2.21	0.41
1:B:267:ALA:HB2	1:B:273:PHE:HE2	1.86	0.41
1:A:139:LEU:CB	1:A:140:PRO:HD2	2.50	0.41
1:A:243:THR:OG1	1:A:244:PRO:CD	2.68	0.41
1:A:308:ASP:OD2	1:A:308:ASP:N	2.26	0.41
1:A:355:GLN:NE2	1:A:355:GLN:HA	2.35	0.41
1:A:420:THR:CG2	1:A:421:MET:N	2.84	0.41
1:A:423:SER:HB3	1:A:427:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:O	1:B:107:ARG:N	2.52	0.41
1:B:260:LEU:CD1	1:B:275:SER:HB3	2.48	0.41
1:B:368:HIS:O	1:B:368:HIS:ND1	2.54	0.41
1:B:392:THR:HG22	1:B:393:LEU:CD2	2.51	0.41
1:A:260:LEU:HD21	1:A:264:ARG:CZ	2.51	0.41
1:B:387:VAL:HG12	1:B:443:VAL:O	2.20	0.41
1:A:266:PHE:HB3	1:A:378:LEU:HD22	2.02	0.40
1:A:372:LEU:HB3	1:A:436:SER:HB2	2.01	0.40
1:B:122:ARG:O	1:B:122:ARG:HG3	2.20	0.40
1:B:294:PRO:HD2	1:B:295:TRP:CE3	2.56	0.40
1:B:395:LEU:O	1:B:397:GLN:N	2.54	0.40
1:A:375:HIS:O	1:A:378:LEU:HB2	2.22	0.40
1:A:481:SER:C	1:A:483:LYS:N	2.78	0.40
1:B:202:LYS:HB3	1:B:324:GLY:HA2	2.04	0.40
1:B:416:GLY:O	1:B:419:GLU:CD	2.64	0.40
1:B:455:LEU:CD1	1:B:455:LEU:C	2.94	0.40
1:A:193:TYR:O	1:A:197:LEU:HB2	2.21	0.40
1:A:263:TRP:CE3	1:A:300:ILE:HD12	2.56	0.40
1:B:122:ARG:CB	1:B:124:GLN:HE21	2.34	0.40
1:B:193:TYR:HB2	1:B:242:PHE:CZ	2.56	0.40
1:A:71:GLU:C	1:A:73:CYS:N	2.77	0.40
1:A:336:LEU:C	1:A:336:LEU:HD23	2.46	0.40
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.86	0.40
1:B:189:ALA:O	1:B:190:LEU:C	2.62	0.40
1:A:190:LEU:O	1:A:191:GLU:C	2.65	0.40
1:B:273:PHE:CE1	1:B:291:TYR:HD1	2.40	0.40
1:B:299:LEU:O	1:B:344:ARG:HD2	2.22	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	358/459 (78%)	246 (69%)	75 (21%)	37 (10%)	0	2
1	B	358/459 (78%)	242 (68%)	73 (20%)	43 (12%)	0	1
All	All	716/918 (78%)	488 (68%)	148 (21%)	80 (11%)	0	2

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	120	VAL
1	A	124	GLN
1	A	131	LEU
1	A	142	ASP
1	A	193	TYR
1	A	309	HIS
1	A	310	GLU
1	A	323	HIS
1	A	389	ARG
1	A	420	THR
1	A	421	MET
1	A	461	THR
1	B	68	ALA
1	B	88	ARG
1	B	104	VAL
1	B	120	VAL
1	B	181	GLY
1	B	281	GLU
1	B	371	VAL
1	B	391	PRO
1	B	393	LEU
1	B	417	TYR
1	B	423	SER
1	B	424	SER
1	B	448	LEU
1	B	461	THR
1	A	90	SER
1	A	121	PHE
1	A	328	ARG
1	A	371	VAL
1	A	391	PRO
1	A	438	LEU
1	A	450	ASN
1	A	469	SER

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Mol	Chain	Res	Type
1	B	121	PHE
1	B	130	ALA
1	B	146	ARG
1	B	191	GLU
1	B	193	TYR
1	B	309	HIS
1	B	421	MET
1	B	438	LEU
1	B	446	THR
1	A	89	ASP
1	A	254	PHE
1	A	271	SER
1	A	321	LYS
1	A	393	LEU
1	A	460	THR
1	B	123	GLU
1	B	124	GLN
1	B	258	HIS
1	B	259	ARG
1	B	285	LYS
1	B	373	LYS
1	B	385	LEU
1	B	396	ARG
1	B	422	GLN
1	B	466	MET
1	A	146	ARG
1	A	294	PRO
1	A	392	THR
1	A	464	GLU
1	B	87	SER
1	B	105	GLU
1	B	321	LYS
1	B	352	ASP
1	B	419	GLU
1	A	280	ASP
1	B	190	LEU
1	B	354	PHE
1	A	140	PRO
1	A	425	LEU
1	B	118	VAL
1	A	376	PRO
1	A	451	GLY

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Mol	Chain	Res	Type
1	B	376	PRO
1	A	104	VAL
1	B	96	HIS

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	323/401 (80%)	271 (84%)	52 (16%)	2	11
1	B	323/401 (80%)	275 (85%)	48 (15%)	3	13
All	All	646/802 (80%)	546 (84%)	100 (16%)	2	12

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	70	LEU
1	A	79	LEU
1	A	85	GLN
1	A	88	ARG
1	A	92	LEU
1	A	95	CYS
1	A	96	HIS
1	A	109	ASN
1	A	116	THR
1	A	118	VAL
1	A	121	PHE
1	A	123	GLU
1	A	124	GLN
1	A	125	VAL
1	A	126	PHE
1	A	128	VAL
1	A	195	ASN
1	A	200	VAL
1	A	206	TYR

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Mol	Chain	Res	Type
1	A	213	VAL
1	A	229	LYS
1	A	231	ILE
1	A	250	GLN
1	A	252	LEU
1	A	277	ASP
1	A	278	CYS
1	A	280	ASP
1	A	298	GLU
1	A	303	LEU
1	A	308	ASP
1	A	330	ASN
1	A	347	LEU
1	A	372	LEU
1	A	378	LEU
1	A	386	ASP
1	A	387	VAL
1	A	389	ARG
1	A	395	LEU
1	A	423	SER
1	A	431	LYS
1	A	443	VAL
1	A	445	GLU
1	A	448	LEU
1	A	449	GLU
1	A	454	HIS
1	A	455	LEU
1	A	460	THR
1	A	468	ILE
1	A	470	LYS
1	A	471	LEU
1	A	481	SER
1	B	70	LEU
1	B	85	GLN
1	B	88	ARG
1	B	95	CYS
1	B	107	ARG
1	B	118	VAL
1	B	124	GLN
1	B	139	LEU
1	B	183	GLU
1	B	199	LEU

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Mol	Chain	Res	Type
1	B	200	VAL
1	B	206	TYR
1	B	230	SER
1	B	248	SER
1	B	252	LEU
1	B	256	LEU
1	B	257	ARG
1	B	258	HIS
1	B	271	SER
1	B	284	ARG
1	B	298	GLU
1	B	311	LEU
1	B	312	LEU
1	B	314	MET
1	B	318	ASN
1	B	322	LEU
1	B	328	ARG
1	B	335	VAL
1	B	338	VAL
1	B	346	MET
1	B	372	LEU
1	B	374	LEU
1	B	377	CYS
1	B	389	ARG
1	B	397	GLN
1	B	426	GLU
1	B	431	LYS
1	B	443	VAL
1	B	445	GLU
1	B	448	LEU
1	B	455	LEU
1	B	459	ASP
1	B	460	THR
1	B	462	MET
1	B	472	LYS
1	B	473	ASP
1	B	481	SER
1	B	484	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	96	HIS
1	A	109	ASN
1	A	184	ASN
1	A	187	HIS
1	A	192	HIS
1	A	201	ASN
1	A	210	GLN
1	A	216	HIS
1	A	249	ASN
1	A	279	GLN
1	A	287	ASN
1	A	305	ASN
1	A	313	HIS
1	A	323	HIS
1	A	400	GLN
1	A	409	ASN
1	A	422	GLN
1	A	427	GLN
1	A	450	ASN
1	A	454	HIS
1	B	77	HIS
1	B	124	GLN
1	B	184	ASN
1	B	192	HIS
1	B	210	GLN
1	B	272	ASN
1	B	279	GLN
1	B	313	HIS
1	B	318	ASN
1	B	323	HIS
1	B	375	HIS
1	B	400	GLN
1	B	454	HIS

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 [i](#)

There are no oligosaccharides 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	364/459 (79%)	-1.41	0 100 100	41, 74, 102, 136	0
1	B	364/459 (79%)	-1.39	0 100 100	48, 73, 108, 127	0
All	All	728/918 (79%)	-1.40	0 100 100	41, 73, 107, 136	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.