



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:04 PM UTC

PDB ID : 1M3J / pdb_00001m3j
Title : CRYSTAL form II of perfringolysin O
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Deposited on : 2002-06-28
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

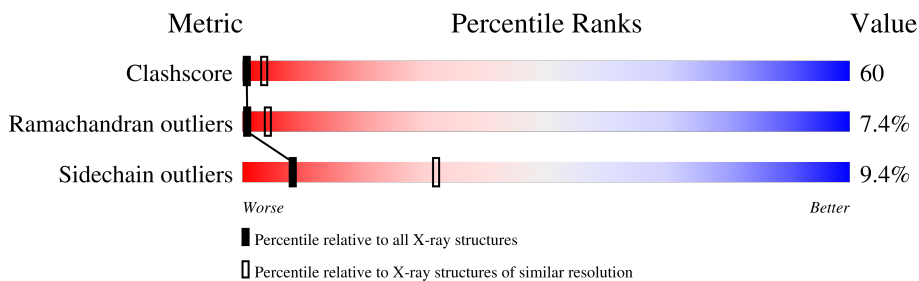
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

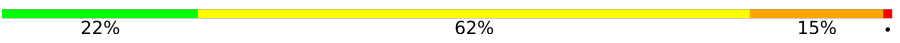
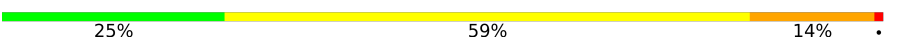
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7467 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 perfringolysin o.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3705	2332	622	746	5			
1	B	471	Total	C	N	O	S	0	0	0
			3705	2332	622	746	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	LEU	PHE	see remark 999	UNP P19995
B	114	LEU	PHE	see remark 999	UNP P19995

- Molecule 2 is water.

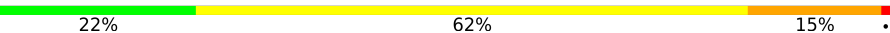
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	31	Total	O	0	0
			31	31		

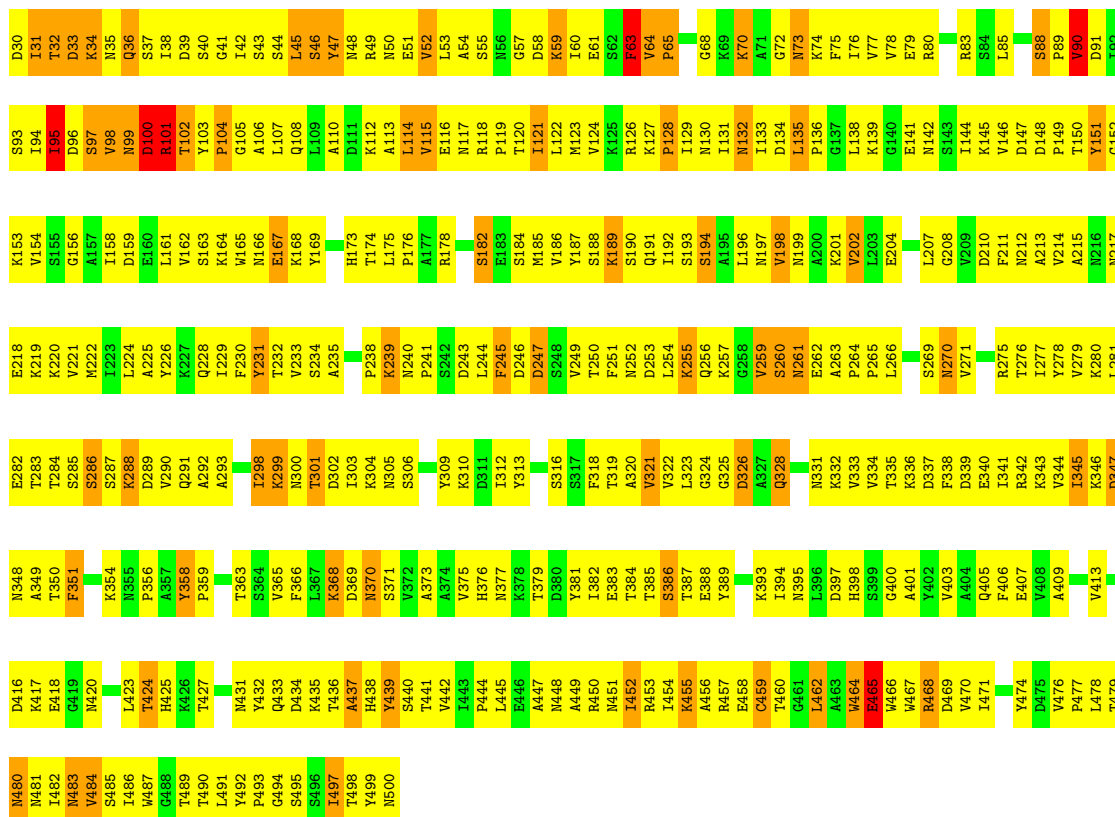
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

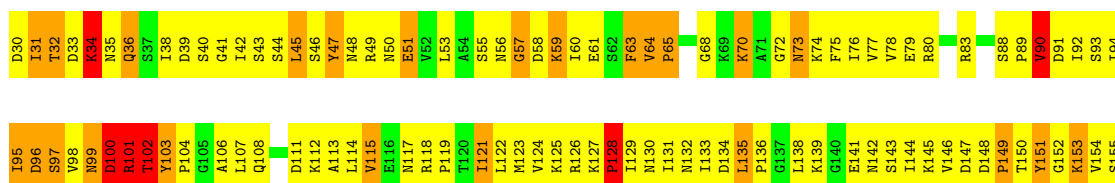
- Molecule 1: perfringolysin o

Chain A: 



- Molecule 1: perfringolysin o

Chain B: 



W487	E418	K354	V290	A225	G156
G488	M420	K355	Q291	Y226	A157
T489		P356	A292	K227	I158
L491	H425	A357	A293	Q228	D159
Y492	K426	Y358	K295	I229	E160
P493	T427	P359	A296	F230	L161
G494		L360	L297	Y231	V162
	M431	S361	K298	T232	S163
I497	Y432	Y362	L299	V233	K164
T498	Q433	T363	K300	S234	V165
Y499	D434	S364	N301	A235	N166
N500		V365	D302	D236	E167
	Q436	F366	K303	K239	K168
	T437	L367	T304	N240	Y169
	H438	F368	K305	P241	T172
	Y439	D369	S306	F245	H173
	S440	K370	Q307	D246	
	T441	S371	K308	D247	R178
	V442	Y372	Y309		
		A373	K310	F248	S182
	E446	A374	D311	T260	E183
	A447	V375	T312	F261	S184
	M448		Y313	Y262	M185
	A449	T379	E314	D263	I186
		D380	N315	L264	Y187
	M451	Y381	S316	K265	S188
	I452	L382	S317	Q266	K189
	R453	E383	F318	K267	S190
	I454	T384	T319	G268	Q191
	R455	K385	A320	V269	I192
	A456	S386	V321	S260	S193
	R457	T387	L322	T261	L196
	E458	E388	L323	E262	N197
	C459	Y389	G324	A263	V198
	T460	S390	G325	P264	
	G461	K391	D326	P265	N199
	L462	G392	A327	L266	V202
	A463	K393	Q328	S269	L203
	R464	L394	N331	N270	E204
	E465	N395	K332	V271	
	W466	L396	V333	A272	L207
	W467	D397	V334	Y273	G208
	R468	H398	T335	G274	V209
	D469	S399	K336	R275	D210
	W470	G400	D337	T276	F211
	I471	A401	F338	I277	N212
		Y402	D339	Y278	A213
		Y403	E340	V279	V214
	D475	A404	T341	K280	A215
	W476	Q405	R342	L281	N216
	P477	F406	K343	F282	N217
	T478	E407	V344	T283	E218
	Y479	W408	I345	T284	K219
	M480	A409	K346	S285	K220
	M481		D347	S286	V221
	I482		N348	S287	M222
	M483	E412		K288	T223
	W484	V413		D289	I224
	S485	V417	T351		
	T186				

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.00Å 214.11Å 47.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , 0.337	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7467	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

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	0.55	0/3776	1.07	32/5127 (0.6%)
1	B	0.55	0/3776	1.09	33/5127 (0.6%)
All	All	0.55	0/7552	1.08	65/10254 (0.6%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	VAL	N-CA-C	-11.26	102.66	112.12
1	A	135	LEU	CA-C-N	9.59	129.64	119.76
1	A	135	LEU	C-N-CA	9.59	129.64	119.76
1	B	64	VAL	CA-C-N	7.86	129.66	119.84
1	B	64	VAL	C-N-CA	7.86	129.66	119.84
1	A	182	SER	N-CA-C	-7.44	98.00	109.24
1	A	189	LYS	N-CA-C	-7.41	103.14	111.07
1	A	64	VAL	CA-C-N	7.40	129.09	119.84
1	A	64	VAL	C-N-CA	7.40	129.09	119.84
1	B	480	ASN	N-CA-C	-7.25	103.38	111.28
1	B	492	TYR	CA-C-N	7.23	127.68	120.52
1	B	492	TYR	C-N-CA	7.23	127.68	120.52
1	B	459	CYS	N-CA-C	7.03	121.60	110.70
1	B	189	LYS	N-CA-C	-6.99	103.59	111.07
1	B	218	GLU	N-CA-C	-6.87	103.54	112.68
1	B	336	LYS	N-CA-C	-6.80	104.80	113.23
1	B	476	VAL	CA-C-N	6.78	127.32	120.14
1	B	476	VAL	C-N-CA	6.78	127.32	120.14
1	B	90	VAL	N-CA-C	-6.74	106.30	111.62
1	B	214	VAL	N-CA-C	-6.63	102.55	111.44
1	B	462	LEU	N-CA-C	6.61	118.14	111.07
1	B	270	ASN	N-CA-C	6.57	118.38	108.46
1	A	459	CYS	N-CA-C	6.47	120.73	110.70
1	A	255	LYS	N-CA-C	-6.44	104.53	112.38
1	B	439	TYR	N-CA-C	-6.42	100.70	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	SER	N-CA-C	6.33	118.39	108.96
1	A	120	THR	N-CA-C	-6.23	102.31	110.53
1	B	135	LEU	CA-C-N	6.16	126.08	119.85
1	B	135	LEU	C-N-CA	6.16	126.08	119.85
1	A	462	LEU	N-CA-C	6.04	117.87	111.28
1	A	480	ASN	N-CA-C	-6.04	104.03	111.33
1	A	194	SER	N-CA-C	-6.00	105.61	113.12
1	B	32	THR	N-CA-C	-6.00	105.06	112.38
1	A	102	THR	N-CA-C	-5.96	100.18	109.72
1	A	101	ARG	N-CA-C	5.93	118.40	108.02
1	B	182	SER	N-CA-C	-5.86	100.44	109.52
1	A	358	TYR	CA-C-N	5.82	125.58	119.76
1	A	358	TYR	C-N-CA	5.82	125.58	119.76
1	A	240	ASN	CA-C-N	5.76	125.23	119.24
1	A	240	ASN	C-N-CA	5.76	125.23	119.24
1	A	336	LYS	N-CA-C	-5.73	105.78	112.89
1	B	101	ARG	N-CA-C	5.72	118.03	108.02
1	A	439	TYR	N-CA-C	-5.70	101.74	109.95
1	A	452	ILE	N-CA-C	5.70	115.75	108.12
1	A	36	GLN	N-CA-C	5.63	117.22	111.14
1	A	261	ASN	N-CA-C	-5.51	106.25	112.87
1	B	103	TYR	N-CA-C	5.49	112.96	108.07
1	B	255	LYS	N-CA-C	-5.45	105.73	112.38
1	A	33	ASP	N-CA-C	-5.42	106.74	113.19
1	B	102	THR	N-CA-C	-5.39	100.98	109.50
1	B	240	ASN	CA-C-N	5.39	124.85	119.24
1	B	240	ASN	C-N-CA	5.39	124.85	119.24
1	A	349	ALA	N-CA-C	-5.36	106.42	113.12
1	A	423	LEU	N-CA-C	5.33	117.40	108.23
1	A	218	GLU	N-CA-C	-5.32	105.60	112.68
1	B	36	GLN	N-CA-C	5.29	118.20	111.69
1	A	221	VAL	N-CA-C	5.25	116.05	108.48
1	B	386	SER	N-CA-C	5.15	116.12	108.60
1	A	32	THR	N-CA-C	-5.11	106.88	113.01
1	B	488	GLY	N-CA-C	5.11	118.22	110.97
1	B	34	LYS	N-CA-C	5.08	118.78	112.47
1	B	481	ASN	N-CA-C	5.05	116.82	108.13
1	B	358	TYR	CA-C-N	5.01	124.92	119.76
1	B	358	TYR	C-N-CA	5.01	124.92	119.76
1	A	270	ASN	N-CA-C	5.01	116.14	108.52

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	3705	0	3656	450	0
1	B	3705	0	3656	440	0
2	A	26	0	0	3	0
2	B	31	0	0	0	0
All	All	7467	0	7312	890	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 60.

All (890) 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:B:96:ASP:HB2	1:B:100:ASP:HB2	1.22	1.17
1:A:96:ASP:HB2	1:A:100:ASP:HB2	1.23	1.16
1:A:481:ASN:HB2	1:A:500:ASN:ND2	1.62	1.12
1:B:70:LYS:H	1:B:70:LYS:HD3	1.08	1.10
1:A:70:LYS:H	1:A:70:LYS:HD3	1.15	1.09
1:A:96:ASP:HB3	1:A:99:ASN:HB2	1.30	1.08
1:B:163:SER:HA	1:B:166:ASN:HD22	1.20	1.06
1:A:449:ALA:C	1:A:450:ARG:HD2	1.84	1.02
1:A:305:ASN:HA	1:A:310:LYS:HE2	1.41	1.02
1:B:339:ASP:HA	1:B:342:ARG:HD2	1.37	1.02
1:A:468:ARG:HH11	1:A:468:ARG:HB3	1.25	1.01
1:B:53:LEU:HD21	1:B:114:LEU:HD23	1.41	1.01
1:A:226:TYR:HB2	1:A:277:ILE:HB	1.42	1.01
1:A:481:ASN:HB2	1:A:500:ASN:HD22	0.87	1.00
1:A:38:ILE:HA	1:A:251:PHE:HB2	1.42	1.00
1:A:59:LYS:HZ2	1:A:59:LYS:HB2	1.26	1.00
1:A:462:LEU:HD22	1:A:466:TRP:HZ3	1.27	0.99
1:A:335:THR:HG22	1:A:337:ASP:H	1.27	0.98
1:B:393:LYS:HD2	1:B:442:VAL:HG11	1.45	0.97
1:B:130:ASN:HD21	1:B:145:LYS:HE2	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:SER:HB2	1:A:225:ALA:HB3	1.48	0.95
1:A:277:ILE:CD1	1:A:345:ILE:HA	1.97	0.94
1:B:335:THR:HG22	1:B:337:ASP:H	1.30	0.94
1:B:59:LYS:HB2	1:B:59:LYS:HZ2	1.30	0.94
1:B:96:ASP:CB	1:B:100:ASP:H	1.82	0.92
1:B:226:TYR:HB2	1:B:277:ILE:HB	1.48	0.92
1:A:96:ASP:HB3	1:A:100:ASP:H	1.33	0.92
1:A:479:THR:HG21	1:A:499:TYR:HB3	1.50	0.92
1:A:462:LEU:HD22	1:A:466:TRP:CZ3	2.05	0.90
1:A:96:ASP:CB	1:A:100:ASP:H	1.83	0.90
1:A:418:GLU:HB2	1:A:420:ASN:ND2	1.88	0.88
1:A:394:ILE:HD11	1:A:445:LEU:HD11	1.54	0.88
1:A:96:ASP:HB2	1:A:100:ASP:CB	2.04	0.87
1:B:107:LEU:HD11	1:B:126:ARG:HH11	1.37	0.87
1:B:96:ASP:HB2	1:B:100:ASP:CB	2.03	0.86
1:B:186:VAL:O	1:B:214:VAL:HG11	1.73	0.86
1:A:343:LYS:HG2	1:A:347:ASP:OD2	1.75	0.86
1:B:277:ILE:HD13	1:B:345:ILE:HA	1.58	0.86
1:A:222:MET:HE2	1:A:281:LEU:HD13	1.57	0.84
1:B:128:PRO:HG3	1:B:147:ASP:HA	1.59	0.84
1:B:182:SER:HB2	1:B:225:ALA:HB3	1.57	0.84
1:B:343:LYS:HA	1:B:346:LYS:HE3	1.58	0.84
1:B:90:VAL:O	1:B:363:THR:HG22	1.78	0.84
1:A:49:ARG:HG3	1:A:50:ASN:ND2	1.93	0.84
1:B:412:GLU:HG3	1:B:426:LYS:HD2	1.60	0.84
1:B:79:GLU:HB2	1:B:385:THR:OG1	1.77	0.83
1:A:277:ILE:HD13	1:A:345:ILE:HA	1.60	0.83
1:B:277:ILE:HG12	1:B:322:VAL:HG22	1.60	0.83
1:B:239:LYS:H	1:B:239:LYS:HD2	1.42	0.83
1:B:403:VAL:HG11	1:B:434:ASP:OD2	1.78	0.83
1:B:398:HIS:HA	1:B:486:ILE:HD11	1.59	0.83
1:B:43:SER:HA	1:B:368:LYS:HG3	1.60	0.82
1:A:103:TYR:CD1	1:A:154:VAL:HG21	2.14	0.82
1:B:449:ALA:C	1:B:450:ARG:HD2	2.03	0.82
1:A:220:LYS:HD2	1:A:290:VAL:HG21	1.62	0.82
1:B:104:PRO:HB2	1:B:235:ALA:HB2	1.61	0.82
1:B:96:ASP:HB2	1:B:100:ASP:H	1.43	0.82
1:A:224:LEU:HB2	1:A:279:VAL:HB	1.60	0.82
1:B:456:ALA:HB3	1:B:471:ILE:HG22	1.60	0.81
1:A:70:LYS:HD3	1:A:70:LYS:N	1.94	0.81
1:A:101:ARG:NE	1:A:101:ARG:H	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:HB	1:A:271:VAL:O	1.81	0.81
1:B:70:LYS:HD3	1:B:70:LYS:N	1.91	0.81
1:B:95:ILE:HG12	1:B:117:ASN:HB2	1.63	0.80
1:A:33:ASP:O	1:A:34:LYS:HG3	1.82	0.80
1:A:398:HIS:ND1	1:A:486:ILE:HD11	1.97	0.80
1:B:224:LEU:HB2	1:B:279:VAL:HB	1.64	0.79
1:B:38:ILE:HA	1:B:251:PHE:HB2	1.64	0.79
1:B:107:LEU:HD11	1:B:126:ARG:NH1	1.98	0.79
1:A:491:LEU:HD22	1:A:492:TYR:CE1	2.18	0.79
1:A:95:ILE:HG22	1:A:96:ASP:N	1.95	0.79
1:B:95:ILE:HG12	1:B:117:ASN:CB	2.13	0.79
1:A:178:ARG:HB2	1:A:229:ILE:HB	1.62	0.78
1:A:59:LYS:HB2	1:A:59:LYS:NZ	1.95	0.78
1:A:465:GLU:CD	1:A:465:GLU:H	1.89	0.78
1:B:148:ASP:O	1:B:153:LYS:HG2	1.83	0.78
1:B:402:TYR:HB3	1:B:490:THR:OG1	1.84	0.78
1:A:104:PRO:HG3	1:A:233:VAL:CG1	2.14	0.78
1:A:124:VAL:HG21	1:A:245:PHE:HD2	1.48	0.78
1:A:413:VAL:HG11	1:A:450:ARG:NH1	1.99	0.78
1:A:80:ARG:HG3	1:A:80:ARG:HH11	1.48	0.77
1:A:150:THR:O	1:A:154:VAL:HG23	1.83	0.77
1:A:458:GLU:O	1:A:467:TRP:HB3	1.84	0.77
1:B:457:ARG:HD3	1:B:469:ASP:OD2	1.84	0.77
1:A:418:GLU:HB2	1:A:420:ASN:HD22	1.48	0.77
1:A:454:ILE:HG21	1:A:484:VAL:HG21	1.67	0.77
1:A:49:ARG:HG3	1:A:50:ASN:HD22	1.49	0.76
1:A:306:SER:O	1:A:310:LYS:HG2	1.85	0.76
1:B:96:ASP:HB3	1:B:100:ASP:H	1.50	0.76
1:B:129:ILE:HG12	1:B:130:ASN:H	1.49	0.76
1:A:98:VAL:HG12	1:A:325:GLY:HA2	1.67	0.76
1:B:135:LEU:HD23	1:B:136:PRO:HD2	1.66	0.76
1:B:96:ASP:HB3	1:B:99:ASN:HB2	1.67	0.76
1:A:101:ARG:H	1:A:101:ARG:HE	1.31	0.76
1:A:104:PRO:HG3	1:A:233:VAL:HG11	1.68	0.76
1:A:305:ASN:HA	1:A:310:LYS:CE	2.15	0.75
1:A:210:ASP:OD2	1:A:213:ALA:HB2	1.87	0.75
1:A:339:ASP:HA	1:A:342:ARG:HD2	1.69	0.74
1:A:263:ALA:N	1:A:264:PRO:HD3	2.02	0.74
1:B:306:SER:O	1:B:310:LYS:HG2	1.88	0.74
1:A:144:ILE:HG13	1:A:145:LYS:H	1.52	0.74
1:A:144:ILE:HB	1:A:161:LEU:HD21	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HD22	1:A:492:TYR:CD1	2.23	0.74
1:B:457:ARG:NH2	1:B:465:GLU:HA	2.03	0.73
1:B:103:TYR:CD1	1:B:154:VAL:HG21	2.23	0.73
1:B:163:SER:HA	1:B:166:ASN:ND2	1.99	0.73
1:B:263:ALA:N	1:B:264:PRO:HD3	2.03	0.73
1:A:96:ASP:HB3	1:A:99:ASN:CB	2.14	0.73
1:B:335:THR:HG22	1:B:337:ASP:N	2.04	0.73
1:B:49:ARG:HG3	1:B:50:ASN:N	2.03	0.73
1:B:91:ASP:OD1	1:B:361:SER:OG	2.06	0.73
1:A:335:THR:HG21	1:A:340:GLU:HG3	1.69	0.73
1:A:34:LYS:C	1:A:34:LYS:HE2	2.14	0.73
1:B:112:LYS:HA	1:B:115:VAL:HG23	1.70	0.73
1:B:222:MET:HE1	1:B:298:ILE:HD11	1.71	0.73
1:B:70:LYS:H	1:B:70:LYS:CD	1.93	0.73
1:B:130:ASN:ND2	1:B:145:LYS:HE2	2.04	0.72
1:A:121:ILE:HD13	1:A:122:LEU:H	1.54	0.72
1:B:365:VAL:HG13	1:B:371:SER:O	1.88	0.72
1:A:158:ILE:O	1:A:162:VAL:HG23	1.89	0.72
1:B:398:HIS:ND1	1:B:486:ILE:HD11	2.04	0.72
1:A:123:MET:H	1:A:257:LYS:HE2	1.51	0.72
1:A:133:ILE:HG13	1:A:232:THR:O	1.89	0.72
1:A:196:LEU:HD22	1:A:225:ALA:HB2	1.72	0.72
1:B:230:PHE:HZ	1:B:275:ARG:NH1	1.88	0.72
1:B:55:SER:HB3	1:B:115:VAL:HG11	1.70	0.72
1:B:95:ILE:HG22	1:B:96:ASP:N	2.02	0.72
1:A:416:ASP:OD1	1:A:420:ASN:HB2	1.90	0.71
1:B:98:VAL:HG12	1:B:358:TYR:HD1	1.56	0.71
1:B:230:PHE:HB3	1:B:351:PHE:CE1	2.25	0.71
1:A:41:GLY:HA3	1:A:251:PHE:CE2	2.25	0.71
1:A:98:VAL:HG12	1:A:358:TYR:CD1	2.25	0.71
1:A:403:VAL:HG11	1:A:434:ASP:OD2	1.91	0.71
1:B:417:LYS:HB2	1:B:417:LYS:NZ	2.06	0.71
1:A:213:ALA:HB1	1:A:219:LYS:HG3	1.71	0.71
1:A:266:LEU:HD23	1:A:366:PHE:HA	1.73	0.71
1:A:468:ARG:HH11	1:A:468:ARG:CB	2.04	0.70
1:B:104:PRO:HG3	1:B:233:VAL:HG12	1.73	0.70
1:A:259:VAL:HG13	1:A:265:PRO:HD3	1.72	0.70
1:B:476:VAL:HG13	1:B:499:TYR:OH	1.91	0.70
1:B:366:PHE:CE1	1:B:373:ALA:HA	2.26	0.70
1:B:458:GLU:O	1:B:467:TRP:HB3	1.92	0.70
1:B:324:GLY:O	1:B:358:TYR:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HG12	1:B:130:ASN:N	2.06	0.70
1:B:96:ASP:HB3	1:B:99:ASN:CB	2.22	0.70
1:B:393:LYS:HD2	1:B:442:VAL:CG1	2.22	0.70
1:A:393:LYS:HD2	1:A:442:VAL:HG11	1.74	0.69
1:B:178:ARG:HB2	1:B:229:ILE:HB	1.73	0.69
1:A:107:LEU:O	1:A:121:ILE:HD13	1.92	0.69
1:B:222:MET:HE3	1:B:224:LEU:HD21	1.74	0.69
1:B:53:LEU:HD21	1:B:114:LEU:CD2	2.20	0.69
1:B:339:ASP:HA	1:B:342:ARG:CD	2.20	0.69
1:A:158:ILE:HD13	1:A:233:VAL:HG21	1.73	0.69
1:B:31:ILE:HD11	1:B:35:ASN:O	1.92	0.69
1:B:123:MET:H	1:B:257:LYS:HE2	1.57	0.69
1:B:287:SER:O	1:B:290:VAL:HG23	1.93	0.69
1:A:114:LEU:HA	1:A:119:PRO:HB3	1.74	0.68
1:B:199:ASN:HB3	1:B:202:VAL:HG23	1.72	0.68
1:B:398:HIS:HA	1:B:486:ILE:CD1	2.23	0.68
1:A:144:ILE:HG13	1:A:145:LYS:N	2.07	0.68
1:B:452:ILE:HD11	1:B:478:LEU:HD13	1.75	0.68
1:A:185:MET:SD	1:A:222:MET:HG3	2.34	0.68
1:B:192:ILE:HG12	1:B:223:ILE:HD12	1.76	0.68
1:A:228:GLN:HE21	1:A:228:GLN:HA	1.57	0.68
1:A:409:ALA:HB2	1:A:427:THR:HG22	1.75	0.67
1:A:134:ASP:CG	1:A:178:ARG:HH22	2.02	0.67
1:B:38:ILE:HG23	1:B:39:ASP:H	1.59	0.67
1:A:98:VAL:CG1	1:A:325:GLY:HA2	2.24	0.67
1:A:427:THR:HB	1:A:431:ASN:ND2	2.10	0.67
1:B:30:ASP:CA	1:B:36:GLN:HG2	2.25	0.67
1:B:46:SER:O	1:B:47:TYR:HB3	1.93	0.67
1:B:96:ASP:CB	1:B:100:ASP:HB2	2.13	0.67
1:B:479:THR:HG21	1:B:499:TYR:HB3	1.77	0.67
1:A:85:LEU:HD23	1:A:194:SER:HB3	1.75	0.67
1:A:94:ILE:HD12	1:A:359:PRO:HB2	1.76	0.66
1:A:107:LEU:HD11	1:A:126:ARG:HH11	1.59	0.66
1:A:110:ALA:HB2	1:A:266:LEU:HD11	1.77	0.66
1:A:46:SER:O	1:A:47:TYR:HB3	1.95	0.66
1:A:129:ILE:C	1:A:130:ASN:HD22	2.02	0.66
1:A:462:LEU:HB3	1:A:466:TRP:CE3	2.29	0.66
1:B:449:ALA:O	1:B:450:ARG:HD2	1.95	0.66
1:B:480:ASN:HB2	1:B:500:ASN:O	1.96	0.66
1:B:73:ASN:C	1:B:74:LYS:HG3	2.20	0.66
1:B:394:ILE:HG12	1:B:482:ILE:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG23	1:A:233:VAL:HG13	1.78	0.66
1:A:144:ILE:HD11	2:A:506:HOH:O	1.96	0.66
1:B:133:ILE:HD11	1:B:231:TYR:CD2	2.30	0.66
1:B:230:PHE:CE1	1:B:351:PHE:HB2	2.31	0.66
1:B:391:LYS:HG2	1:B:447:ALA:H	1.60	0.66
1:A:124:VAL:HG21	1:A:245:PHE:CD2	2.31	0.66
1:A:452:ILE:CD1	1:A:478:LEU:HD13	2.26	0.65
1:A:457:ARG:HG2	1:A:467:TRP:HB2	1.76	0.65
1:A:452:ILE:HD11	1:A:478:LEU:HD13	1.78	0.65
1:B:277:ILE:CD1	1:B:345:ILE:HA	2.27	0.65
1:A:312:ILE:HA	2:A:524:HOH:O	1.95	0.65
1:A:318:PHE:HD1	1:A:335:THR:O	1.79	0.65
1:A:97:SER:HB3	1:A:324:GLY:HA2	1.79	0.65
1:A:134:ASP:OD1	1:A:232:THR:HG23	1.97	0.65
1:A:68:GLY:HA2	1:A:76:ILE:O	1.97	0.64
1:B:49:ARG:HG3	1:B:50:ASN:H	1.62	0.64
1:B:413:VAL:HG11	1:B:450:ARG:NH1	2.12	0.64
1:A:98:VAL:HG12	1:A:358:TYR:HD1	1.62	0.64
1:A:96:ASP:HB2	1:A:100:ASP:H	1.62	0.64
1:A:366:PHE:CE1	1:A:373:ALA:HA	2.32	0.64
1:B:30:ASP:HA	1:B:36:GLN:HG2	1.80	0.64
1:A:130:ASN:C	1:A:131:ILE:HD12	2.22	0.64
1:A:199:ASN:HB3	1:A:202:VAL:HG23	1.79	0.64
1:A:309:TYR:HB3	1:A:313:TYR:CE1	2.32	0.64
1:B:135:LEU:CD2	1:B:136:PRO:HD2	2.26	0.64
1:B:96:ASP:HB2	1:B:100:ASP:N	2.10	0.64
1:B:128:PRO:HA	1:B:146:VAL:O	1.98	0.64
1:A:477:PRO:O	1:A:482:ILE:HD11	1.98	0.64
1:B:275:ARG:HD2	1:B:322:VAL:CG1	2.28	0.64
1:B:259:VAL:HG13	1:B:265:PRO:HD3	1.79	0.64
1:A:337:ASP:OD2	1:A:339:ASP:HB2	1.99	0.64
1:B:461:GLY:C	1:B:467:TRP:HE1	2.06	0.64
1:A:182:SER:HB2	1:A:225:ALA:CB	2.24	0.63
1:B:98:VAL:HG12	1:B:358:TYR:CD1	2.33	0.63
1:A:95:ILE:HG12	1:A:117:ASN:CB	2.29	0.63
1:A:305:ASN:CA	1:A:310:LYS:HE2	2.25	0.63
1:B:30:ASP:CG	1:B:36:GLN:HB3	2.23	0.63
1:B:305:ASN:HA	1:B:310:LYS:HE2	1.81	0.63
1:B:45:LEU:O	1:B:368:LYS:NZ	2.22	0.63
1:B:212:ASN:HA	1:B:215:ALA:HB3	1.80	0.63
1:A:449:ALA:O	1:A:450:ARG:HD2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASP:HA	1:A:342:ARG:CD	2.29	0.63
1:A:394:ILE:HG23	1:A:482:ILE:O	1.98	0.63
1:B:457:ARG:HH21	1:B:465:GLU:HA	1.63	0.63
1:A:31:ILE:HD11	1:A:35:ASN:O	1.98	0.62
1:A:75:PHE:HB3	1:A:389:TYR:HB2	1.81	0.62
1:B:291:GLN:O	1:B:295:LYS:HG3	2.00	0.62
1:A:107:LEU:N	1:A:107:LEU:HD12	2.15	0.62
1:A:187:TYR:HD1	1:A:381:TYR:HE1	1.46	0.62
1:A:409:ALA:HB1	1:A:425:HIS:CE1	2.34	0.62
1:A:138:LEU:CD1	1:A:141:GLU:HG3	2.30	0.62
1:B:319:THR:HA	1:B:333:VAL:O	2.00	0.62
1:A:103:TYR:OH	1:A:150:THR:HA	2.00	0.62
1:B:60:ILE:HG12	1:B:61:GLU:N	2.14	0.62
1:B:369:ASP:OD2	1:B:371:SER:HB3	1.99	0.62
1:A:95:ILE:CG2	1:A:96:ASP:N	2.62	0.61
1:A:269:SER:HB3	1:A:365:VAL:HG23	1.82	0.61
1:A:130:ASN:HD21	1:A:145:LYS:HE2	1.65	0.61
1:A:138:LEU:HD12	1:A:141:GLU:HG3	1.82	0.61
1:A:222:MET:O	1:A:281:LEU:HD12	2.00	0.61
1:A:413:VAL:HG12	1:A:448:ASN:O	2.00	0.61
1:B:394:ILE:HA	1:B:482:ILE:O	2.00	0.61
1:B:486:ILE:HD12	1:B:486:ILE:O	2.01	0.61
1:B:465:GLU:CD	1:B:465:GLU:H	2.08	0.61
1:A:298:ILE:C	1:A:300:ASN:H	2.09	0.61
1:B:486:ILE:HD12	1:B:486:ILE:C	2.25	0.61
1:A:89:PRO:HD2	1:A:375:VAL:O	2.01	0.60
1:A:90:VAL:O	1:A:363:THR:HG22	2.00	0.60
1:A:491:LEU:C	1:A:493:PRO:HD3	2.25	0.60
1:B:48:ASN:HD22	1:B:51:GLU:HB2	1.66	0.60
1:B:230:PHE:CD1	1:B:351:PHE:HB2	2.36	0.60
1:B:89:PRO:HD2	1:B:375:VAL:O	2.01	0.60
1:A:107:LEU:HD11	1:A:126:ARG:NH1	2.17	0.60
1:A:222:MET:HE1	1:A:298:ILE:HD11	1.83	0.60
1:A:275:ARG:HH21	1:A:348:ASN:C	2.09	0.60
1:B:220:LYS:HD2	1:B:290:VAL:HG21	1.83	0.60
1:B:263:ALA:N	1:B:264:PRO:CD	2.62	0.60
1:B:369:ASP:CG	1:B:371:SER:HB3	2.27	0.60
1:B:401:ALA:HB3	1:B:489:THR:HA	1.84	0.60
1:A:53:LEU:O	1:A:375:VAL:HA	2.02	0.59
1:B:154:VAL:O	1:B:158:ILE:HG13	2.02	0.59
1:B:198:VAL:HG11	1:B:278:TYR:OH	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLN:HE21	1:B:295:LYS:HD2	1.65	0.59
1:A:397:ASP:HB3	1:A:485:SER:OG	2.02	0.59
1:B:125:LYS:HD3	1:B:246:ASP:OD2	2.01	0.59
1:A:30:ASP:CA	1:A:36:GLN:HG2	2.32	0.59
1:B:33:ASP:O	1:B:34:LYS:HG3	2.01	0.59
1:B:263:ALA:H	1:B:264:PRO:HD3	1.67	0.59
1:B:454:ILE:HG21	1:B:484:VAL:HG21	1.83	0.59
1:B:462:LEU:HD23	1:B:462:LEU:O	2.02	0.59
1:B:259:VAL:HG12	1:B:260:SER:N	2.18	0.59
1:A:95:ILE:HG22	1:A:96:ASP:H	1.66	0.59
1:A:104:PRO:HG3	1:A:233:VAL:HG12	1.85	0.59
1:B:189:LYS:HG2	1:B:211:PHE:CZ	2.38	0.59
1:B:293:ALA:HB1	1:B:313:TYR:CE2	2.38	0.59
1:B:133:ILE:HD13	1:B:135:LEU:HD12	1.85	0.59
1:B:207:LEU:HD22	1:B:280:LYS:HB2	1.85	0.59
1:A:49:ARG:CG	1:A:50:ASN:ND2	2.64	0.59
1:A:319:THR:HA	1:A:333:VAL:O	2.03	0.59
1:A:462:LEU:O	1:A:462:LEU:HD23	2.03	0.59
1:B:68:GLY:HA2	1:B:76:ILE:O	2.03	0.59
1:B:124:VAL:HG21	1:B:245:PHE:HD2	1.68	0.59
1:A:228:GLN:HA	1:A:228:GLN:NE2	2.17	0.58
1:B:134:ASP:OD1	1:B:232:THR:HG23	2.03	0.58
1:B:391:LYS:HG2	1:B:447:ALA:N	2.18	0.58
1:B:491:LEU:HD22	1:B:492:TYR:CE1	2.38	0.58
1:A:41:GLY:HA3	1:A:251:PHE:CD2	2.39	0.58
1:A:114:LEU:O	1:A:114:LEU:HD12	2.04	0.58
1:B:222:MET:HE1	1:B:298:ILE:CD1	2.34	0.58
1:A:97:SER:C	1:A:99:ASN:H	2.11	0.58
1:A:254:LEU:O	1:A:259:VAL:HG23	2.03	0.58
1:B:60:ILE:CD1	1:B:382:ILE:HD11	2.34	0.58
1:A:263:ALA:N	1:A:264:PRO:CD	2.67	0.58
1:A:275:ARG:HB2	1:A:323:LEU:O	2.04	0.58
1:B:275:ARG:HB2	1:B:323:LEU:O	2.04	0.58
1:A:79:GLU:HB2	1:A:385:THR:OG1	2.04	0.58
1:A:207:LEU:HD21	1:A:278:TYR:O	2.02	0.58
1:B:83:ARG:NE	1:B:383:GLU:OE2	2.37	0.58
1:B:346:LYS:C	1:B:348:ASN:H	2.12	0.58
1:A:275:ARG:HH21	1:A:348:ASN:CA	2.16	0.57
1:B:365:VAL:HG13	1:B:371:SER:C	2.29	0.57
1:A:48:ASN:O	1:A:52:VAL:HG13	2.03	0.57
1:B:111:ASP:O	1:B:114:LEU:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:TRP:C	1:B:466:TRP:H	2.13	0.57
1:A:30:ASP:CB	1:A:36:GLN:HG2	2.35	0.57
1:A:38:ILE:HG23	1:A:39:ASP:H	1.69	0.57
1:A:80:ARG:HH11	1:A:80:ARG:CG	2.17	0.57
1:A:239:LYS:H	1:A:239:LYS:HD2	1.69	0.57
1:B:96:ASP:HB3	1:B:99:ASN:CG	2.30	0.57
1:A:230:PHE:CE1	1:A:351:PHE:HB2	2.40	0.57
1:A:413:VAL:HG11	1:A:450:ARG:CZ	2.35	0.57
1:A:484:VAL:CG2	1:A:497:ILE:HD12	2.34	0.57
1:A:133:ILE:HD11	1:A:231:TYR:CD2	2.40	0.57
1:A:432:TYR:O	1:A:433:GLN:HG3	2.04	0.57
1:B:77:VAL:O	1:B:386:SER:HA	2.05	0.57
1:B:284:THR:OG1	1:B:315:ASN:HB3	2.04	0.57
1:A:98:VAL:HA	1:A:358:TYR:CD1	2.39	0.57
1:A:287:SER:O	1:A:290:VAL:HG23	2.04	0.57
1:A:409:ALA:CB	1:A:427:THR:HG22	2.34	0.57
1:B:104:PRO:CB	1:B:235:ALA:HB2	2.34	0.56
1:A:471:ILE:HD13	1:A:495:SER:HB2	1.85	0.56
1:B:103:TYR:HB2	1:B:104:PRO:HD2	1.87	0.56
1:A:158:ILE:CD1	1:A:233:VAL:HG21	2.35	0.56
1:A:365:VAL:HG13	1:A:371:SER:O	2.05	0.56
1:A:394:ILE:HA	1:A:482:ILE:O	2.05	0.56
1:B:95:ILE:CG1	1:B:117:ASN:HB2	2.35	0.56
1:B:230:PHE:CE2	1:B:274:GLY:HA2	2.40	0.56
1:A:298:ILE:HG22	1:A:299:LYS:N	2.20	0.56
1:B:112:LYS:O	1:B:113:ALA:C	2.47	0.56
1:B:468:ARG:HB3	1:B:468:ARG:HH11	1.69	0.56
1:A:31:ILE:HD12	1:A:31:ILE:H	1.70	0.56
1:A:134:ASP:OD2	1:A:231:TYR:HB2	2.04	0.56
1:B:96:ASP:HB3	1:B:99:ASN:OD1	2.04	0.56
1:A:226:TYR:CB	1:A:277:ILE:HB	2.27	0.56
1:A:401:ALA:HB3	1:A:489:THR:HA	1.87	0.56
1:B:104:PRO:HG3	1:B:233:VAL:CG1	2.34	0.56
1:B:230:PHE:CD2	1:B:274:GLY:HA2	2.41	0.56
1:B:60:ILE:HD11	1:B:382:ILE:HD11	1.88	0.56
1:B:150:THR:O	1:B:154:VAL:HG23	2.06	0.55
1:B:101:ARG:H	1:B:101:ARG:NE	2.04	0.55
1:B:293:ALA:HB1	1:B:313:TYR:HE2	1.71	0.55
1:A:346:LYS:C	1:A:348:ASN:H	2.13	0.55
1:A:189:LYS:O	1:A:193:SER:HB2	2.06	0.55
1:A:238:PRO:HB3	1:A:244:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ASN:CB	1:A:500:ASN:ND2	2.54	0.55
1:B:207:LEU:HD21	1:B:278:TYR:O	2.07	0.55
1:A:230:PHE:HZ	1:A:275:ARG:NH1	2.05	0.55
1:B:209:VAL:HG12	1:B:211:PHE:H	1.72	0.55
1:A:186:VAL:O	1:A:214:VAL:HG11	2.07	0.54
1:B:94:ILE:HD13	1:B:359:PRO:HB2	1.88	0.54
1:B:138:LEU:HD12	1:B:141:GLU:HG3	1.89	0.54
1:A:407:GLU:HA	1:A:431:ASN:OD1	2.08	0.54
1:B:151:TYR:O	1:B:152:GLY:C	2.47	0.54
1:B:452:ILE:O	1:B:476:VAL:N	2.37	0.54
1:A:163:SER:HA	1:A:166:ASN:ND2	2.22	0.54
1:B:226:TYR:CE1	1:B:345:ILE:HD13	2.42	0.54
1:B:166:ASN:O	1:B:169:TYR:C	2.51	0.54
1:B:464:TRP:HA	1:B:467:TRP:CE3	2.42	0.54
1:B:189:LYS:HG2	1:B:211:PHE:CE1	2.42	0.54
1:B:456:ALA:H	1:B:471:ILE:HG23	1.72	0.54
1:A:298:ILE:C	1:A:300:ASN:N	2.64	0.54
1:A:452:ILE:O	1:A:476:VAL:N	2.33	0.54
1:A:465:GLU:CD	1:A:465:GLU:N	2.65	0.54
1:B:259:VAL:O	1:B:260:SER:HB3	2.08	0.54
1:B:72:GLY:O	1:B:74:LYS:N	2.38	0.54
1:A:156:GLY:O	1:A:159:ASP:HB2	2.08	0.53
1:A:214:VAL:HA	1:A:219:LYS:O	2.09	0.53
1:A:281:LEU:HD12	1:A:281:LEU:N	2.23	0.53
1:B:38:ILE:HG23	1:B:39:ASP:N	2.22	0.53
1:B:304:LYS:HA	1:B:309:TYR:HD2	1.74	0.53
1:B:457:ARG:CD	1:B:469:ASP:OD2	2.55	0.53
1:A:42:ILE:O	1:A:45:LEU:HB2	2.09	0.53
1:A:63:PHE:CD1	1:A:63:PHE:C	2.85	0.53
1:A:186:VAL:HG22	1:A:192:ILE:HD13	1.89	0.53
1:B:59:LYS:HB2	1:B:59:LYS:NZ	2.10	0.53
1:B:72:GLY:C	1:B:74:LYS:H	2.16	0.53
1:B:107:LEU:HB2	1:B:122:LEU:HB2	1.90	0.53
1:B:276:THR:CG2	1:B:278:TYR:CE1	2.92	0.53
1:A:187:TYR:HD1	1:A:381:TYR:CE1	2.25	0.53
1:B:83:ARG:CB	1:B:381:TYR:CZ	2.91	0.53
1:B:456:ALA:HB3	1:B:471:ILE:CG2	2.34	0.53
1:A:167:GLU:N	1:A:167:GLU:OE2	2.41	0.53
1:A:259:VAL:O	1:A:260:SER:HB3	2.09	0.53
1:A:259:VAL:HG12	1:A:260:SER:N	2.23	0.53
1:A:394:ILE:HG23	1:A:482:ILE:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TRP:C	1:A:466:TRP:H	2.16	0.53
1:B:58:ASP:OD2	1:B:190:SER:CB	2.56	0.53
1:B:207:LEU:HD11	1:B:278:TYR:HB3	1.90	0.53
1:A:99:ASN:N	1:A:99:ASN:OD1	2.42	0.53
1:B:391:LYS:HG3	1:B:447:ALA:HB2	1.90	0.53
1:B:491:LEU:HD22	1:B:492:TYR:CD1	2.44	0.53
1:A:41:GLY:HA3	1:A:251:PHE:CZ	2.44	0.52
1:A:113:ALA:HA	1:A:118:ARG:NH1	2.24	0.52
1:A:129:ILE:HG12	1:A:130:ASN:H	1.74	0.52
1:A:335:THR:HG22	1:A:337:ASP:N	2.10	0.52
1:A:457:ARG:HD3	1:A:469:ASP:OD2	2.08	0.52
1:B:253:ASP:O	1:B:257:LYS:HG3	2.08	0.52
1:B:189:LYS:O	1:B:193:SER:HB2	2.08	0.52
1:B:491:LEU:O	1:B:493:PRO:HD3	2.09	0.52
1:A:63:PHE:C	1:A:63:PHE:HD1	2.18	0.52
1:A:114:LEU:HD12	1:A:114:LEU:C	2.34	0.52
1:A:188:SER:O	1:A:192:ILE:HG22	2.09	0.52
1:A:107:LEU:HB2	1:A:122:LEU:HB2	1.91	0.52
1:B:366:PHE:CZ	1:B:373:ALA:HA	2.44	0.52
1:A:30:ASP:HA	1:A:36:GLN:HG2	1.90	0.52
1:B:48:ASN:ND2	1:B:51:GLU:HB2	2.24	0.52
1:B:93:SER:O	1:B:117:ASN:ND2	2.40	0.52
1:B:208:GLY:O	1:B:280:LYS:NZ	2.41	0.52
1:A:33:ASP:C	1:A:34:LYS:HG3	2.35	0.52
1:A:480:ASN:HB2	1:A:500:ASN:O	2.10	0.52
1:B:224:LEU:HD11	1:B:281:LEU:HD11	1.92	0.52
1:B:427:THR:HB	1:B:431:ASN:ND2	2.25	0.52
1:B:433:GLN:O	1:B:435:LYS:NZ	2.41	0.52
1:A:103:TYR:CE1	1:A:154:VAL:HG21	2.45	0.52
1:A:325:GLY:HA3	1:A:358:TYR:CD1	2.45	0.52
1:B:150:THR:HB	1:B:153:LYS:HB2	1.92	0.52
1:B:230:PHE:HB3	1:B:351:PHE:CZ	2.43	0.52
1:A:96:ASP:CB	1:A:99:ASN:HB2	2.22	0.52
1:B:224:LEU:CD1	1:B:281:LEU:HD11	2.39	0.52
1:B:269:SER:OG	1:B:365:VAL:HG23	2.09	0.52
1:B:441:THR:CG2	1:B:442:VAL:N	2.72	0.52
1:A:77:VAL:O	1:A:386:SER:HA	2.09	0.52
1:A:290:VAL:O	1:A:291:GLN:C	2.51	0.52
1:B:402:TYR:HB3	1:B:490:THR:HG1	1.74	0.52
1:B:434:ASP:O	1:B:435:LYS:HD3	2.10	0.52
1:A:275:ARG:HD2	1:A:322:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HD12	1:A:345:ILE:HA	1.89	0.52
1:B:222:MET:HE2	1:B:281:LEU:HD13	1.92	0.52
1:A:85:LEU:CD2	1:A:194:SER:HB3	2.40	0.51
1:B:130:ASN:HB2	1:B:236:ASP:OD1	2.10	0.51
1:B:144:ILE:HG13	1:B:145:LYS:H	1.75	0.51
1:A:60:ILE:HD11	1:A:382:ILE:HD11	1.92	0.51
1:A:298:ILE:O	1:A:300:ASN:N	2.43	0.51
1:A:450:ARG:HD2	1:A:450:ARG:N	2.25	0.51
1:B:78:VAL:HG11	1:B:80:ARG:HE	1.74	0.51
1:B:403:VAL:CG1	1:B:434:ASP:OD2	2.55	0.51
1:A:103:TYR:HB2	1:A:104:PRO:HD2	1.92	0.51
1:A:31:ILE:HG13	1:A:252:ASN:CG	2.36	0.51
1:A:57:GLY:HA3	1:A:379:THR:HB	1.93	0.51
1:A:133:ILE:HD13	1:A:135:LEU:HD12	1.93	0.51
1:B:219:LYS:HA	1:B:283:THR:O	2.11	0.51
1:B:318:PHE:O	1:B:341:ILE:HD11	2.11	0.51
1:A:228:GLN:HE21	1:A:228:GLN:CA	2.18	0.51
1:A:340:GLU:O	1:A:344:VAL:HG23	2.10	0.51
1:B:254:LEU:O	1:B:259:VAL:HG23	2.10	0.51
1:B:481:ASN:HB2	1:B:500:ASN:HD22	1.74	0.51
1:A:343:LYS:HA	1:A:346:LYS:HE3	1.93	0.51
1:A:394:ILE:O	1:A:442:VAL:HA	2.11	0.51
1:B:101:ARG:HB2	1:B:151:TYR:CE1	2.45	0.51
1:B:131:ILE:HG23	1:B:233:VAL:HG13	1.93	0.51
1:A:497:ILE:O	1:A:497:ILE:HG23	2.10	0.51
1:B:112:LYS:HA	1:B:115:VAL:CG2	2.39	0.51
1:A:83:ARG:NE	1:A:383:GLU:OE2	2.44	0.51
1:A:409:ALA:HB1	1:A:425:HIS:HE1	1.76	0.51
1:B:95:ILE:O	1:B:97:SER:N	2.44	0.51
1:B:214:VAL:HA	1:B:219:LYS:O	2.11	0.51
1:A:366:PHE:O	1:A:370:ASN:HA	2.11	0.51
1:A:462:LEU:HB3	1:A:466:TRP:HE3	1.76	0.51
1:B:128:PRO:HG3	1:B:147:ASP:CA	2.36	0.51
1:A:318:PHE:O	1:A:341:ILE:HD11	2.11	0.50
1:B:126:ARG:HB3	1:B:149:PRO:HD2	1.92	0.50
1:B:256:GLN:OE1	1:B:256:GLN:HA	2.11	0.50
1:A:104:PRO:HB2	1:A:235:ALA:HB2	1.93	0.50
1:A:324:GLY:O	1:A:358:TYR:HB2	2.11	0.50
1:B:32:THR:C	1:B:34:LYS:H	2.19	0.50
1:B:42:ILE:O	1:B:45:LEU:HB2	2.11	0.50
1:B:446:GLU:O	1:B:448:ASN:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:GLU:OE1	1:A:460:THR:HB	2.12	0.50
1:B:45:LEU:HD11	1:B:259:VAL:HG12	1.92	0.50
1:B:114:LEU:HA	1:B:119:PRO:HB3	1.93	0.50
1:B:222:MET:CE	1:B:224:LEU:HD21	2.41	0.50
1:A:134:ASP:OD1	1:A:178:ARG:NH2	2.45	0.50
1:A:436:THR:O	1:A:437:ALA:C	2.55	0.50
1:B:107:LEU:N	1:B:107:LEU:HD12	2.27	0.50
1:B:226:TYR:CB	1:B:277:ILE:HB	2.33	0.50
1:B:232:THR:HB	1:B:271:VAL:O	2.12	0.50
1:A:130:ASN:HD22	1:A:130:ASN:N	2.08	0.50
1:B:98:VAL:HG12	1:B:325:GLY:HA2	1.93	0.50
1:A:73:ASN:C	1:A:74:LYS:HG3	2.36	0.50
1:B:409:ALA:HB1	1:B:425:HIS:CE1	2.46	0.50
1:A:132:ASN:OD1	1:A:234:SER:O	2.30	0.50
1:A:304:LYS:HA	1:A:309:TYR:HD2	1.76	0.50
1:A:319:THR:OG1	1:A:334:VAL:HG13	2.12	0.50
1:B:30:ASP:CB	1:B:36:GLN:HG2	2.41	0.50
1:B:49:ARG:HG3	1:B:50:ASN:CG	2.36	0.50
1:A:94:ILE:CD1	1:A:359:PRO:HB2	2.42	0.50
1:B:210:ASP:O	1:B:211:PHE:C	2.55	0.50
1:A:105:GLY:O	1:A:106:ALA:C	2.55	0.49
1:A:133:ILE:HG23	1:A:135:LEU:H	1.77	0.49
1:B:30:ASP:HA	1:B:36:GLN:CG	2.41	0.49
1:B:185:MET:SD	1:B:291:GLN:HG3	2.52	0.49
1:A:112:LYS:HA	1:A:115:VAL:HG23	1.94	0.49
1:A:186:VAL:HG13	1:A:192:ILE:HB	1.93	0.49
1:B:417:LYS:HB2	1:B:417:LYS:HZ2	1.74	0.49
1:B:63:PHE:HD1	1:B:64:VAL:N	2.10	0.49
1:B:277:ILE:HD11	1:B:348:ASN:HB2	1.94	0.49
1:B:441:THR:HG22	1:B:442:VAL:N	2.26	0.49
1:A:464:TRP:O	1:A:466:TRP:N	2.46	0.49
1:B:292:ALA:O	1:B:293:ALA:C	2.55	0.49
1:B:138:LEU:HG	1:B:142:ASN:HB3	1.93	0.49
1:B:224:LEU:HD12	1:B:279:VAL:HB	1.95	0.49
1:B:343:LYS:HG2	1:B:347:ASP:OD2	2.12	0.49
1:B:491:LEU:C	1:B:493:PRO:HD3	2.38	0.49
1:A:182:SER:HB3	1:A:196:LEU:HD23	1.94	0.49
1:A:96:ASP:CB	1:A:100:ASP:HB2	2.16	0.49
1:A:127:LYS:HD2	1:A:246:ASP:HA	1.94	0.49
1:A:131:ILE:HD12	1:A:131:ILE:N	2.27	0.49
1:B:228:GLN:NE2	1:B:228:GLN:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:O	1:B:233:VAL:HG23	2.12	0.49
1:B:335:THR:HG21	1:B:340:GLU:HG3	1.94	0.49
1:B:407:GLU:HG3	1:B:432:TYR:CE2	2.48	0.49
1:A:61:GLU:HG3	1:A:61:GLU:O	2.13	0.49
1:B:129:ILE:CG1	1:B:130:ASN:N	2.76	0.49
1:B:320:ALA:HB2	1:B:341:ILE:HD12	1.94	0.49
1:B:92:ILE:O	1:B:361:SER:HA	2.13	0.49
1:B:150:THR:O	1:B:154:VAL:N	2.39	0.49
1:A:441:THR:HG22	1:A:442:VAL:N	2.27	0.48
1:A:457:ARG:NH2	1:A:464:TRP:CE2	2.81	0.48
1:B:265:PRO:CG	1:B:367:LEU:HD12	2.43	0.48
1:A:98:VAL:HG12	1:A:358:TYR:CE1	2.47	0.48
1:A:219:LYS:HA	1:A:283:THR:O	2.12	0.48
1:A:454:ILE:HD11	1:A:482:ILE:HG21	1.94	0.48
1:B:112:LYS:O	1:B:115:VAL:HG23	2.13	0.48
1:B:265:PRO:HG2	1:B:367:LEU:HD12	1.95	0.48
1:B:457:ARG:HG2	1:B:467:TRP:HB2	1.94	0.48
1:A:168:LYS:HD3	1:A:169:TYR:HE1	1.77	0.48
1:A:433:GLN:HB3	1:A:435:LYS:NZ	2.28	0.48
1:A:480:ASN:CB	1:A:500:ASN:O	2.61	0.48
1:B:158:ILE:O	1:B:162:VAL:HG23	2.13	0.48
1:A:491:LEU:O	1:A:493:PRO:HD3	2.13	0.48
1:B:405:GLN:HG2	1:B:433:GLN:C	2.38	0.48
1:A:74:LYS:HA	1:A:389:TYR:O	2.13	0.48
1:A:275:ARG:HD2	1:A:322:VAL:HG13	1.95	0.48
1:A:318:PHE:CD1	1:A:335:THR:O	2.64	0.48
1:B:356:PRO:HB2	1:B:358:TYR:CE2	2.49	0.48
1:A:230:PHE:CD1	1:A:351:PHE:HB2	2.48	0.48
1:A:457:ARG:HH21	1:A:464:TRP:CD1	2.32	0.48
1:B:41:GLY:HA3	1:B:251:PHE:CE1	2.49	0.48
1:B:150:THR:O	1:B:151:TYR:C	2.57	0.48
1:B:217:ASN:HB2	1:B:384:THR:HG21	1.94	0.48
1:B:259:VAL:HG12	1:B:260:SER:H	1.75	0.48
1:B:275:ARG:HA	1:B:324:GLY:HA3	1.94	0.48
1:B:327:ALA:O	1:B:328:GLN:C	2.56	0.48
1:B:436:THR:O	1:B:437:ALA:C	2.56	0.48
1:A:135:LEU:CD2	1:A:136:PRO:HD2	2.43	0.48
1:A:261:ASN:HB2	1:A:262:GLU:OE2	2.14	0.48
1:B:281:LEU:HD12	1:B:281:LEU:N	2.28	0.48
1:B:398:HIS:NE2	1:B:435:LYS:O	2.46	0.48
1:B:427:THR:HB	1:B:431:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:N	1:A:101:ARG:CD	2.77	0.48
1:B:446:GLU:C	1:B:448:ASN:H	2.21	0.48
1:A:453:ARG:HH11	1:A:453:ARG:HG2	1.78	0.48
1:B:156:GLY:O	1:B:159:ASP:HB2	2.14	0.48
1:A:74:LYS:NZ	1:A:388:GLU:HB3	2.27	0.47
1:A:163:SER:HA	1:A:166:ASN:HD22	1.77	0.47
1:A:196:LEU:HD22	1:A:225:ALA:CB	2.43	0.47
1:A:328:GLN:O	1:A:331:ASN:HB3	2.14	0.47
1:A:456:ALA:HB3	1:A:471:ILE:HG22	1.96	0.47
1:B:83:ARG:O	1:B:380:ASP:HA	2.13	0.47
1:B:230:PHE:CZ	1:B:275:ARG:NH1	2.77	0.47
1:A:70:LYS:H	1:A:70:LYS:CD	2.01	0.47
1:A:151:TYR:O	1:A:152:GLY:C	2.56	0.47
1:A:453:ARG:HD2	1:A:474:TYR:HE2	1.78	0.47
1:B:226:TYR:CZ	1:B:345:ILE:HD13	2.48	0.47
1:B:307:GLN:O	1:B:311:ASP:OD1	2.32	0.47
1:A:88:SER:HA	1:A:375:VAL:O	2.14	0.47
1:A:483:ASN:OD1	1:A:498:THR:O	2.32	0.47
1:A:60:ILE:CD1	1:A:382:ILE:HD11	2.43	0.47
1:A:31:ILE:HD12	1:A:31:ILE:N	2.30	0.47
1:A:212:ASN:HA	1:A:215:ALA:HB3	1.96	0.47
1:A:286:SER:HB2	1:A:388:GLU:HG2	1.96	0.47
1:A:464:TRP:HA	1:A:467:TRP:CE3	2.50	0.47
1:B:259:VAL:O	1:B:260:SER:CB	2.62	0.47
1:B:287:SER:O	1:B:289:ASP:N	2.47	0.47
1:B:56:ASN:HD21	1:B:59:LYS:NZ	2.13	0.47
1:B:297:LEU:HD13	1:B:313:TYR:CZ	2.50	0.47
1:A:96:ASP:HB2	1:A:100:ASP:N	2.30	0.47
1:B:325:GLY:HA3	1:B:358:TYR:CD1	2.50	0.47
1:B:152:GLY:O	1:B:153:LYS:C	2.57	0.47
1:B:433:GLN:HB3	1:B:435:LYS:HZ1	1.80	0.47
1:A:253:ASP:O	1:A:257:LYS:HG3	2.14	0.46
1:B:30:ASP:OD2	1:B:36:GLN:HB3	2.15	0.46
1:B:133:ILE:HG13	1:B:232:THR:O	2.14	0.46
1:B:266:LEU:HD23	1:B:366:PHE:HA	1.96	0.46
1:B:297:LEU:HD12	1:B:304:LYS:HD2	1.97	0.46
1:B:328:GLN:O	1:B:331:ASN:HB3	2.15	0.46
1:A:124:VAL:HG11	1:A:254:LEU:CD2	2.45	0.46
1:A:150:THR:C	1:A:154:VAL:HG23	2.40	0.46
1:A:168:LYS:HG2	1:A:169:TYR:CE1	2.50	0.46
1:A:174:THR:HB	1:A:350:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ASN:CB	1:B:500:ASN:O	2.63	0.46
1:A:343:LYS:HA	1:A:346:LYS:CE	2.45	0.46
1:A:416:ASP:OD2	1:A:420:ASN:N	2.37	0.46
1:A:457:ARG:HB3	1:A:464:TRP:CZ3	2.50	0.46
1:B:78:VAL:HG12	1:B:79:GLU:N	2.30	0.46
1:A:54:ALA:HA	1:A:376:HIS:HB2	1.96	0.46
1:A:351:PHE:CD1	1:A:351:PHE:C	2.93	0.46
1:B:83:ARG:HB2	1:B:381:TYR:CZ	2.50	0.46
1:B:168:LYS:HD3	1:B:169:TYR:HE1	1.79	0.46
1:B:464:TRP:O	1:B:466:TRP:N	2.48	0.46
1:A:80:ARG:CG	1:A:80:ARG:NH1	2.78	0.46
1:A:123:MET:N	1:A:257:LYS:HE2	2.25	0.46
1:A:174:THR:HB	1:A:350:THR:CG2	2.45	0.46
1:A:383:GLU:O	1:A:383:GLU:HG2	2.15	0.46
1:A:405:GLN:HG3	1:A:459:CYS:SG	2.56	0.46
1:A:454:ILE:O	1:A:455:LYS:HB2	2.16	0.46
1:B:89:PRO:HG2	1:B:375:VAL:HB	1.97	0.46
1:B:303:ILE:C	1:B:305:ASN:H	2.23	0.46
1:B:332:LYS:HG2	1:B:333:VAL:N	2.30	0.46
1:A:281:LEU:HD12	1:A:281:LEU:H	1.80	0.46
1:B:74:LYS:HZ1	1:B:388:GLU:CD	2.23	0.46
1:B:88:SER:HA	1:B:375:VAL:O	2.15	0.46
1:B:106:ALA:HB1	1:B:121:ILE:HD11	1.97	0.46
1:A:491:LEU:O	1:A:491:LEU:HD23	2.16	0.46
1:B:45:LEU:HD11	1:B:259:VAL:CG1	2.46	0.46
1:B:398:HIS:O	1:B:438:HIS:N	2.48	0.46
1:B:453:ARG:O	1:B:453:ARG:HG3	2.15	0.46
1:A:165:TRP:CZ3	1:A:169:TYR:HB2	2.51	0.46
1:A:246:ASP:O	1:A:249:VAL:N	2.36	0.46
1:A:173:HIS:CE1	1:A:354:LYS:NZ	2.83	0.46
1:A:78:VAL:HG11	1:A:80:ARG:NH2	2.31	0.45
1:A:204:GLU:O	1:A:204:GLU:HG2	2.15	0.45
1:B:172:THR:O	1:B:173:HIS:HD2	1.99	0.45
1:A:318:PHE:O	1:A:334:VAL:HA	2.16	0.45
1:B:63:PHE:CD1	1:B:63:PHE:C	2.94	0.45
1:B:130:ASN:ND2	1:B:145:LYS:HG3	2.31	0.45
1:B:417:LYS:HB2	1:B:417:LYS:HZ3	1.79	0.45
1:B:418:GLU:HB2	1:B:420:ASN:ND2	2.31	0.45
1:B:462:LEU:HD23	1:B:462:LEU:C	2.41	0.45
1:A:32:THR:C	1:A:34:LYS:H	2.25	0.45
1:A:101:ARG:H	1:A:101:ARG:CD	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:HG22	1:A:151:TYR:N	2.31	0.45
1:A:224:LEU:HD12	1:A:279:VAL:HB	1.98	0.45
1:B:129:ILE:CG1	1:B:130:ASN:H	2.22	0.45
1:A:96:ASP:HB3	1:A:100:ASP:N	2.16	0.45
1:A:321:VAL:HG12	1:A:332:LYS:HG3	1.97	0.45
1:A:356:PRO:HB2	1:A:358:TYR:HE2	1.82	0.45
1:A:458:GLU:HB2	1:A:470:VAL:CG2	2.46	0.45
1:B:476:VAL:CG1	1:B:477:PRO:HD2	2.47	0.45
1:A:38:ILE:HA	1:A:251:PHE:CB	2.30	0.45
1:A:453:ARG:HG2	1:A:453:ARG:NH1	2.32	0.45
1:B:125:LYS:HD3	1:B:246:ASP:CB	2.47	0.45
1:B:228:GLN:HA	1:B:228:GLN:HE21	1.81	0.45
1:A:304:LYS:O	1:A:310:LYS:NZ	2.47	0.45
1:A:441:THR:CG2	1:A:442:VAL:N	2.79	0.45
1:B:58:ASP:OD2	1:B:190:SER:HB3	2.16	0.45
1:B:73:ASN:O	1:B:74:LYS:HG3	2.16	0.45
1:A:30:ASP:HB3	1:A:36:GLN:HG2	1.98	0.45
1:A:72:GLY:C	1:A:74:LYS:H	2.24	0.45
1:A:462:LEU:HD23	1:A:462:LEU:C	2.42	0.45
1:B:60:ILE:CG1	1:B:61:GLU:N	2.80	0.45
1:B:102:THR:OG1	1:B:108:GLN:NE2	2.49	0.45
1:B:346:LYS:C	1:B:348:ASN:N	2.74	0.45
1:A:58:ASP:OD2	1:A:190:SER:CB	2.64	0.45
1:B:40:SER:O	1:B:44:SER:CB	2.65	0.45
1:B:96:ASP:CB	1:B:100:ASP:N	2.65	0.45
1:B:298:ILE:C	1:B:300:ASN:H	2.24	0.45
1:A:31:ILE:HG12	1:A:255:LYS:NZ	2.32	0.45
1:A:93:SER:O	1:A:117:ASN:ND2	2.50	0.45
1:A:121:ILE:CD1	1:A:122:LEU:H	2.26	0.45
1:A:269:SER:HB3	1:A:365:VAL:CG2	2.46	0.45
1:B:49:ARG:HG3	1:B:50:ASN:ND2	2.32	0.45
1:B:212:ASN:HA	1:B:215:ALA:CB	2.45	0.45
1:B:389:TYR:O	1:B:447:ALA:HB1	2.16	0.45
1:A:51:GLU:C	1:A:53:LEU:N	2.75	0.45
1:A:283:THR:OG1	1:A:284:THR:N	2.48	0.45
1:A:398:HIS:C	1:A:400:GLY:H	2.23	0.45
1:B:83:ARG:HB3	1:B:381:TYR:CZ	2.52	0.45
1:B:132:ASN:ND2	1:B:143:SER:OG	2.50	0.45
1:A:78:VAL:C	1:A:79:GLU:CG	2.91	0.44
1:B:40:SER:O	1:B:44:SER:HB3	2.17	0.44
1:B:182:SER:HB3	1:B:196:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:TYR:HD1	1:B:381:TYR:CE1	2.36	0.44
1:B:325:GLY:O	1:B:326:ASP:C	2.60	0.44
1:B:432:TYR:CD2	1:B:432:TYR:N	2.84	0.44
1:A:192:ILE:HD11	1:A:196:LEU:HD12	2.00	0.44
1:A:262:GLU:N	1:A:262:GLU:CD	2.75	0.44
1:B:214:VAL:HG22	1:B:221:VAL:HG23	1.99	0.44
1:B:468:ARG:CZ	1:B:493:PRO:HG2	2.47	0.44
1:B:277:ILE:HG21	1:B:345:ILE:HG12	1.99	0.44
1:A:189:LYS:O	1:A:193:SER:CB	2.66	0.44
1:B:42:ILE:HG22	1:B:368:LYS:HB2	1.99	0.44
1:B:95:ILE:HG12	1:B:117:ASN:HB3	1.95	0.44
1:B:163:SER:OG	1:B:164:LYS:N	2.50	0.44
1:B:224:LEU:CB	1:B:279:VAL:HB	2.42	0.44
1:B:263:ALA:O	1:B:264:PRO:C	2.59	0.44
1:B:283:THR:HB	1:B:316:SER:OG	2.18	0.44
1:A:131:ILE:N	1:A:131:ILE:CD1	2.80	0.44
1:A:210:ASP:OD2	1:A:213:ALA:CB	2.60	0.44
1:B:113:ALA:HB1	1:B:118:ARG:O	2.17	0.44
1:B:173:HIS:CE1	1:B:354:LYS:HZ1	2.36	0.44
1:B:298:ILE:C	1:B:300:ASN:N	2.75	0.44
1:B:299:LYS:HB2	1:B:301:THR:HG22	2.00	0.44
1:A:219:LYS:HD3	1:A:282:GLU:OE2	2.17	0.44
1:B:72:GLY:C	1:B:74:LYS:N	2.76	0.44
1:B:150:THR:O	1:B:153:LYS:HB3	2.17	0.44
1:B:155:SER:O	1:B:159:ASP:OD2	2.36	0.44
1:B:189:LYS:NZ	1:B:204:GLU:OE1	2.40	0.44
1:B:319:THR:OG1	1:B:334:VAL:HG22	2.18	0.44
1:A:132:ASN:HA	1:A:142:ASN:O	2.17	0.44
1:A:254:LEU:C	1:A:256:GLN:N	2.75	0.44
1:A:341:ILE:O	1:A:344:VAL:HB	2.17	0.44
1:A:427:THR:HB	1:A:431:ASN:HD22	1.81	0.44
1:B:118:ARG:HG3	1:B:118:ARG:HH11	1.81	0.44
1:B:126:ARG:CB	1:B:149:PRO:HD2	2.46	0.44
1:B:239:LYS:HB3	1:B:239:LYS:HE3	1.83	0.44
1:A:97:SER:C	1:A:99:ASN:N	2.75	0.44
1:A:292:ALA:O	1:A:293:ALA:C	2.60	0.44
1:A:346:LYS:C	1:A:348:ASN:N	2.76	0.44
1:B:49:ARG:NH2	1:B:369:ASP:OD2	2.51	0.44
1:B:96:ASP:HB2	1:B:100:ASP:CA	2.48	0.44
1:B:97:SER:C	1:B:99:ASN:H	2.25	0.44
1:B:113:ALA:HA	1:B:118:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:CG	1:B:142:ASN:HB3	2.47	0.44
1:B:173:HIS:CD2	1:B:354:LYS:HZ1	2.35	0.44
1:A:166:ASN:O	1:A:169:TYR:C	2.60	0.44
1:A:366:PHE:HB2	1:A:369:ASP:OD1	2.18	0.44
1:B:78:VAL:HA	1:B:385:THR:O	2.17	0.44
1:A:49:ARG:HB2	1:A:366:PHE:CZ	2.53	0.43
1:A:163:SER:CA	1:A:166:ASN:HD22	2.30	0.43
1:A:175:LEU:HD22	1:A:176:PRO:HD2	2.00	0.43
1:A:198:VAL:HG11	1:A:278:TYR:OH	2.18	0.43
1:A:285:SER:OG	1:A:286:SER:N	2.51	0.43
1:A:487:TRP:O	1:A:494:GLY:N	2.51	0.43
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.82	0.43
1:B:148:ASP:HB3	1:B:153:LYS:HE2	1.98	0.43
1:B:276:THR:N	1:B:323:LEU:O	2.46	0.43
1:A:129:ILE:HG12	1:A:130:ASN:N	2.32	0.43
1:A:144:ILE:CG1	1:A:145:LYS:H	2.27	0.43
1:A:150:THR:O	1:A:151:TYR:C	2.61	0.43
1:A:168:LYS:C	1:A:169:TYR:CD1	2.96	0.43
1:A:277:ILE:HD11	1:A:348:ASN:HB2	2.00	0.43
1:A:301:THR:O	1:A:303:ILE:N	2.51	0.43
1:A:325:GLY:O	1:A:326:ASP:C	2.60	0.43
1:B:124:VAL:HG12	1:B:257:LYS:HD2	2.00	0.43
1:B:266:LEU:HD13	1:B:364:SER:OG	2.17	0.43
1:A:128:PRO:HA	1:A:146:VAL:O	2.18	0.43
1:B:453:ARG:NH1	1:B:453:ARG:HG2	2.33	0.43
1:A:64:VAL:HA	1:A:65:PRO:HD2	1.65	0.43
1:A:89:PRO:HG2	1:A:375:VAL:HB	2.01	0.43
1:A:103:TYR:CE2	1:A:151:TYR:N	2.87	0.43
1:B:39:ASP:OD1	1:B:241:PRO:HD2	2.18	0.43
1:B:162:VAL:O	1:B:163:SER:C	2.61	0.43
1:B:398:HIS:C	1:B:400:GLY:H	2.27	0.43
1:B:398:HIS:CA	1:B:486:ILE:HD11	2.40	0.43
1:A:134:ASP:OD1	1:A:178:ARG:NH1	2.50	0.43
1:A:210:ASP:CG	1:A:210:ASP:O	2.61	0.43
1:A:293:ALA:HB1	1:A:313:TYR:CE2	2.54	0.43
1:B:114:LEU:HD11	1:B:362:TYR:OH	2.19	0.43
1:B:132:ASN:HA	1:B:142:ASN:O	2.17	0.43
1:B:489:THR:O	1:B:490:THR:C	2.61	0.43
1:A:83:ARG:HG3	1:A:383:GLU:HB2	2.01	0.43
1:A:301:THR:C	1:A:303:ILE:H	2.27	0.43
1:B:296:ALA:HA	1:B:301:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:ND2	1:A:255:LYS:HD2	2.34	0.43
1:B:101:ARG:H	1:B:101:ARG:HE	1.67	0.43
1:B:262:GLU:CD	1:B:262:GLU:N	2.77	0.43
1:B:346:LYS:O	1:B:348:ASN:N	2.52	0.43
1:A:260:SER:C	1:A:262:GLU:N	2.76	0.43
1:A:434:ASP:O	1:A:435:LYS:HD3	2.18	0.43
1:A:288:LYS:HE3	1:A:387:THR:HG23	2.01	0.43
1:A:358:TYR:HB3	1:A:359:PRO:HD2	1.99	0.43
1:B:42:ILE:O	1:B:45:LEU:N	2.52	0.43
1:B:483:ASN:OD1	1:B:498:THR:O	2.37	0.43
1:A:104:PRO:HD3	1:A:271:VAL:CG2	2.49	0.42
1:A:338:PHE:O	1:A:342:ARG:HG3	2.19	0.42
1:B:283:THR:OG1	1:B:284:THR:N	2.52	0.42
1:B:407:GLU:HG3	1:B:432:TYR:HE2	1.83	0.42
1:B:446:GLU:C	1:B:448:ASN:N	2.77	0.42
1:B:458:GLU:OE2	1:B:460:THR:N	2.52	0.42
1:A:95:ILE:HG12	1:A:117:ASN:HB2	2.01	0.42
1:A:118:ARG:HG3	1:A:118:ARG:O	2.19	0.42
1:B:33:ASP:C	1:B:34:LYS:HG3	2.44	0.42
1:B:125:LYS:HD3	1:B:246:ASP:HB3	2.00	0.42
1:B:343:LYS:HA	1:B:346:LYS:CE	2.38	0.42
1:B:452:ILE:HB	1:B:476:VAL:O	2.19	0.42
1:A:95:ILE:HD13	1:A:95:ILE:HA	1.78	0.42
1:A:130:ASN:ND2	1:A:145:LYS:HE2	2.33	0.42
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.74	0.42
1:A:199:ASN:OD1	1:A:201:LYS:HB2	2.19	0.42
1:A:207:LEU:HD22	1:A:280:LYS:HB2	2.01	0.42
1:B:64:VAL:HA	1:B:65:PRO:HD2	1.60	0.42
1:B:413:VAL:HG11	1:B:450:ARG:CZ	2.49	0.42
1:A:457:ARG:NH2	1:A:464:TRP:NE1	2.68	0.42
1:A:464:TRP:C	1:A:466:TRP:N	2.77	0.42
1:A:484:VAL:HG23	1:A:497:ILE:HD12	2.00	0.42
1:A:32:THR:HG21	2:A:517:HOH:O	2.19	0.42
1:A:128:PRO:HG3	1:A:147:ASP:HA	2.02	0.42
1:B:209:VAL:HG12	1:B:211:PHE:N	2.33	0.42
1:B:276:THR:HB	1:B:278:TYR:HE1	1.82	0.42
1:B:305:ASN:HA	1:B:310:LYS:CE	2.48	0.42
1:A:50:ASN:HD22	1:A:50:ASN:N	2.17	0.42
1:A:276:THR:HG21	1:A:278:TYR:CZ	2.55	0.42
1:A:418:GLU:CB	1:A:420:ASN:ND2	2.72	0.42
1:B:99:ASN:O	1:B:100:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:CG2	1:B:132:ASN:N	2.83	0.42
1:B:163:SER:O	1:B:164:LYS:C	2.61	0.42
1:B:409:ALA:CB	1:B:427:THR:HG22	2.50	0.42
1:A:38:ILE:HG23	1:A:39:ASP:N	2.34	0.42
1:B:227:LYS:HA	1:B:276:THR:HG23	2.01	0.42
1:A:34:LYS:HE2	1:A:34:LYS:O	2.19	0.42
1:A:290:VAL:C	1:A:292:ALA:N	2.73	0.42
1:A:343:LYS:HA	1:A:346:LYS:NZ	2.35	0.42
1:B:217:ASN:O	1:B:217:ASN:CG	2.62	0.42
1:B:250:THR:O	1:B:251:PHE:C	2.62	0.42
1:A:30:ASP:HA	1:A:36:GLN:CG	2.49	0.42
1:A:50:ASN:HA	1:A:376:HIS:NE2	2.35	0.42
1:A:165:TRP:O	1:A:168:LYS:N	2.52	0.42
1:A:232:THR:CB	1:A:271:VAL:O	2.61	0.42
1:B:220:LYS:HB2	1:B:283:THR:HG23	2.02	0.42
1:B:271:VAL:HG12	1:B:273:TYR:CE1	2.55	0.42
1:A:60:ILE:HG12	1:A:61:GLU:N	2.34	0.42
1:A:83:ARG:CZ	1:A:383:GLU:OE2	2.67	0.42
1:A:241:PRO:C	1:A:243:ASP:H	2.28	0.42
1:A:275:ARG:NH2	1:A:348:ASN:O	2.52	0.42
1:A:450:ARG:O	1:A:451:ASN:HB2	2.20	0.42
1:B:43:SER:O	1:B:368:LYS:HE3	2.20	0.42
1:B:338:PHE:CE1	1:B:341:ILE:HG21	2.54	0.41
1:A:424:THR:O	1:A:424:THR:HG22	2.19	0.41
1:B:144:ILE:HG13	1:B:145:LYS:N	2.34	0.41
1:B:239:LYS:H	1:B:239:LYS:CD	2.14	0.41
1:A:449:ALA:O	1:A:478:LEU:HD22	2.21	0.41
1:B:127:LYS:HD2	1:B:246:ASP:HA	2.02	0.41
1:A:287:SER:O	1:A:289:ASP:N	2.53	0.41
1:A:398:HIS:C	1:A:400:GLY:N	2.79	0.41
1:B:246:ASP:O	1:B:247:ASP:C	2.63	0.41
1:B:273:TYR:CD1	1:B:273:TYR:N	2.87	0.41
1:B:396:LEU:HA	1:B:484:VAL:O	2.19	0.41
1:A:96:ASP:CB	1:A:100:ASP:N	2.66	0.41
1:B:75:PHE:HB3	1:B:389:TYR:HB2	2.02	0.41
1:B:266:LEU:HA	1:B:365:VAL:O	2.20	0.41
1:B:487:TRP:O	1:B:494:GLY:N	2.53	0.41
1:A:43:SER:HA	1:A:368:LYS:HG3	2.03	0.41
1:A:113:ALA:HA	1:A:116:GLU:OE1	2.20	0.41
1:A:182:SER:CB	1:A:225:ALA:HB3	2.35	0.41
1:A:320:ALA:HB2	1:A:341:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:THR:HG22	1:B:151:TYR:N	2.36	0.41
1:B:163:SER:O	1:B:167:GLU:OE1	2.39	0.41
1:B:319:THR:HG23	1:B:333:VAL:O	2.21	0.41
1:B:456:ALA:H	1:B:471:ILE:CG2	2.33	0.41
1:B:461:GLY:CA	1:B:467:TRP:HE1	2.33	0.41
1:A:37:SER:HB3	1:A:40:SER:CB	2.51	0.41
1:A:75:PHE:O	1:A:389:TYR:HD1	2.03	0.41
1:A:103:TYR:CE2	1:A:151:TYR:CA	3.04	0.41
1:A:333:VAL:C	1:A:334:VAL:CG2	2.93	0.41
1:A:398:HIS:HD2	1:A:436:THR:O	2.03	0.41
1:A:31:ILE:HG23	1:A:252:ASN:OD1	2.20	0.41
1:A:55:SER:OG	1:A:377:ASN:HA	2.21	0.41
1:A:162:VAL:O	1:A:163:SER:C	2.63	0.41
1:A:166:ASN:ND2	1:A:166:ASN:H	2.19	0.41
1:A:196:LEU:O	1:A:197:ASN:HB3	2.21	0.41
1:A:457:ARG:HD2	1:A:467:TRP:O	2.21	0.41
1:B:95:ILE:HD11	1:B:199:ASN:HB2	2.03	0.41
1:B:343:LYS:O	1:B:347:ASP:OD2	2.39	0.41
1:B:391:LYS:CG	1:B:447:ALA:H	2.29	0.41
1:B:398:HIS:HB3	1:B:439:TYR:H	1.86	0.41
1:A:80:ARG:HG3	1:A:80:ARG:NH1	2.25	0.41
1:A:107:LEU:HA	1:A:266:LEU:O	2.20	0.41
1:A:148:ASP:O	1:A:153:LYS:HG2	2.20	0.41
1:A:282:GLU:O	1:A:316:SER:HA	2.21	0.41
1:A:303:ILE:C	1:A:305:ASN:H	2.28	0.41
1:A:342:ARG:O	1:A:346:LYS:HG2	2.21	0.41
1:B:83:ARG:HG3	1:B:383:GLU:HB2	2.03	0.41
1:B:94:ILE:HD12	1:B:360:ILE:N	2.36	0.41
1:B:161:LEU:O	1:B:162:VAL:C	2.64	0.41
1:B:405:GLN:HG2	1:B:434:ASP:N	2.35	0.41
1:B:433:GLN:C	1:B:435:LYS:NZ	2.79	0.41
1:B:79:GLU:HB2	1:B:385:THR:HG1	1.84	0.40
1:A:191:GLN:HG3	1:A:381:TYR:CD1	2.55	0.40
1:A:99:ASN:O	1:A:100:ASP:C	2.64	0.40
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.93	0.40
1:A:439:TYR:CG	1:A:440:SER:N	2.90	0.40
1:B:38:ILE:HA	1:B:251:PHE:CB	2.44	0.40
1:B:163:SER:C	1:B:167:GLU:OE1	2.64	0.40
1:B:192:ILE:HD11	1:B:196:LEU:CD1	2.51	0.40
1:A:90:VAL:HG23	1:A:91:ASP:N	2.37	0.40
1:A:138:LEU:O	1:A:139:LYS:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:O	1:A:164:LYS:HB3	2.22	0.40
1:B:57:GLY:HA3	1:B:379:THR:HB	2.03	0.40
1:B:78:VAL:CG1	1:B:80:ARG:HE	2.34	0.40
1:A:126:ARG:HB3	1:A:149:PRO:HD2	2.04	0.40
1:A:217:ASN:OD1	1:A:384:THR:HG21	2.22	0.40
1:A:406:PHE:CD1	1:A:406:PHE:N	2.89	0.40
1:B:101:ARG:CD	1:B:101:ARG:N	2.85	0.40
1:B:318:PHE:CD1	1:B:318:PHE:N	2.89	0.40
1:B:461:GLY:N	1:B:467:TRP:HE1	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/471 (100%)	358 (76%)	77 (16%)	34 (7%)	1	4
1	B	469/471 (100%)	358 (76%)	76 (16%)	35 (8%)	1	4
All	All	938/942 (100%)	716 (76%)	153 (16%)	69 (7%)	1	4

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ILE
1	B	288	LYS
1	B	438	HIS
1	A	151	TYR
1	A	259	VAL
1	A	288	LYS
1	A	438	HIS
1	A	464	TRP
1	A	465	GLU

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Mol	Chain	Res	Type
1	B	47	TYR
1	B	95	ILE
1	B	96	ASP
1	B	151	TYR
1	B	259	VAL
1	B	260	SER
1	B	347	ASP
1	B	447	ALA
1	B	464	TRP
1	B	465	GLU
1	A	47	TYR
1	A	97	SER
1	A	100	ASP
1	A	247	ASP
1	A	299	LYS
1	A	302	ASP
1	A	345	ILE
1	A	347	ASP
1	A	447	ALA
1	B	63	PHE
1	B	65	PRO
1	B	73	ASN
1	B	97	SER
1	B	100	ASP
1	B	128	PRO
1	B	153	LYS
1	B	211	PHE
1	B	302	ASP
1	A	63	PHE
1	A	73	ASN
1	A	211	PHE
1	A	231	TYR
1	A	368	LYS
1	A	437	ALA
1	B	139	LYS
1	B	208	GLY
1	B	437	ALA
1	A	65	PRO
1	A	260	SER
1	A	328	GLN
1	A	455	LYS
1	B	51	GLU

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Mol	Chain	Res	Type
1	B	57	GLY
1	B	327	ALA
1	B	368	LYS
1	A	95	ILE
1	A	208	GLY
1	B	162	VAL
1	B	231	TYR
1	B	310	LYS
1	B	328	GLN
1	B	298	ILE
1	B	345	ILE
1	A	52	VAL
1	A	104	PRO
1	A	202	VAL
1	A	128	PRO
1	A	98	VAL
1	A	497	ILE
1	B	149	PRO

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	418/418 (100%)	375 (90%)	43 (10%)	7	28
1	B	418/418 (100%)	382 (91%)	36 (9%)	10	36
All	All	836/836 (100%)	757 (91%)	79 (9%)	8	32

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	34	LYS
1	A	44	SER
1	A	45	LEU
1	A	46	SER

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Mol	Chain	Res	Type
1	A	59	LYS
1	A	63	PHE
1	A	70	LYS
1	A	88	SER
1	A	90	VAL
1	A	95	ILE
1	A	99	ASN
1	A	100	ASP
1	A	101	ARG
1	A	102	THR
1	A	108	GLN
1	A	114	LEU
1	A	115	VAL
1	A	121	ILE
1	A	132	ASN
1	A	167	GLU
1	A	184	SER
1	A	198	VAL
1	A	239	LYS
1	A	245	PHE
1	A	247	ASP
1	A	250	THR
1	A	270	ASN
1	A	286	SER
1	A	301	THR
1	A	321	VAL
1	A	326	ASP
1	A	351	PHE
1	A	370	ASN
1	A	395	ASN
1	A	417	LYS
1	A	424	THR
1	A	444	PRO
1	A	465	GLU
1	A	468	ARG
1	A	483	ASN
1	A	484	VAL
1	A	490	THR
1	B	31	ILE
1	B	34	LYS
1	B	45	LEU
1	B	59	LYS

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Mol	Chain	Res	Type
1	B	70	LYS
1	B	90	VAL
1	B	99	ASN
1	B	100	ASP
1	B	101	ARG
1	B	102	THR
1	B	115	VAL
1	B	121	ILE
1	B	128	PRO
1	B	163	SER
1	B	184	SER
1	B	223	ILE
1	B	239	LYS
1	B	250	THR
1	B	286	SER
1	B	289	ASP
1	B	301	THR
1	B	326	ASP
1	B	351	PHE
1	B	370	ASN
1	B	371	SER
1	B	395	ASN
1	B	407	GLU
1	B	417	LYS
1	B	453	ARG
1	B	457	ARG
1	B	465	GLU
1	B	468	ARG
1	B	475	ASP
1	B	483	ASN
1	B	484	VAL
1	B	497	ILE

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	36	GLN
1	A	50	ASN
1	A	56	ASN
1	A	108	GLN
1	A	130	ASN
1	A	166	ASN

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Mol	Chain	Res	Type
1	A	173	HIS
1	A	197	ASN
1	A	228	GLN
1	A	252	ASN
1	A	270	ASN
1	A	291	GLN
1	A	420	ASN
1	A	433	GLN
1	A	451	ASN
1	A	480	ASN
1	A	500	ASN
1	B	48	ASN
1	B	50	ASN
1	B	56	ASN
1	B	108	GLN
1	B	130	ASN
1	B	132	ASN
1	B	166	ASN
1	B	197	ASN
1	B	228	GLN
1	B	252	ASN
1	B	291	GLN
1	B	300	ASN
1	B	405	GLN
1	B	420	ASN
1	B	433	GLN
1	B	451	ASN
1	B	500	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.