



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:08 PM GMT

PDB ID : 1JSW  
Title : NATIVE L-ASPARTATE AMMONIA LYASE  
Authors : Shi, W.; Dunbar, J.; Farber, G.K.  
Deposited on : 1997-02-19  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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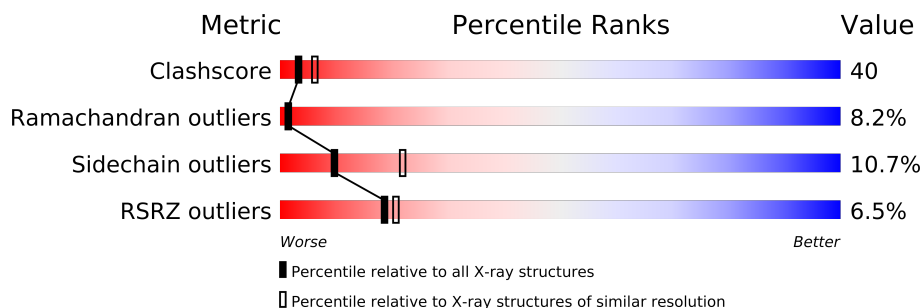
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	478	
1	B	478	
1	C	478	
1	D	478	

## 2 Entry composition i

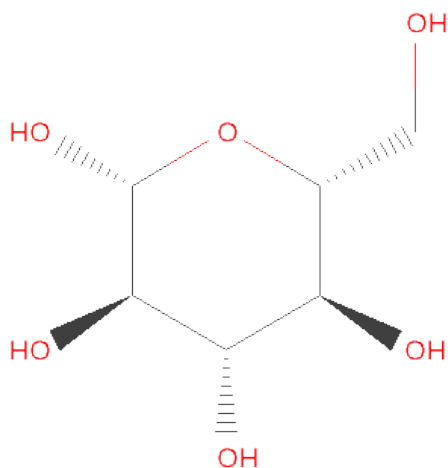
There are 4 unique types of molecules in this entry. The entry contains 13764 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-ASPARTATE AMMONIA-LYASE.

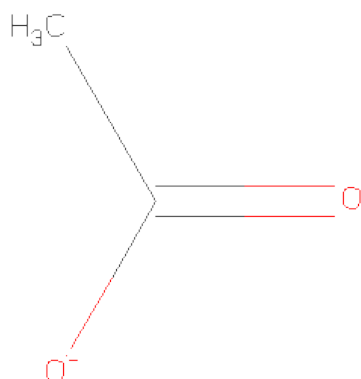
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			
1	B	460	Total	C	N	O	S	0	0	0
			3511	2210	597	678	26			
1	C	413	Total	C	N	O	S	0	0	0
			3152	1988	534	606	24			
1	D	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

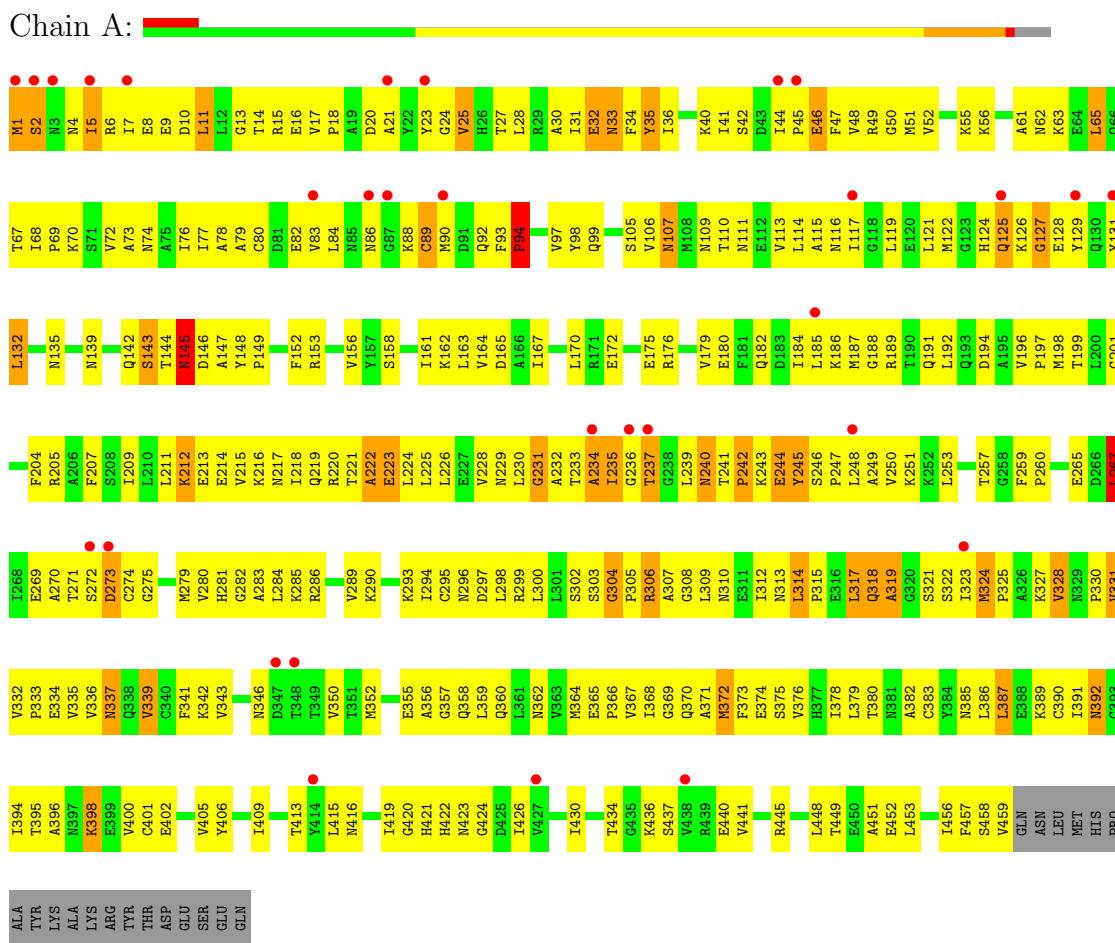
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	16	Total	O	0	0
			16	16		
4	C	11	Total	O	0	0
			11	11		
4	D	23	Total	O	0	0
			23	23		

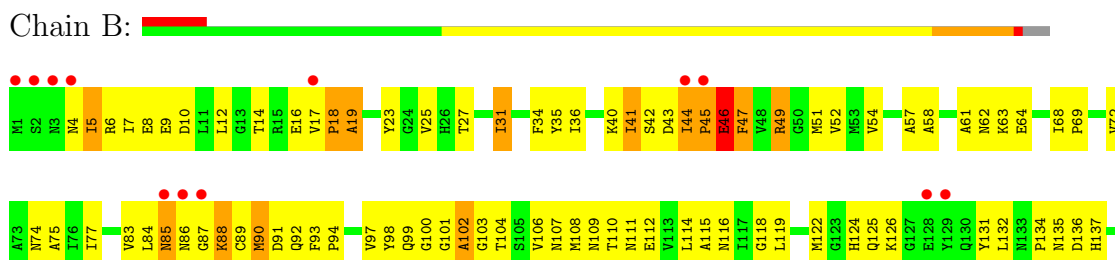
### 3 Residue-property plots

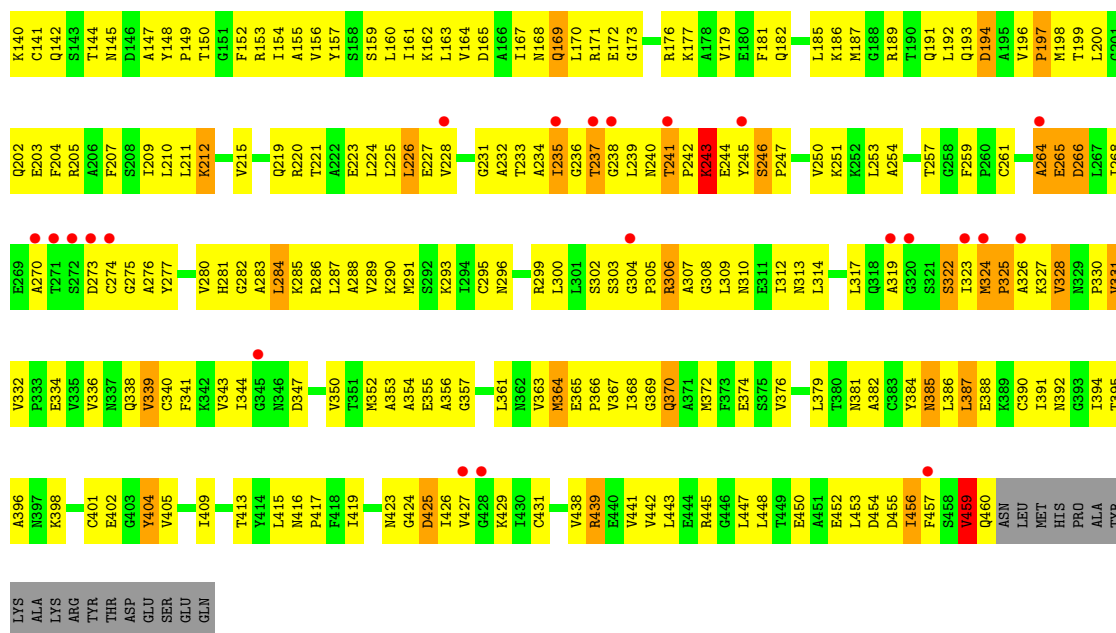
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: L-ASPARTATE AMMONIA-LYASE



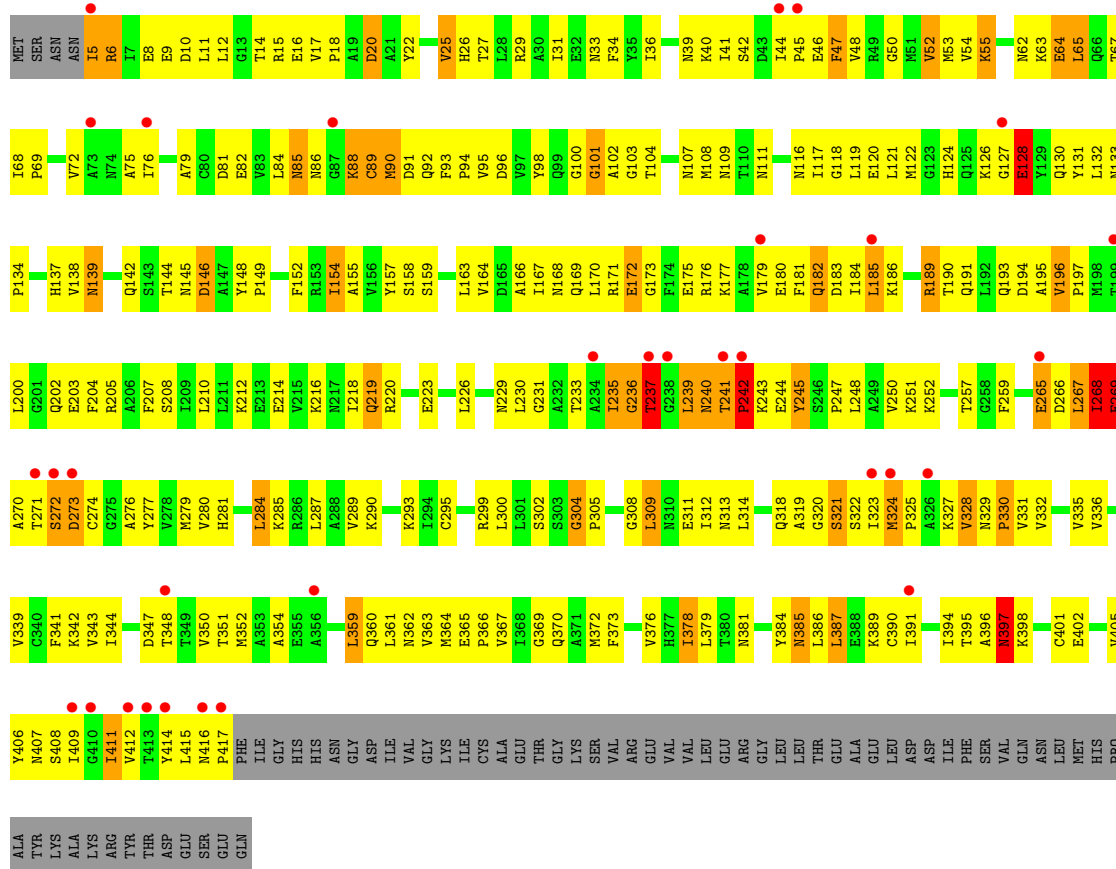
#### • Molecule 1: L-ASPARTATE AMMONIA-LYASE





### • Molecule 1: L-ASPARTATE AMMONIA-LYASE

Chain C:



### • Molecule 1: L-ASPARTATE AMMONIA-LYASE

Chain D:

ALA	Y406	V335	A270	E203	L132	L65	M1
LYS	N407	V336	T271	F204	M133	Q66	S2
ARG	S408		S272	R205	P134	T67	M3
TYR	I409	V339	D273	A206	M135	I68	N4
THR	G410	C340	C274	F207	D136	P69	I5
ASP	I411	F341	G275	S208	H137	K70	R6
GLU	V412	K342	A276	I209	V138	S71	I7
SER	T413	G345	V278	L210	Q142	A72	E8
GLN	Y414	N346	V279	L211	N145	V73	E9
	L415	D347	V280	K212			D10
	N416	H281	H281	E213	Y148	I76	L11
	P417	V350		E214	P149	I77	L12
	F418	A353	L284	K216	T150	A78	G13
	I419	A356	K285	N217	G151	A79	T14
	H422		R286	Q219	F152	C80	R15
	G424	L359	L287	R220	R153	V83	E16
	D425	V283	A288	T221	I154	L84	E17
	I426	Q360	K290	A222	A155	N85	P18
	V427	L361	S292	E223	V156	G87	A21
	G428	N362	K293	L226	Y157	K88	Y22
	K429	M364	C295	E227	S158	C89	Y23
	I430	E365	I294	V228	I160	N90	G24
	C431	P366	N296		I161	D91	V25
	A432	V367		T233	K162	P94	H26
	E433	I368	R299	A234	V164	V95	T27
	K436	G369	L300	G236	N168	V97	L28
	S437	Q370	S303	T237	Q169	G100	A30
	V438	A371	C304	C238	L170	G101	I31
	R439	M372	F305	L239	R171	A102	E32
	E440	F373	R306	N240	E172	G103	N33
	V441	V376	A307	T241	G173	T104	F94
	L442	L379	G308	P242	R176	S105	Y35
	E444	T380	L309	K243		V106	I36
	R445	N381	T312	E244	F181	N107	N39
	G446	N385	L314	Y245	Q182	M108	K40
	L447	L386	P315	P247	D183	T110	I41
	L448	E387	E316	L248	I184	L114	D43
	A451	E388	A319	A249	L185	A115	I44
	E452	K389	G320	V250	K186	N116	P45
	L453	C390	S321	L253	M187	I117	E46
	D454	I391	S322	V256	R189	G118	F47
	D455	I394	K324	T257	T190	L119	V48
	I456	T395	A325		Q191	E120	G50
	F457	A396	A326	P260	L192	L121	M51
	S458	N397	K327	C261	Q193	H124	V52
	V459	K398	V328	V262	D194	Q125	M53
	GLN	E399	N329	A264	A195	K126	V54
	ASN	V400	E265	E265	V196	G127	K55
	LEU	C401	P330	D266	P197	E128	K56
	MET	E402	V331	L267	M198	Y129	A57
	HIS	G403	V332	T268	L200	Q130	A58
	PRO	Y404	P333	E269			M62
	ALA	LYS	E334				K63
	TYR						E64

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.50Å 146.20Å 103.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 46.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 75.6 (46.38-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.216 , 0.371 0.256 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 79.2	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 43803 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.48	0/3553	0.76	1/4815 (0.0%)
1	B	0.47	0/3562	0.73	0/4827
1	C	0.47	0/3199	0.75	2/4338 (0.0%)
1	D	0.47	0/3553	0.74	0/4815
All	All	0.47	0/13867	0.74	3/18795 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	GLU	N-CA-C	5.93	127.02	111.00
1	C	240	ASN	N-CA-C	5.63	126.21	111.00
1	A	132	LEU	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3539	338	0
1	B	3511	0	3547	299	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3152	0	3191	268	0
1	D	3502	0	3539	318	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	4	0	3	0	0
4	A	19	0	0	1	0
4	B	16	0	0	0	0
4	C	11	0	0	0	0
4	D	23	0	0	1	0
All	All	13764	0	13843	1112	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

All (1112) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:GLU:HG3	1:A:270:ALA:H	1.20	1.05
1:D:273:ASP:HB2	1:D:362:ASN:HD22	1.22	1.04
1:B:319:ALA:HB2	1:D:26:HIS:CE1	1.94	1.02
1:B:119:LEU:HG	1:B:132:LEU:HB3	1.42	1.01
1:A:83:VAL:HG13	1:A:90:MET:HB3	1.43	1.01
1:A:284:LEU:HD21	1:A:376:VAL:HG22	1.40	1.00
1:A:323:ILE:HB	1:A:324:MET:SD	2.02	0.99
1:A:241:THR:N	1:A:242:PRO:HD2	1.78	0.98
1:D:431:CYS:SG	1:D:441:VAL:HG21	2.05	0.95
1:B:314:LEU:HD12	1:B:390:CYS:SG	2.07	0.93
1:A:416:ASN:HD21	1:A:424:GLY:HA3	1.32	0.93
1:C:185:LEU:HB3	1:C:405:VAL:HG11	1.50	0.93
1:D:235:ILE:HD12	1:D:236:GLY:H	1.34	0.92
1:B:439:ARG:HH22	1:B:454:ASP:HB3	1.35	0.91
1:D:287:LEU:HD23	1:D:379:LEU:HD13	1.53	0.91
1:D:253:LEU:HD12	1:D:261:CYS:SG	2.11	0.91
1:C:200:LEU:HD22	1:C:401:CYS:SG	2.11	0.91
1:A:52:VAL:HG21	1:A:83:VAL:HG11	1.53	0.91
1:A:5:ILE:HG22	1:A:18:PRO:HA	1.53	0.89
1:A:226:LEU:HD11	1:A:259:PHE:HB3	1.52	0.89
1:D:323:ILE:HG12	1:D:324:MET:SD	2.12	0.89
1:C:185:LEU:HB2	1:C:402:GLU:HG2	1.54	0.89
1:B:93:PHE:HA	1:B:109:ASN:HD21	1.37	0.89
1:A:269:GLU:CG	1:A:270:ALA:H	1.87	0.88
1:D:445:ARG:HG2	1:D:445:ARG:HH11	1.36	0.88
1:D:233:THR:HA	1:D:238:GLY:HA2	1.55	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:44:ILE:H	1:B:45:PRO:HD2	1.38	0.88
1:C:152:PHE:HE2	1:C:369:GLY:HA2	1.37	0.87
1:C:172:GLU:HB3	1:C:176:ARG:HH21	1.38	0.87
1:B:323:ILE:HB	1:B:324:MET:SD	2.16	0.86
1:B:12:LEU:HD13	1:D:319:ALA:HA	1.58	0.86
1:B:35:TYR:CE1	1:D:385:ASN:HA	2.11	0.85
1:A:135:ASN:HA	1:A:139:ASN:HB3	1.59	0.84
1:B:199:THR:HG23	1:B:202:GLN:H	1.41	0.84
1:B:35:TYR:HE1	1:D:385:ASN:HA	1.43	0.84
1:B:319:ALA:HB2	1:D:26:HIS:HE1	1.38	0.83
1:D:409:ILE:H	1:D:409:ILE:HD12	1.40	0.83
1:D:409:ILE:O	1:D:412:VAL:HG23	1.78	0.83
1:C:179:VAL:O	1:C:182:GLN:HG2	1.79	0.82
1:C:104:THR:HG22	1:C:144:THR:HG21	1.60	0.82
1:B:277:TYR:HA	1:B:280:VAL:HG22	1.61	0.82
1:C:408:SER:O	1:C:411:ILE:HG23	1.80	0.82
1:A:416:ASN:ND2	1:A:424:GLY:HA3	1.95	0.81
1:D:85:ASN:OD1	1:D:88:LYS:HB2	1.79	0.81
1:B:238:GLY:HA3	1:B:242:PRO:HG2	1.59	0.81
1:D:49:ARG:HG2	1:D:84:LEU:HD23	1.63	0.81
1:B:9:GLU:HB2	1:B:14:THR:HG22	1.62	0.80
1:B:104:THR:HA	1:B:144:THR:HG21	1.63	0.80
1:B:338:GLN:HE21	1:D:367:VAL:HB	1.46	0.80
1:A:6:ARG:HH11	1:A:17:VAL:HG13	1.47	0.79
1:C:119:LEU:HD23	1:C:132:LEU:HB3	1.64	0.79
1:C:247:PRO:O	1:C:251:LYS:HG2	1.83	0.79
1:A:270:ALA:HA	1:A:274:CYS:HG	1.47	0.79
1:C:152:PHE:CE2	1:C:369:GLY:HA2	2.18	0.79
1:A:270:ALA:HA	1:A:274:CYS:SG	2.23	0.78
1:B:239:LEU:O	1:B:242:PRO:HD2	1.83	0.78
1:D:40:LYS:HA	1:D:96:ASP:HA	1.65	0.78
1:C:8:GLU:HB2	1:C:25:VAL:HG13	1.63	0.78
1:C:412:VAL:HA	1:C:415:LEU:HB3	1.65	0.78
1:C:235:ILE:HA	1:C:360:GLN:HG2	1.66	0.78
1:D:207:PHE:O	1:D:210:LEU:HB3	1.84	0.77
1:B:243:LYS:HE3	1:B:244:GLU:H	1.49	0.77
1:A:215:VAL:HG12	1:A:219:GLN:HE21	1.49	0.77
1:B:439:ARG:HG3	1:B:439:ARG:HH11	1.49	0.77
1:B:364:MET:O	1:B:367:VAL:HG12	1.84	0.77
1:D:272:SER:HA	1:D:361:LEU:HA	1.66	0.77
1:A:204:PHE:HA	1:A:207:PHE:HD2	1.49	0.77
1:D:242:PRO:HA	1:D:246:SER:OG	1.85	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:187:MET:HE3	1:B:405:VAL:HA	1.67	0.76
1:C:300:LEU:HD11	1:D:300:LEU:HD11	1.64	0.76
1:D:72:VAL:HB	1:D:132:LEU:HD13	1.67	0.76
1:A:99:GLN:OE1	1:A:105:SER:HB2	1.86	0.76
1:C:327:LYS:O	1:C:328:VAL:HG23	1.86	0.75
1:D:323:ILE:H	1:D:323:ILE:HD13	1.51	0.75
1:D:425:ASP:O	1:D:429:LYS:HG2	1.85	0.75
1:B:93:PHE:HA	1:B:109:ASN:ND2	2.01	0.75
1:D:414:TYR:O	1:D:417:PRO:HD2	1.87	0.75
1:A:217:ASN:HD21	1:D:279:MET:HG3	1.52	0.74
1:A:305:PRO:HD3	1:B:193:GLN:HE22	1.53	0.74
1:A:93:PHE:HA	1:A:109:ASN:HD21	1.52	0.74
1:B:150:THR:O	1:B:154:ILE:HG12	1.88	0.73
1:A:343:VAL:HG21	1:A:379:LEU:HG	1.67	0.73
1:B:49:ARG:HA	1:B:52:VAL:HG22	1.69	0.73
1:A:10:ASP:HB3	1:A:25:VAL:HG11	1.68	0.73
1:A:47:PHE:HE2	1:A:106:VAL:HG11	1.53	0.73
1:D:210:LEU:HD21	1:D:290:LYS:HB3	1.71	0.73
1:D:436:LYS:HB3	1:D:440:GLU:HG3	1.70	0.73
1:B:8:GLU:HB3	1:B:25:VAL:HG22	1.69	0.73
1:D:11:LEU:H	1:D:11:LEU:HD22	1.53	0.73
1:D:130:GLN:N	1:D:130:GLN:HE21	1.86	0.73
1:A:198:MET:HB3	1:D:235:ILE:HD13	1.71	0.72
1:D:204:PHE:HA	1:D:207:PHE:HD2	1.54	0.72
1:A:21:ALA:HA	1:A:92:GLN:OE1	1.90	0.72
1:A:152:PHE:O	1:A:156:VAL:HG23	1.89	0.72
1:C:324:MET:N	1:C:324:MET:SD	2.62	0.72
1:A:285:LYS:O	1:A:289:VAL:HG23	1.90	0.72
1:A:230:LEU:HD23	1:A:249:ALA:HB1	1.71	0.72
1:D:204:PHE:HA	1:D:207:PHE:CD2	2.25	0.72
1:D:28:LEU:HA	1:D:31:ILE:HD12	1.72	0.72
1:C:416:ASN:HB2	1:C:417:PRO:HD3	1.72	0.72
1:D:284:LEU:HD21	1:D:376:VAL:HG12	1.70	0.71
1:D:241:THR:N	1:D:242:PRO:HD2	2.05	0.71
1:B:5:ILE:HD13	1:B:5:ILE:H	1.54	0.71
1:C:152:PHE:HE2	1:C:369:GLY:CA	2.03	0.71
1:B:210:LEU:HD21	1:B:290:LYS:HD2	1.72	0.71
1:D:414:TYR:CD2	1:D:456:ILE:HG12	2.26	0.71
1:B:341:PHE:CE2	1:D:353:ALA:HA	2.26	0.71
1:C:202:GLN:O	1:C:205:ARG:HG2	1.89	0.71
1:A:8:GLU:HB3	1:A:25:VAL:HG22	1.71	0.71
1:A:359:LEU:HD11	1:D:300:LEU:HD23	1.73	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:456:ILE:HG13	1:B:457:PHE:H	1.55	0.71
1:C:40:LYS:HD3	1:C:94:PRO:HA	1.71	0.71
1:B:51:MET:O	1:B:54:VAL:HG12	1.89	0.71
1:A:61:ALA:O	1:A:65:LEU:HB2	1.89	0.71
1:A:69:PRO:HB2	1:A:72:VAL:HG13	1.73	0.71
1:D:296:ASN:HA	1:D:299:ARG:HE	1.55	0.70
1:D:51:MET:O	1:D:54:VAL:HG12	1.91	0.70
1:A:449:THR:HG22	1:A:451:ALA:H	1.56	0.70
1:A:51:MET:O	1:A:55:LYS:HG2	1.92	0.70
1:C:182:GLN:HG3	1:C:183:ASP:H	1.57	0.70
1:A:230:LEU:HD22	1:A:253:LEU:HD12	1.72	0.70
1:D:56:LYS:HD3	1:D:256:VAL:HG21	1.73	0.70
1:B:63:LYS:HZ2	1:B:74:ASN:HD21	1.38	0.70
1:D:129:TYR:CD2	1:D:131:TYR:HE2	2.10	0.70
1:D:47:PHE:HA	1:D:155:ALA:CB	2.21	0.70
1:A:269:GLU:HG3	1:A:270:ALA:N	2.01	0.69
1:D:76:ILE:HG13	1:D:132:LEU:HD11	1.73	0.69
1:B:235:ILE:HG13	1:C:196:VAL:HG13	1.74	0.69
1:B:221:THR:O	1:B:224:LEU:HG	1.92	0.69
1:B:176:ARG:O	1:B:179:VAL:HG12	1.93	0.69
1:C:323:ILE:HG22	1:C:324:MET:SD	2.31	0.69
1:B:233:THR:HB	1:B:238:GLY:HA2	1.73	0.69
1:A:56:LYS:HB2	1:A:80:CYS:SG	2.31	0.69
1:A:339:VAL:HG21	1:A:382:ALA:HB2	1.74	0.69
1:D:250:VAL:HG21	1:D:263:PRO:HG3	1.74	0.69
1:D:130:GLN:HE21	1:D:130:GLN:CA	2.06	0.69
1:C:189:ARG:HH21	1:C:309:LEU:HD11	1.58	0.69
1:C:53:MET:SD	1:C:257:THR:HA	2.33	0.68
1:C:146:ASP:HB2	1:C:229:ASN:OD1	1.92	0.68
1:A:122:MET:SD	1:A:132:LEU:CD1	2.81	0.68
1:A:109:ASN:O	1:A:113:VAL:HG23	1.93	0.68
1:B:7:ILE:HA	1:B:16:GLU:HA	1.74	0.68
1:C:235:ILE:HD12	1:C:236:GLY:N	2.09	0.68
1:D:150:THR:O	1:D:154:ILE:HG12	1.94	0.68
1:D:6:ARG:NH1	1:D:127:GLY:HA2	2.07	0.68
1:B:341:PHE:HE2	1:D:353:ALA:HA	1.59	0.67
1:B:72:VAL:HG21	1:B:137:HIS:CD2	2.29	0.67
1:B:90:MET:HG3	1:B:91:ASP:H	1.58	0.67
1:C:182:GLN:HG3	1:C:183:ASP:N	2.09	0.67
1:C:164:VAL:HG21	1:C:219:GLN:OE1	1.95	0.67
1:D:23:TYR:HB2	1:D:27:THR:HB	1.76	0.67
1:C:22:TYR:HB2	1:C:92:GLN:HG3	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:LEU:HD22	1:A:11:LEU:H	1.60	0.67
1:A:215:VAL:HG12	1:A:219:GLN:NE2	2.10	0.67
1:A:336:VAL:HA	1:A:339:VAL:HG13	1.75	0.67
1:C:44:ILE:H	1:C:45:PRO:HD2	1.60	0.66
1:A:9:GLU:HG3	1:A:13:GLY:O	1.95	0.66
1:C:281:HIS:HA	1:C:284:LEU:HD22	1.76	0.66
1:B:322:SER:O	1:B:325:PRO:HG3	1.96	0.66
1:A:305:PRO:HD3	1:B:193:GLN:NE2	2.10	0.66
1:A:187:MET:SD	1:A:197:PRO:HD3	2.35	0.66
1:B:431:CYS:SG	1:B:441:VAL:HG21	2.35	0.66
1:A:212:LYS:O	1:A:216:LYS:HG3	1.96	0.66
1:C:273:ASP:HB2	1:C:362:ASN:HD22	1.61	0.66
1:A:318:GLN:HG3	1:A:319:ALA:H	1.61	0.66
1:A:34:PHE:HZ	1:C:331:VAL:HG22	1.60	0.66
1:D:414:TYR:CE2	1:D:456:ILE:HG12	2.30	0.66
1:C:409:ILE:HD11	1:D:306:ARG:HB2	1.77	0.66
1:C:101:GLY:O	1:C:104:THR:HG23	1.96	0.66
1:B:314:LEU:CD1	1:B:390:CYS:SG	2.83	0.65
1:A:318:GLN:CG	1:A:319:ALA:H	2.08	0.65
1:D:246:SER:HB2	1:D:247:PRO:HD3	1.76	0.65
1:B:63:LYS:NZ	1:B:74:ASN:HD21	1.93	0.65
1:D:188:GLY:O	1:D:195:ALA:HB3	1.96	0.65
1:B:439:ARG:HH21	1:B:450:GLU:HG3	1.62	0.65
1:B:44:ILE:H	1:B:45:PRO:CD	2.09	0.65
1:C:126:LYS:HG2	1:C:127:GLY:H	1.62	0.65
1:A:34:PHE:CZ	1:C:331:VAL:HG22	2.31	0.65
1:A:122:MET:SD	1:A:132:LEU:HD13	2.37	0.65
1:B:85:ASN:CG	1:B:86:ASN:H	2.00	0.65
1:A:241:THR:N	1:A:242:PRO:CD	2.58	0.65
1:D:323:ILE:HD13	1:D:323:ILE:N	2.12	0.65
1:D:210:LEU:HD13	1:D:294:ILE:HD11	1.77	0.65
1:D:158:SER:HA	1:D:161:ILE:HD12	1.79	0.65
1:D:285:LYS:O	1:D:289:VAL:HG23	1.97	0.65
1:B:220:ARG:O	1:B:223:GLU:HG2	1.96	0.65
1:B:425:ASP:O	1:B:429:LYS:HG2	1.97	0.64
1:D:332:VAL:O	1:D:335:VAL:HG12	1.96	0.64
1:A:68:ILE:HD12	1:A:72:VAL:HG23	1.78	0.64
1:B:34:PHE:HZ	1:D:331:VAL:HG22	1.62	0.64
1:A:286:ARG:HH11	1:D:279:MET:HG2	1.63	0.64
1:A:214:GLU:O	1:A:218:ILE:HG12	1.97	0.64
1:C:267:LEU:HD23	1:C:267:LEU:H	1.63	0.64
1:A:92:GLN:O	1:A:94:PRO:HD3	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:163:LEU:O	1:B:167:ILE:HG13	1.96	0.64
1:B:381:ASN:O	1:B:385:ASN:HB2	1.98	0.64
1:D:47:PHE:HA	1:D:155:ALA:HB1	1.78	0.64
1:D:150:THR:HG23	1:D:228:VAL:HB	1.78	0.64
1:D:220:ARG:O	1:D:223:GLU:HB3	1.97	0.64
1:B:317:LEU:HB3	1:D:33:ASN:ND2	2.13	0.64
1:B:239:LEU:HD21	1:C:196:VAL:HG11	1.80	0.64
1:B:324:MET:N	1:B:324:MET:SD	2.71	0.64
1:A:63:LYS:HE3	1:A:70:LYS:HG3	1.79	0.64
1:B:443:LEU:HD13	1:B:453:LEU:HD22	1.79	0.63
1:B:235:ILE:CG1	1:C:196:VAL:HG13	2.28	0.63
1:D:145:ASN:O	1:D:149:PRO:HG2	1.97	0.63
1:C:189:ARG:NH2	1:C:309:LEU:HD11	2.13	0.63
1:D:323:ILE:CD1	1:D:323:ILE:H	2.11	0.63
1:A:379:LEU:O	1:A:382:ALA:HB3	1.99	0.63
1:C:407:ASN:ND2	1:D:306:ARG:HH21	1.97	0.63
1:D:158:SER:O	1:D:161:ILE:HB	1.99	0.63
1:A:332:VAL:O	1:A:335:VAL:HG12	1.99	0.63
1:B:87:GLY:C	1:B:89:CYS:H	2.02	0.63
1:C:402:GLU:HB3	1:C:406:TYR:HE2	1.62	0.63
1:C:372:MET:O	1:C:376:VAL:HG23	1.98	0.63
1:B:209:ILE:HG13	1:C:268:ILE:HD12	1.80	0.63
1:A:30:ALA:HA	1:A:33:ASN:HD22	1.63	0.63
1:B:275:GLY:HA3	1:C:290:LYS:HZ1	1.64	0.63
1:C:280:VAL:HG23	1:C:372:MET:SD	2.39	0.63
1:D:285:LYS:HD3	1:D:347:ASP:CG	2.19	0.63
1:B:231:GLY:HA2	1:B:241:THR:HG22	1.81	0.63
1:D:7:ILE:HA	1:D:16:GLU:HA	1.81	0.63
1:A:331:VAL:HG22	1:C:100:GLY:HA3	1.79	0.63
1:C:72:VAL:HG21	1:C:137:HIS:CD2	2.34	0.63
1:C:20:ASP:HA	1:C:126:LYS:HZ2	1.64	0.62
1:C:82:GLU:O	1:C:88:LYS:HB3	1.99	0.62
1:B:119:LEU:N	1:B:132:LEU:HD23	2.14	0.62
1:C:343:VAL:CG2	1:C:378:ILE:HD11	2.28	0.62
1:C:130:GLN:NE2	1:C:133:ASN:HA	2.14	0.62
1:A:207:PHE:CE1	1:A:294:ILE:HG23	2.34	0.62
1:A:145:ASN:HD22	1:A:234:ALA:HB2	1.64	0.62
1:A:182:GLN:HA	1:A:201:GLY:HA3	1.80	0.62
1:B:257:THR:HB	1:B:259:PHE:CD2	2.34	0.62
1:B:319:ALA:HB1	1:D:11:LEU:HD23	1.81	0.62
1:B:313:ASN:O	1:B:394:ILE:HA	2.00	0.62
1:D:184:ILE:O	1:D:200:LEU:N	2.31	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:CYS:HB3	1:B:245:TYR:CE2	2.34	0.62
1:A:409:ILE:HG23	1:B:306:ARG:HD2	1.81	0.62
1:B:415:LEU:HD22	1:B:448:LEU:HD21	1.81	0.62
1:D:31:ILE:HD11	1:D:94:PRO:HG2	1.82	0.62
1:D:52:VAL:HG13	1:D:114:LEU:HD11	1.82	0.62
1:B:416:ASN:HB2	1:B:417:PRO:HD3	1.81	0.62
1:C:212:LYS:O	1:C:216:LYS:HG2	2.00	0.61
1:D:221:THR:HG22	1:D:280:VAL:HG12	1.82	0.61
1:B:150:THR:HG23	1:B:228:VAL:HB	1.80	0.61
1:A:343:VAL:HG23	1:A:378:ILE:HD11	1.82	0.61
1:A:218:ILE:HD13	1:A:283:ALA:HB1	1.80	0.61
1:A:341:PHE:CD1	1:C:352:MET:HB3	2.36	0.61
1:D:156:VAL:O	1:D:160:LEU:HG	1.99	0.61
1:B:119:LEU:CG	1:B:132:LEU:HB3	2.24	0.61
1:D:11:LEU:H	1:D:11:LEU:CD2	2.14	0.61
1:C:128:GLU:O	1:C:130:GLN:HG2	2.01	0.61
1:D:173:GLY:O	1:D:176:ARG:HB3	2.00	0.61
1:D:323:ILE:HG12	1:D:324:MET:H	1.65	0.61
1:A:437:SER:OG	1:A:440:GLU:HG3	2.01	0.61
1:B:102:ALA:HB2	1:B:363:VAL:HA	1.82	0.61
1:D:119:LEU:HB2	1:D:124:HIS:HB2	1.83	0.61
1:C:53:MET:SD	1:C:257:THR:HG22	2.41	0.61
1:C:269:GLU:HA	1:C:272:SER:OG	2.00	0.61
1:B:225:LEU:HG	1:B:280:VAL:HG11	1.83	0.61
1:C:281:HIS:CD2	1:C:350:VAL:HG21	2.36	0.60
1:D:292:SER:HB2	1:D:340:CYS:SG	2.40	0.60
1:B:254:ALA:HB2	1:B:261:CYS:SG	2.41	0.60
1:D:423:ASN:HD22	1:D:447:LEU:HD11	1.66	0.60
1:B:363:VAL:O	1:B:366:PRO:HD2	2.01	0.60
1:B:6:ARG:HD2	1:B:17:VAL:CG1	2.31	0.60
1:A:416:ASN:O	1:A:420:GLY:N	2.34	0.60
1:C:218:ILE:HD11	1:C:287:LEU:HD22	1.83	0.60
1:B:211:LEU:O	1:B:215:VAL:HG23	2.01	0.60
1:A:47:PHE:HZ	1:A:148:TYR:CE1	2.18	0.60
1:A:119:LEU:CD1	1:A:126:LYS:HA	2.32	0.60
1:D:76:ILE:CG1	1:D:132:LEU:HD11	2.31	0.60
1:A:152:PHE:CE1	1:A:369:GLY:HA2	2.37	0.60
1:C:40:LYS:HD3	1:C:94:PRO:CA	2.32	0.60
1:A:318:GLN:HG3	1:A:319:ALA:N	2.17	0.60
1:A:176:ARG:O	1:A:180:GLU:HG3	2.01	0.60
1:C:205:ARG:HB2	1:C:205:ARG:NH1	2.17	0.60
1:B:312:ILE:HB	1:B:394:ILE:CG2	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:LEU:HA	1:A:31:ILE:HD12	1.84	0.60
1:A:346:ASN:O	1:A:350:VAL:HG23	2.02	0.60
1:D:73:ALA:O	1:D:77:ILE:HG23	2.02	0.60
1:D:39:ASN:O	1:D:97:VAL:HG22	2.02	0.59
1:D:127:GLY:O	1:D:129:TYR:N	2.35	0.59
1:A:119:LEU:HA	1:A:122:MET:HB2	1.85	0.59
1:D:148:TYR:HB3	1:D:149:PRO:HD3	1.84	0.59
1:A:369:GLY:O	1:A:373:PHE:HD1	1.84	0.59
1:C:248:LEU:O	1:C:252:LYS:HG2	2.02	0.59
1:B:295:CYS:O	1:B:299:ARG:HG3	2.02	0.59
1:A:8:GLU:OE1	1:A:17:VAL:HG11	2.03	0.59
1:D:49:ARG:O	1:D:53:MET:HG3	2.02	0.59
1:B:149:PRO:O	1:B:153:ARG:HG3	2.02	0.59
1:D:314:LEU:HD23	1:D:394:ILE:HD12	1.83	0.59
1:D:226:LEU:HD23	1:D:260:PRO:HG2	1.84	0.59
1:C:364:MET:O	1:C:367:VAL:HG12	2.03	0.59
1:A:306:ARG:NE	1:A:306:ARG:HA	2.18	0.59
1:C:69:PRO:O	1:C:72:VAL:HG22	2.02	0.59
1:C:68:ILE:HD12	1:C:72:VAL:HG23	1.85	0.59
1:A:241:THR:H	1:A:242:PRO:HD2	1.66	0.59
1:C:130:GLN:NE2	1:C:130:GLN:HA	2.17	0.59
1:A:244:GLU:HB3	1:A:248:LEU:HD22	1.85	0.59
1:C:327:LYS:NZ	1:C:329:ASN:HD21	2.00	0.58
1:B:62:ASN:HB3	1:B:68:ILE:HG12	1.85	0.58
1:A:223:GLU:HA	1:A:226:LEU:HD23	1.85	0.58
1:B:233:THR:CB	1:B:238:GLY:HA2	2.34	0.58
1:A:370:GLN:HG3	1:A:371:ALA:N	2.16	0.58
1:A:334:GLU:O	1:A:337:ASN:HB2	2.03	0.58
1:B:324:MET:N	1:B:325:PRO:HD3	2.18	0.58
1:B:343:VAL:HG21	1:B:379:LEU:HD21	1.84	0.58
1:A:65:LEU:HD22	1:A:245:TYR:HD1	1.68	0.58
1:D:234:ALA:CB	1:D:239:LEU:HD23	2.33	0.58
1:C:343:VAL:HG21	1:C:379:LEU:HG	1.85	0.58
1:B:314:LEU:HD13	1:B:394:ILE:HG12	1.86	0.58
1:D:186:LYS:HA	1:D:401:CYS:O	2.03	0.58
1:D:402:GLU:HA	1:D:405:VAL:HG12	1.84	0.58
1:A:405:VAL:HG23	1:A:406:TYR:N	2.18	0.58
1:D:427:VAL:HG11	1:D:438:VAL:HG13	1.86	0.58
1:D:221:THR:CG2	1:D:280:VAL:HA	2.34	0.58
1:B:6:ARG:HD2	1:B:17:VAL:HG13	1.85	0.58
1:C:241:THR:O	1:C:243:LYS:N	2.37	0.58
1:D:129:TYR:C	1:D:130:GLN:HE21	2.07	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:132:LEU:O	1:D:137:HIS:HB2	2.03	0.58
1:A:72:VAL:O	1:A:76:ILE:HG12	2.03	0.58
1:B:181:PHE:CZ	1:B:395:THR:HA	2.39	0.58
1:B:353:ALA:O	1:B:356:ALA:HB3	2.03	0.58
1:D:426:ILE:O	1:D:430:ILE:HG12	2.03	0.58
1:C:20:ASP:HA	1:C:126:LYS:NZ	2.19	0.57
1:D:130:GLN:HG3	1:D:133:ASN:HA	1.85	0.57
1:A:146:ASP:HB2	1:A:229:ASN:O	2.04	0.57
1:B:35:TYR:OH	1:D:389:LYS:HG2	2.04	0.57
1:A:441:VAL:O	1:A:445:ARG:HG3	2.04	0.57
1:B:285:LYS:O	1:B:288:ALA:HB3	2.04	0.57
1:A:330:PRO:O	1:A:333:PRO:HD2	2.04	0.57
1:A:389:LYS:NZ	1:C:33:ASN:HA	2.19	0.57
1:C:313:ASN:N	1:C:395:THR:O	2.34	0.57
1:D:221:THR:HG21	1:D:280:VAL:HA	1.85	0.57
1:A:204:PHE:HA	1:A:207:PHE:CD2	2.36	0.57
1:C:189:ARG:HB2	1:C:189:ARG:HH11	1.68	0.57
1:B:98:TYR:CD2	1:D:339:VAL:HG12	2.40	0.57
1:C:11:LEU:HD22	1:C:11:LEU:H	1.69	0.57
1:C:45:PRO:HB2	1:C:159:SER:OG	2.04	0.57
1:A:97:VAL:HG23	1:A:98:TYR:CE1	2.38	0.57
1:D:295:CYS:SG	1:D:336:VAL:HB	2.43	0.57
1:A:162:LYS:HD2	4:A:709:HOH:O	2.04	0.57
1:B:452:GLU:O	1:B:455:ASP:HB2	2.05	0.57
1:C:177:LYS:HE3	1:C:391:ILE:O	2.04	0.57
1:D:445:ARG:NH1	1:D:445:ARG:HG2	2.14	0.57
1:B:235:ILE:HG12	1:C:196:VAL:O	2.04	0.57
1:C:214:GLU:OE1	1:C:287:LEU:HA	2.05	0.57
1:D:52:VAL:HG21	1:D:83:VAL:HG11	1.87	0.57
1:D:233:THR:OG1	1:D:234:ALA:N	2.37	0.57
1:D:346:ASN:O	1:D:350:VAL:HG23	2.05	0.57
1:D:124:HIS:HB3	1:D:129:TYR:HD2	1.70	0.57
1:B:365:GLU:N	1:B:366:PRO:HD2	2.20	0.57
1:A:21:ALA:HB1	1:A:23:TYR:CE1	2.40	0.56
1:A:248:LEU:HD12	1:A:251:LYS:HD3	1.86	0.56
1:B:104:THR:HA	1:B:144:THR:CG2	2.34	0.56
1:C:94:PRO:HD2	1:C:109:ASN:HD21	1.69	0.56
1:B:107:ASN:ND2	1:B:147:ALA:HB3	2.19	0.56
1:D:200:LEU:HD21	1:D:312:ILE:CG2	2.36	0.56
1:B:200:LEU:HD11	1:B:204:PHE:HE1	1.70	0.56
1:A:56:LYS:HB2	1:A:80:CYS:CB	2.35	0.56
1:B:273:ASP:O	1:C:290:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:241:THR:O	1:C:243:LYS:HG2	2.05	0.56
1:A:79:ALA:O	1:A:82:GLU:HB2	2.05	0.56
1:A:358:GLN:NE2	1:C:299:ARG:HH12	2.03	0.56
1:C:311:GLU:HB3	1:C:401:CYS:SG	2.46	0.56
1:D:119:LEU:HD23	1:D:132:LEU:HB3	1.87	0.56
1:D:120:GLU:HA	1:D:124:HIS:O	2.05	0.56
1:D:127:GLY:C	1:D:129:TYR:H	2.09	0.56
1:A:234:ALA:O	1:A:235:ILE:HG23	2.05	0.56
1:D:419:ILE:HD11	1:D:424:GLY:HA2	1.88	0.56
1:B:88:LYS:C	1:B:89:CYS:SG	2.84	0.56
1:B:161:ILE:O	1:B:164:VAL:HG22	2.05	0.56
1:B:159:SER:HB3	1:B:376:VAL:HG11	1.87	0.56
1:D:204:PHE:HZ	1:D:312:ILE:HD13	1.71	0.56
1:B:350:VAL:HG13	1:B:368:ILE:HG12	1.86	0.56
1:D:391:ILE:HA	1:D:394:ILE:HG12	1.88	0.56
1:B:108:MET:O	1:B:112:GLU:HG3	2.05	0.56
1:A:391:ILE:HA	1:A:394:ILE:HG13	1.88	0.56
1:A:257:THR:HB	1:A:259:PHE:CD2	2.40	0.56
1:D:6:ARG:O	1:D:17:VAL:N	2.39	0.56
1:A:11:LEU:HD23	1:C:319:ALA:HA	1.87	0.56
1:C:247:PRO:HA	1:C:250:VAL:HG22	1.87	0.56
1:A:34:PHE:HZ	1:C:331:VAL:CG2	2.19	0.56
1:B:189:ARG:HB2	1:C:359:LEU:HD12	1.86	0.56
1:D:295:CYS:SG	1:D:336:VAL:CG1	2.94	0.56
1:D:6:ARG:HG2	1:D:17:VAL:O	2.06	0.55
1:A:40:LYS:HD3	1:A:94:PRO:O	2.06	0.55
1:A:237:THR:HA	1:A:267:LEU:HD23	1.88	0.55
1:A:107:ASN:OD1	1:A:147:ALA:HB3	2.05	0.55
1:D:13:GLY:HA3	1:D:15:ARG:HH12	1.70	0.55
1:A:419:ILE:O	1:A:423:ASN:HB2	2.06	0.55
1:C:11:LEU:HD22	1:C:11:LEU:N	2.21	0.55
1:A:196:VAL:HG23	1:D:235:ILE:HG12	1.87	0.55
1:C:173:GLY:O	1:C:177:LYS:HG2	2.07	0.55
1:A:423:ASN:O	1:A:426:ILE:HG23	2.07	0.55
1:C:302:SER:HB3	1:C:314:LEU:HD13	1.87	0.55
1:C:329:ASN:O	1:C:331:VAL:N	2.39	0.55
1:B:268:ILE:HD13	1:C:205:ARG:HD3	1.88	0.55
1:C:90:MET:O	1:C:92:GLN:N	2.38	0.55
1:D:168:ASN:HD22	1:D:171:ARG:HD3	1.71	0.55
1:C:81:ASP:O	1:C:85:ASN:HB3	2.06	0.55
1:D:356:ALA:HB3	1:D:364:MET:HG3	1.88	0.55
1:A:97:VAL:HG23	1:A:98:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:350:VAL:HG13	1:B:368:ILE:HG23	1.87	0.55
1:C:241:THR:OG1	1:C:242:PRO:HD3	2.06	0.55
1:B:419:ILE:HG21	1:B:448:LEU:HD21	1.87	0.55
1:D:315:PRO:HD3	1:D:394:ILE:HD13	1.87	0.55
1:A:119:LEU:HD12	1:A:126:LYS:HA	1.88	0.55
1:A:314:LEU:HD21	1:A:333:PRO:HG2	1.89	0.55
1:B:288:ALA:HB1	1:B:344:ILE:HG13	1.89	0.55
1:A:328:VAL:HG12	1:A:328:VAL:O	2.06	0.55
1:D:11:LEU:N	1:D:11:LEU:HD22	2.20	0.55
1:C:402:GLU:HB3	1:C:406:TYR:CE2	2.41	0.55
1:D:385:ASN:C	1:D:385:ASN:HD22	2.10	0.55
1:C:267:LEU:O	1:C:268:ILE:HG23	2.06	0.55
1:B:116:ASN:CG	1:B:126:LYS:HB2	2.27	0.55
1:B:156:VAL:O	1:B:160:LEU:HG	2.07	0.55
1:B:327:LYS:O	1:B:328:VAL:HG23	2.07	0.55
1:B:116:ASN:OD1	1:B:126:LYS:HB2	2.06	0.55
1:A:207:PHE:O	1:A:211:LEU:HG	2.08	0.55
1:D:281:HIS:CD2	1:D:350:VAL:HG21	2.42	0.55
1:A:364:MET:HG2	1:C:341:PHE:CE2	2.42	0.55
1:A:332:VAL:O	1:A:336:VAL:HG23	2.07	0.54
1:B:431:CYS:SG	1:B:441:VAL:CG2	2.95	0.54
1:C:267:LEU:CD2	1:C:267:LEU:H	2.21	0.54
1:C:134:PRO:HA	1:C:138:VAL:HG23	1.90	0.54
1:B:370:GLN:O	1:B:374:GLU:HB2	2.08	0.54
1:A:110:THR:HG22	1:A:114:LEU:HD11	1.89	0.54
1:D:170:LEU:HD23	1:D:211:LEU:HG	1.90	0.54
1:D:40:LYS:HE2	1:D:94:PRO:O	2.06	0.54
1:D:241:THR:N	1:D:242:PRO:CD	2.66	0.54
1:D:168:ASN:O	1:D:172:GLU:HG3	2.07	0.54
1:C:386:LEU:O	1:C:390:CYS:HB3	2.06	0.54
1:B:102:ALA:HB2	1:B:363:VAL:HG12	1.90	0.54
1:B:36:ILE:HG12	1:D:339:VAL:HG11	1.88	0.54
1:A:415:LEU:O	1:A:419:ILE:HG12	2.08	0.54
1:D:126:LYS:HZ3	1:D:126:LYS:HB3	1.73	0.54
1:B:23:TYR:HB2	1:B:27:THR:HG21	1.90	0.54
1:B:308:GLY:O	1:B:310:ASN:N	2.40	0.54
1:A:115:ALA:O	1:A:119:LEU:HG	2.08	0.54
1:B:243:LYS:CE	1:B:244:GLU:H	2.18	0.54
1:D:246:SER:HB2	1:D:247:PRO:CD	2.37	0.54
1:A:378:ILE:HG13	1:A:379:LEU:N	2.23	0.54
1:B:423:ASN:O	1:B:426:ILE:HG22	2.06	0.54
1:A:281:HIS:CD2	1:A:350:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:339:VAL:O	1:B:343:VAL:HG23	2.08	0.54
1:A:272:SER:HA	1:A:362:ASN:N	2.22	0.54
1:A:237:THR:HA	1:A:267:LEU:CD2	2.38	0.53
1:D:152:PHE:CE1	1:D:369:GLY:HA2	2.43	0.53
1:B:88:LYS:O	1:B:89:CYS:SG	2.66	0.53
1:A:331:VAL:HG13	1:C:34:PHE:HE1	1.72	0.53
1:B:363:VAL:CG1	1:C:191:GLN:HG2	2.38	0.53
1:B:439:ARG:HG3	1:B:439:ARG:NH1	2.22	0.53
1:A:34:PHE:HA	1:C:385:ASN:OD1	2.08	0.53
1:C:6:ARG:HH11	1:C:127:GLY:HA3	1.73	0.53
1:D:321:SER:OG	1:D:325:PRO:HA	2.09	0.53
1:C:325:PRO:O	1:D:409:ILE:HD13	2.09	0.53
1:D:280:VAL:HG23	1:D:281:HIS:N	2.24	0.53
1:A:295:CYS:O	1:A:299:ARG:HG3	2.08	0.53
1:A:451:ALA:C	1:A:453:LEU:H	2.11	0.53
1:A:153:ARG:HD3	1:A:228:VAL:HG12	1.91	0.53
1:A:324:MET:N	1:A:324:MET:SD	2.82	0.53
1:B:52:VAL:HG12	1:B:114:LEU:HD21	1.90	0.53
1:B:5:ILE:HD13	1:B:5:ILE:N	2.22	0.53
1:B:205:ARG:O	1:B:209:ILE:HG12	2.07	0.53
1:C:27:THR:O	1:C:31:ILE:HG13	2.08	0.53
1:C:154:ILE:HG13	1:C:259:PHE:HD2	1.73	0.53
1:C:62:ASN:HD22	1:C:67:THR:HG21	1.72	0.53
1:D:246:SER:O	1:D:250:VAL:HG13	2.09	0.53
1:A:359:LEU:HD12	1:A:359:LEU:N	2.23	0.53
1:B:191:GLN:O	1:B:192:LEU:HB2	2.09	0.53
1:C:200:LEU:O	1:C:203:GLU:HB3	2.09	0.53
1:D:22:TYR:O	1:D:116:ASN:ND2	2.40	0.53
1:C:193:GLN:HB2	1:D:327:LYS:NZ	2.23	0.53
1:B:45:PRO:O	1:B:46:GLU:HB2	2.09	0.52
1:A:299:ARG:HB3	1:B:192:LEU:HD12	1.92	0.52
1:A:370:GLN:HG3	1:A:371:ALA:H	1.75	0.52
1:A:327:LYS:O	1:A:328:VAL:HG23	2.09	0.52
1:A:35:TYR:HE1	1:C:389:LYS:HD2	1.73	0.52
1:D:185:LEU:HA	1:D:198:MET:O	2.09	0.52
1:D:28:LEU:O	1:D:31:ILE:HB	2.09	0.52
1:D:210:LEU:HD22	1:D:294:ILE:HD11	1.91	0.52
1:D:296:ASN:HA	1:D:299:ARG:NE	2.24	0.52
1:D:46:GLU:OE2	1:D:155:ALA:HA	2.09	0.52
1:C:276:ALA:O	1:C:280:VAL:HG13	2.09	0.52
1:B:181:PHE:HZ	1:B:395:THR:HA	1.73	0.52
1:D:101:GLY:O	1:D:104:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:275:GLY:HA3	1:D:286:ARG:NE	2.24	0.52
1:D:439:ARG:HA	1:D:453:LEU:HD21	1.91	0.52
1:B:323:ILE:C	1:B:325:PRO:HD3	2.30	0.52
1:B:199:THR:HG23	1:B:202:GLN:N	2.18	0.52
1:A:294:ILE:O	1:A:298:LEU:HG	2.09	0.52
1:B:305:PRO:O	1:B:306:ARG:HB3	2.09	0.52
1:D:365:GLU:N	1:D:366:PRO:CD	2.72	0.52
1:D:247:PRO:O	1:D:250:VAL:HG22	2.09	0.52
1:B:189:ARG:HA	1:B:193:GLN:O	2.09	0.52
1:A:235:ILE:HD13	1:D:196:VAL:HG23	1.91	0.52
1:A:322:SER:CB	1:B:429:LYS:HZ1	2.23	0.52
1:D:314:LEU:HD23	1:D:394:ILE:CD1	2.40	0.52
1:A:188:GLY:HA2	1:D:360:GLN:OE1	2.10	0.52
1:D:119:LEU:HD22	1:D:129:TYR:O	2.09	0.52
1:C:44:ILE:HB	1:C:45:PRO:HD3	1.91	0.52
1:A:267:LEU:N	1:A:267:LEU:HD22	2.24	0.52
1:A:327:LYS:HG2	1:A:328:VAL:H	1.73	0.52
1:A:275:GLY:HA3	1:D:286:ARG:CZ	2.39	0.52
1:C:148:TYR:HB3	1:C:149:PRO:HD3	1.92	0.52
1:B:196:VAL:O	1:C:235:ILE:HG21	2.10	0.52
1:D:117:ILE:O	1:D:121:LEU:HG	2.10	0.52
1:A:350:VAL:HG13	1:A:368:ILE:HG23	1.92	0.52
1:C:391:ILE:HA	1:C:394:ILE:HG13	1.90	0.52
1:C:332:VAL:O	1:C:335:VAL:HG12	2.10	0.52
1:B:31:ILE:HG22	1:B:31:ILE:O	2.10	0.52
1:D:55:LYS:HG3	1:D:110:THR:CG2	2.39	0.52
1:D:415:LEU:HA	1:D:418:PHE:HD2	1.74	0.52
1:A:68:ILE:HD11	1:A:73:ALA:HA	1.92	0.52
1:D:295:CYS:SG	1:D:336:VAL:HG11	2.50	0.52
1:C:11:LEU:H	1:C:11:LEU:CD2	2.22	0.52
1:A:5:ILE:HD13	1:A:5:ILE:N	2.25	0.51
1:C:88:LYS:C	1:C:90:MET:H	2.14	0.51
1:C:149:PRO:O	1:C:152:PHE:HB3	2.10	0.51
1:A:359:LEU:HD11	1:D:300:LEU:CD2	2.40	0.51
1:B:83:VAL:HA	1:B:87:GLY:HA2	1.92	0.51
1:A:74:ASN:O	1:A:78:ALA:HB2	2.10	0.51
1:A:434:THR:HB	1:A:436:LYS:HG3	1.92	0.51
1:A:365:GLU:N	1:A:366:PRO:HD2	2.25	0.51
1:C:119:LEU:CD2	1:C:132:LEU:HB3	2.37	0.51
1:B:185:LEU:HB3	1:B:405:VAL:HG21	1.93	0.51
1:A:458:SER:O	1:A:459:VAL:HB	2.09	0.51
1:B:41:ILE:HD11	1:B:99:GLN:HE22	1.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:302:SER:HB3	1:B:312:ILE:HG13	1.92	0.51
1:B:281:HIS:O	1:B:284:LEU:N	2.43	0.51
1:D:415:LEU:O	1:D:419:ILE:HG23	2.10	0.51
1:A:286:ARG:HH11	1:D:279:MET:CG	2.22	0.51
1:B:413:THR:HA	1:B:416:ASN:OD1	2.11	0.51
1:A:364:MET:HG2	1:C:341:PHE:HE2	1.74	0.51
1:A:342:LYS:NZ	1:C:342:LYS:NZ	2.58	0.51
1:C:220:ARG:O	1:C:223:GLU:HG3	2.09	0.51
1:A:125:GLN:NE2	1:A:129:TYR:HB2	2.25	0.51
1:A:389:LYS:HZ3	1:C:33:ASN:HA	1.75	0.51
1:A:240:ASN:C	1:A:242:PRO:HD2	2.31	0.51
1:C:402:GLU:O	1:C:405:VAL:HG12	2.10	0.51
1:C:175:GLU:O	1:C:179:VAL:HG23	2.10	0.51
1:A:271:THR:HG23	1:A:272:SER:N	2.25	0.51
1:D:55:LYS:HG3	1:D:110:THR:HG21	1.93	0.51
1:D:323:ILE:HG12	1:D:324:MET:N	2.25	0.51
1:A:163:LEU:O	1:A:167:ILE:HG13	2.10	0.51
1:A:269:GLU:CG	1:A:270:ALA:N	2.63	0.51
1:A:23:TYR:HB2	1:A:27:THR:HG21	1.92	0.51
1:D:235:ILE:CD1	1:D:236:GLY:H	2.13	0.51
1:B:186:LYS:HE3	1:B:203:GLU:OE1	2.10	0.51
1:B:69:PRO:HB2	1:B:72:VAL:HG13	1.93	0.51
1:A:387:LEU:HA	1:A:391:ILE:HG13	1.93	0.51
1:B:445:ARG:HB3	1:B:447:LEU:HD13	1.93	0.51
1:B:200:LEU:CD2	1:B:396:ALA:HB2	2.41	0.50
1:C:139:ASN:ND2	1:C:142:GLN:HB2	2.27	0.50
1:C:168:ASN:O	1:C:171:ARG:HB2	2.11	0.50
1:A:5:ILE:HG13	1:A:16:GLU:HB3	1.93	0.50
1:C:274:CYS:HB2	1:C:277:TYR:CE2	2.46	0.50
1:A:185:LEU:H	1:A:402:GLU:HG2	1.75	0.50
1:D:273:ASP:CB	1:D:362:ASN:HD22	2.08	0.50
1:D:431:CYS:SG	1:D:441:VAL:CG2	2.91	0.50
1:D:381:ASN:O	1:D:385:ASN:HB2	2.10	0.50
1:A:113:VAL:O	1:A:117:ILE:HG13	2.10	0.50
1:C:26:HIS:ND1	1:C:108:MET:HG2	2.26	0.50
1:B:415:LEU:HB3	1:B:419:ILE:CD1	2.40	0.50
1:B:231:GLY:HA2	1:B:241:THR:CG2	2.41	0.50
1:D:413:THR:O	1:D:417:PRO:HD3	2.10	0.50
1:B:157:TYR:O	1:B:161:ILE:HG13	2.10	0.50
1:B:40:LYS:O	1:B:42:SER:N	2.44	0.50
1:B:401:CYS:O	1:B:404:TYR:HB2	2.11	0.50
1:D:244:GLU:OE2	1:D:248:LEU:HD22	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:250:VAL:HA	1:B:253:LEU:CB	2.42	0.50
1:A:339:VAL:HG21	1:A:382:ALA:CB	2.40	0.50
1:D:214:GLU:OE1	1:D:287:LEU:HA	2.12	0.50
1:C:120:GLU:C	1:C:122:MET:H	2.15	0.50
1:B:250:VAL:HA	1:B:253:LEU:HB3	1.92	0.50
1:A:131:TYR:O	1:A:132:LEU:HD12	2.11	0.50
1:A:302:SER:OG	1:A:314:LEU:HD13	2.11	0.50
1:D:126:LYS:HZ3	1:D:126:LYS:CB	2.24	0.50
1:D:444:GLU:HG3	1:D:445:ARG:N	2.27	0.50
1:D:130:GLN:HE21	1:D:130:GLN:HA	1.76	0.50
1:B:85:ASN:ND2	1:B:88:LYS:NZ	2.60	0.50
1:A:172:GLU:O	1:A:176:ARG:HG3	2.11	0.50
1:C:10:ASP:HB3	1:C:29:ARG:HH21	1.77	0.50
1:D:85:ASN:O	1:D:86:ASN:HB3	2.12	0.50
1:D:210:LEU:HD22	1:D:294:ILE:CD1	2.42	0.50
1:A:216:LYS:O	1:A:220:ARG:HB2	2.12	0.50
1:B:439:ARG:HG2	1:B:453:LEU:HD21	1.94	0.49
1:B:72:VAL:O	1:B:75:ALA:HB3	2.11	0.49
1:D:134:PRO:HG2	1:D:135:ASN:H	1.77	0.49
1:C:117:ILE:O	1:C:121:LEU:HG	2.11	0.49
1:D:445:ARG:CG	1:D:445:ARG:HH11	2.12	0.49
1:A:152:PHE:CZ	1:A:369:GLY:HA2	2.47	0.49
1:B:275:GLY:HA3	1:C:290:LYS:NZ	2.25	0.49
1:C:108:MET:HA	1:C:111:ASN:HD22	1.78	0.49
1:A:413:THR:O	1:A:413:THR:HG22	2.12	0.49
1:A:222:ALA:O	1:A:224:LEU:N	2.45	0.49
1:D:323:ILE:CG1	1:D:324:MET:SD	2.94	0.49
1:C:45:PRO:HG2	1:C:373:PHE:CD1	2.47	0.49
1:C:48:VAL:O	1:C:52:VAL:HG12	2.12	0.49
1:A:192:LEU:HD13	1:B:300:LEU:HA	1.93	0.49
1:A:247:PRO:O	1:A:250:VAL:HG22	2.13	0.49
1:D:373:PHE:HA	1:D:376:VAL:HG22	1.94	0.49
1:B:456:ILE:O	1:B:457:PHE:HB2	2.12	0.49
1:A:68:ILE:HD12	1:A:72:VAL:CG2	2.40	0.49
1:A:235:ILE:HG22	1:D:188:GLY:HA3	1.94	0.49
1:A:199:THR:C	1:A:201:GLY:H	2.16	0.49
1:A:110:THR:O	1:A:114:LEU:HG	2.12	0.49
1:C:304:GLY:HA2	1:D:193:GLN:HA	1.93	0.49
1:A:122:MET:C	1:A:124:HIS:H	2.14	0.49
1:B:331:VAL:HG23	1:D:101:GLY:N	2.28	0.49
1:A:191:GLN:HG2	1:D:363:VAL:CG1	2.42	0.49
1:B:442:VAL:HG11	1:B:448:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:205:ARG:CZ	1:C:205:ARG:HB2	2.43	0.49
1:C:257:THR:HB	1:C:259:PHE:CD2	2.47	0.49
1:A:126:LYS:HG3	1:A:127:GLY:N	2.28	0.49
1:B:85:ASN:HD22	1:B:88:LYS:HZ1	1.61	0.49
1:B:336:VAL:HA	1:B:339:VAL:HG13	1.94	0.49
1:A:191:GLN:HG2	1:D:363:VAL:HG11	1.95	0.49
1:D:303:SER:HG	1:D:309:LEU:HB2	1.78	0.49
1:B:354:ALA:CB	1:C:289:VAL:HG11	2.42	0.49
1:C:196:VAL:HG23	1:C:197:PRO:HD2	1.94	0.49
1:C:119:LEU:O	1:C:122:MET:HB2	2.13	0.49
1:A:296:ASN:O	1:A:300:LEU:HB2	2.13	0.49
1:D:161:ILE:O	1:D:164:VAL:HG22	2.13	0.49
1:C:69:PRO:HB2	1:C:72:VAL:HG13	1.94	0.49
1:D:269:GLU:HA	1:D:272:SER:OG	2.13	0.49
1:D:241:THR:H	1:D:242:PRO:HD2	1.78	0.49
1:B:5:ILE:HA	1:B:19:ALA:HB2	1.95	0.49
1:B:85:ASN:ND2	1:B:88:LYS:HZ1	2.11	0.49
1:A:405:VAL:CG2	1:A:406:TYR:N	2.76	0.49
1:A:322:SER:HA	1:B:429:LYS:HZ3	1.78	0.49
1:A:272:SER:HA	1:A:362:ASN:H	1.78	0.49
1:D:274:CYS:SG	1:D:276:ALA:HB3	2.53	0.49
1:B:324:MET:O	1:B:326:ALA:N	2.46	0.48
1:A:125:GLN:HE22	1:A:131:TYR:HE1	1.61	0.48
1:A:327:LYS:HG2	1:A:328:VAL:N	2.28	0.48
1:D:83:VAL:HG22	1:D:89:CYS:HB2	1.95	0.48
1:B:52:VAL:HG23	1:B:84:LEU:HD21	1.95	0.48
1:A:145:ASN:HB2	1:A:233:THR:O	2.13	0.48
1:C:406:TYR:C	1:C:408:SER:H	2.15	0.48
1:D:129:TYR:CD2	1:D:131:TYR:CE2	2.97	0.48
1:A:93:PHE:HA	1:A:109:ASN:ND2	2.24	0.48
1:D:56:LYS:HB2	1:D:80:CYS:SG	2.53	0.48
1:A:36:ILE:HG23	1:C:378:ILE:HB	1.93	0.48
1:B:108:MET:CE	1:B:111:ASN:HD22	2.26	0.48
1:B:58:ALA:HB1	1:B:142:GLN:HE22	1.79	0.48
1:D:273:ASP:HB2	1:D:362:ASN:ND2	2.07	0.48
1:A:343:VAL:HG22	1:A:375:SER:HA	1.94	0.48
1:D:47:PHE:N	1:D:155:ALA:HB1	2.27	0.48
1:C:272:SER:HA	1:C:362:ASN:N	2.29	0.48
1:D:13:GLY:HA3	1:D:15:ARG:NH1	2.28	0.48
1:A:307:ALA:HB3	1:B:194:ASP:OD2	2.13	0.48
1:B:419:ILE:CG2	1:B:448:LEU:HD21	2.43	0.48
1:D:79:ALA:HB1	1:D:117:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:290:LYS:HZ3	1:D:273:ASP:CG	2.17	0.48
1:D:23:TYR:HB2	1:D:27:THR:CB	2.43	0.48
1:B:387:LEU:HG	1:B:388:GLU:N	2.29	0.48
1:B:293:LYS:HA	1:B:296:ASN:HB2	1.95	0.48
1:A:226:LEU:CD1	1:A:259:PHE:HB3	2.35	0.48
1:B:49:ARG:HA	1:B:52:VAL:CG2	2.43	0.48
1:B:177:LYS:HE3	1:B:391:ILE:O	2.13	0.48
1:A:98:TYR:N	1:A:98:TYR:CD1	2.80	0.48
1:A:146:ASP:CG	1:A:231:GLY:H	2.17	0.48
1:B:227:GLU:HB3	1:B:264:ALA:HA	1.96	0.48
1:C:5:ILE:HG22	1:C:18:PRO:HA	1.93	0.48
1:A:184:ILE:HG23	1:A:398:LYS:HA	1.95	0.48
1:D:264:ALA:C	1:D:266:ASP:H	2.15	0.48
1:D:41:ILE:HG13	1:D:95:VAL:O	2.13	0.48
1:B:241:THR:HB	1:B:242:PRO:HD3	1.95	0.48
1:B:459:VAL:HG22	1:B:460:GLN:H	1.77	0.48
1:D:325:PRO:O	1:D:326:ALA:HB2	2.14	0.48
1:A:47:PHE:CZ	1:A:148:TYR:CE1	3.01	0.48
1:B:173:GLY:C	1:B:391:ILE:HD12	2.34	0.48
1:B:176:ARG:NH2	1:B:392:ASN:ND2	2.62	0.48
1:A:126:LYS:HG3	1:A:127:GLY:H	1.79	0.48
1:D:274:CYS:SG	1:D:276:ALA:CB	3.02	0.48
1:A:242:PRO:O	1:A:243:LYS:HB3	2.14	0.48
1:D:234:ALA:HB2	1:D:239:LEU:HD23	1.96	0.48
1:B:124:HIS:HD2	1:B:131:TYR:CE1	2.32	0.48
1:D:190:THR:O	1:D:191:GLN:HB2	2.14	0.48
1:A:235:ILE:HG13	1:A:236:GLY:H	1.79	0.47
1:A:364:MET:O	1:A:367:VAL:HG12	2.14	0.47
1:C:285:LYS:HD3	1:C:347:ASP:CB	2.44	0.47
1:D:26:HIS:HD2	1:D:108:MET:HG3	1.79	0.47
1:C:126:LYS:HG2	1:C:127:GLY:N	2.28	0.47
1:C:8:GLU:HA	1:C:128:GLU:HG2	1.96	0.47
1:B:87:GLY:C	1:B:89:CYS:N	2.67	0.47
1:A:331:VAL:HG13	1:C:34:PHE:CE1	2.49	0.47
1:C:241:THR:N	1:C:242:PRO:HD2	2.30	0.47
1:C:166:ALA:HA	1:C:384:TYR:CE1	2.49	0.47
1:D:9:GLU:HB2	1:D:14:THR:HG22	1.97	0.47
1:A:368:ILE:O	1:A:372:MET:HB2	2.13	0.47
1:A:369:GLY:O	1:A:372:MET:HB3	2.14	0.47
1:D:423:ASN:O	1:D:427:VAL:HG23	2.14	0.47
1:D:185:LEU:HA	1:D:199:THR:HA	1.96	0.47
1:C:295:CYS:SG	1:C:336:VAL:HG11	2.54	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:8:GLU:HB2	1:C:25:VAL:CG1	2.39	0.47
1:A:185:LEU:HD22	1:A:406:TYR:HE1	1.78	0.47
1:D:423:ASN:HD22	1:D:447:LEU:HD21	1.80	0.47
1:C:79:ALA:HB2	1:C:118:GLY:CA	2.43	0.47
1:C:323:ILE:C	1:C:324:MET:SD	2.92	0.47
1:C:378:ILE:HD13	1:C:379:LEU:H	1.80	0.47
1:A:342:LYS:HZ2	1:C:342:LYS:NZ	2.12	0.47
1:B:152:PHE:CE1	1:B:369:GLY:HA2	2.48	0.47
1:B:415:LEU:HD13	1:B:442:VAL:HG21	1.97	0.47
1:D:214:GLU:O	1:D:218:ILE:HG13	2.15	0.47
1:B:225:LEU:CG	1:B:280:VAL:HG11	2.44	0.47
1:D:204:PHE:CZ	1:D:312:ILE:HD13	2.49	0.47
1:B:187:MET:HE2	1:B:405:VAL:HG22	1.95	0.47
1:D:456:ILE:O	1:D:457:PHE:CG	2.67	0.47
1:A:9:GLU:HG3	1:A:13:GLY:C	2.34	0.47
1:D:102:ALA:HB2	1:D:363:VAL:HB	1.94	0.47
1:C:47:PHE:O	1:C:50:GLY:N	2.47	0.47
1:D:399:GLU:O	1:D:403:GLY:N	2.48	0.47
1:A:56:LYS:HB2	1:A:80:CYS:HB3	1.96	0.47
1:C:280:VAL:O	1:C:284:LEU:HD13	2.15	0.47
1:A:194:ASP:OD2	1:B:305:PRO:O	2.33	0.47
1:A:419:ILE:O	1:A:423:ASN:ND2	2.47	0.47
1:A:205:ARG:HH21	1:A:209:ILE:HD11	1.80	0.47
1:A:83:VAL:CG1	1:A:90:MET:HB3	2.31	0.47
1:C:299:ARG:HG2	1:C:330:PRO:HB2	1.97	0.47
1:D:5:ILE:HD13	1:D:5:ILE:N	2.30	0.47
1:C:170:LEU:HA	1:C:387:LEU:HD13	1.96	0.47
1:C:104:THR:HG22	1:C:144:THR:CG2	2.37	0.47
1:B:51:MET:HB3	1:B:110:THR:HG21	1.97	0.47
1:A:145:ASN:ND2	1:A:234:ALA:HB2	2.30	0.47
1:D:168:ASN:ND2	1:D:171:ARG:HD3	2.30	0.47
1:A:243:LYS:HG2	1:A:244:GLU:N	2.30	0.46
1:A:196:VAL:HG23	1:D:235:ILE:CG1	2.44	0.46
1:B:439:ARG:NH2	1:B:450:GLU:HG3	2.28	0.46
1:D:54:VAL:HG13	1:D:55:LYS:N	2.30	0.46
1:B:323:ILE:C	1:B:324:MET:SD	2.93	0.46
1:B:9:GLU:CG	1:B:10:ASP:N	2.78	0.46
1:D:27:THR:O	1:D:31:ILE:HG13	2.15	0.46
1:C:327:LYS:HE2	1:C:329:ASN:OD1	2.15	0.46
1:A:164:VAL:HB	1:A:215:VAL:HG13	1.97	0.46
1:A:45:PRO:O	1:A:46:GLU:HB2	2.15	0.46
1:D:372:MET:O	1:D:376:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:63:LYS:HG3	1:B:64:GLU:N	2.30	0.46
1:A:330:PRO:O	1:A:334:GLU:HG3	2.16	0.46
1:A:35:TYR:CE1	1:C:389:LYS:HD2	2.51	0.46
1:C:157:TYR:CE2	1:C:226:LEU:HD11	2.51	0.46
1:D:197:PRO:HB3	1:D:405:VAL:HG23	1.97	0.46
1:B:99:GLN:HE22	1:B:106:VAL:CG2	2.29	0.46
1:B:118:GLY:O	1:B:122:MET:HG3	2.15	0.46
1:A:241:THR:O	1:A:242:PRO:O	2.33	0.46
1:D:324:MET:N	1:D:324:MET:SD	2.88	0.46
1:B:45:PRO:HB2	1:B:159:SER:OG	2.16	0.46
1:B:280:VAL:O	1:B:284:LEU:HD22	2.14	0.46
1:B:61:ALA:O	1:B:64:GLU:HB3	2.16	0.46
1:B:281:HIS:HA	1:B:284:LEU:CD2	2.46	0.46
1:C:365:GLU:HB2	1:C:366:PRO:HD3	1.98	0.46
1:A:290:LYS:NZ	1:D:273:ASP:CG	2.69	0.46
1:D:207:PHE:CD1	1:D:294:ILE:HG23	2.50	0.46
1:D:250:VAL:HG21	1:D:263:PRO:CG	2.45	0.46
1:D:116:ASN:O	1:D:120:GLU:HB2	2.15	0.46
1:D:69:PRO:O	1:D:72:VAL:HG22	2.15	0.46
1:D:186:LYS:O	1:D:405:VAL:HB	2.15	0.46
1:B:330:PRO:O	1:B:334:GLU:HG3	2.16	0.46
1:B:101:GLY:O	1:B:104:THR:HG23	2.15	0.46
1:C:312:ILE:HG13	1:C:312:ILE:O	2.15	0.46
1:D:439:ARG:HH22	1:D:454:ASP:HB3	1.80	0.46
1:A:204:PHE:O	1:A:207:PHE:HB2	2.16	0.46
1:B:186:LYS:HG2	1:B:187:MET:N	2.29	0.46
1:A:175:GLU:O	1:A:179:VAL:HG23	2.15	0.46
1:B:431:CYS:SG	1:B:438:VAL:HA	2.56	0.46
1:C:231:GLY:CA	1:C:241:THR:HG21	2.46	0.46
1:A:35:TYR:CD1	1:A:35:TYR:N	2.84	0.46
1:C:223:GLU:O	1:C:226:LEU:HB2	2.16	0.46
1:A:273:ASP:OD1	1:A:274:CYS:N	2.49	0.45
1:B:326:ALA:O	1:B:327:LYS:HG3	2.16	0.45
1:D:436:LYS:HZ1	1:D:440:GLU:HB2	1.80	0.45
1:A:355:GLU:C	1:A:357:GLY:H	2.19	0.45
1:C:233:THR:HB	1:C:237:THR:O	2.16	0.45
1:D:253:LEU:CD1	1:D:261:CYS:SG	2.94	0.45
1:C:186:LYS:HD3	1:C:200:LEU:HA	1.99	0.45
1:C:116:ASN:O	1:C:120:GLU:HG3	2.16	0.45
1:B:170:LEU:HD12	1:B:391:ILE:HD13	1.97	0.45
1:C:277:TYR:HA	1:C:280:VAL:HG22	1.98	0.45
1:B:49:ARG:CA	1:B:52:VAL:HG22	2.43	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:46:GLU:HG2	1:A:49:ARG:HD3	1.97	0.45
1:C:92:GLN:O	1:C:94:PRO:HD3	2.17	0.45
1:A:318:GLN:O	1:C:12:LEU:HD22	2.16	0.45
1:D:25:VAL:O	1:D:29:ARG:N	2.41	0.45
1:A:170:LEU:HD11	1:A:386:LEU:HD23	1.99	0.45
1:D:53:MET:SD	1:D:257:THR:HG22	2.57	0.45
1:C:328:VAL:HG12	1:C:328:VAL:O	2.16	0.45
1:C:273:ASP:N	1:C:362:ASN:HB2	2.31	0.45
1:A:322:SER:HA	1:B:429:LYS:NZ	2.32	0.45
1:B:324:MET:C	1:B:326:ALA:H	2.20	0.45
1:B:241:THR:CB	1:B:242:PRO:HD3	2.47	0.45
1:C:339:VAL:HB	1:C:378:ILE:HG12	1.98	0.45
1:A:225:LEU:HD21	1:A:280:VAL:HG11	1.98	0.45
1:C:348:THR:O	1:C:351:THR:HB	2.15	0.45
1:A:6:ARG:HG2	1:A:7:ILE:N	2.31	0.45
1:C:194:ASP:OD1	1:D:307:ALA:HB3	2.16	0.45
1:D:138:VAL:O	1:D:142:GLN:NE2	2.49	0.45
1:D:239:LEU:HB3	1:D:240:ASN:H	1.64	0.45
1:D:406:TYR:HE1	1:D:457:PHE:HB3	1.82	0.45
1:A:245:TYR:CD2	1:A:246:SER:N	2.85	0.45
1:A:212:LYS:HG3	1:A:213:GLU:N	2.31	0.45
1:C:409:ILE:CD1	1:D:306:ARG:HB2	2.47	0.45
1:B:209:ILE:HG13	1:C:268:ILE:CD1	2.47	0.45
1:D:160:LEU:O	1:D:163:LEU:HB3	2.17	0.45
1:D:336:VAL:O	1:D:340:CYS:SG	2.62	0.45
1:A:142:GLN:O	1:A:143:SER:HB3	2.16	0.45
1:A:207:PHE:CD1	1:A:294:ILE:HG23	2.52	0.45
1:A:336:VAL:HA	1:A:339:VAL:CG1	2.46	0.45
1:D:151:GLY:O	1:D:154:ILE:HB	2.16	0.45
1:D:65:LEU:O	1:D:66:GLN:HB2	2.16	0.45
1:A:6:ARG:HD3	1:A:8:GLU:HG3	1.99	0.45
1:A:92:GLN:C	1:A:94:PRO:HD3	2.37	0.45
1:C:416:ASN:CB	1:C:417:PRO:HD3	2.42	0.45
1:A:312:ILE:HB	1:A:394:ILE:CG2	2.47	0.45
1:A:279:MET:O	1:A:282:GLY:N	2.49	0.45
1:B:442:VAL:HG11	1:B:453:LEU:HD13	1.99	0.44
1:B:85:ASN:CG	1:B:86:ASN:N	2.69	0.44
1:A:70:LYS:HG2	1:A:74:ASN:ND2	2.31	0.44
1:C:50:GLY:O	1:C:54:VAL:HG23	2.16	0.44
1:B:251:LYS:HA	1:B:251:LYS:HD2	1.83	0.44
1:B:198:MET:HB2	1:B:198:MET:HE3	1.91	0.44
1:C:323:ILE:CG2	1:C:324:MET:SD	3.03	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:PHE:HA	1:B:207:PHE:CD2	2.52	0.44
1:C:93:PHE:HA	1:C:109:ASN:HD21	1.82	0.44
1:B:423:ASN:O	1:B:427:VAL:HG23	2.17	0.44
1:C:62:ASN:ND2	1:C:245:TYR:HE1	2.15	0.44
1:A:32:GLU:HG2	1:A:32:GLU:H	1.56	0.44
1:B:442:VAL:CG1	1:B:448:LEU:HD23	2.47	0.44
1:B:235:ILE:CD1	1:B:236:GLY:N	2.81	0.44
1:C:116:ASN:ND2	1:C:127:GLY:HA2	2.32	0.44
1:D:132:LEU:O	1:D:133:ASN:O	2.34	0.44
1:D:72:VAL:HB	1:D:132:LEU:CD1	2.41	0.44
1:A:122:MET:SD	1:A:132:LEU:HD11	2.57	0.44
1:D:423:ASN:ND2	1:D:447:LEU:HD11	2.32	0.44
1:A:323:ILE:HG12	1:B:425:ASP:OD1	2.17	0.44
1:D:181:PHE:CD1	1:D:184:ILE:HD12	2.52	0.44
1:A:122:MET:HB3	1:A:124:HIS:ND1	2.32	0.44
1:B:247:PRO:O	1:B:251:LYS:HG2	2.17	0.44
1:B:382:ALA:HA	1:D:36:ILE:HD12	1.99	0.44
1:D:323:ILE:O	1:D:325:PRO:HD3	2.17	0.44
1:C:116:ASN:HA	1:C:119:LEU:HD12	1.98	0.44
1:D:47:PHE:CE2	1:D:106:VAL:HG11	2.53	0.44
1:D:157:TYR:CE2	1:D:226:LEU:HD22	2.53	0.44
1:D:226:LEU:HA	1:D:226:LEU:HD12	1.60	0.44
1:B:246:SER:CB	1:B:247:PRO:HD3	2.48	0.44
1:D:451:ALA:O	1:D:455:ASP:N	2.50	0.44
1:B:171:ARG:NH2	1:B:212:LYS:NZ	2.65	0.44
1:B:118:GLY:HA3	1:B:132:LEU:HD21	2.00	0.44
1:A:323:ILE:HG12	1:B:425:ASP:OD2	2.17	0.44
1:B:281:HIS:C	1:B:283:ALA:N	2.70	0.44
1:D:205:ARG:O	1:D:209:ILE:HG12	2.18	0.44
1:A:56:LYS:CA	1:A:80:CYS:SG	3.05	0.44
1:A:116:ASN:HB3	1:A:126:LYS:HD2	1.99	0.44
1:A:36:ILE:HD12	1:C:339:VAL:HG11	1.99	0.44
1:C:239:LEU:O	1:C:242:PRO:HD2	2.17	0.44
1:C:285:LYS:HD2	1:C:344:ILE:HG23	2.00	0.44
1:C:47:PHE:HA	1:C:155:ALA:CB	2.47	0.44
1:C:230:LEU:HD12	1:C:230:LEU:HA	1.59	0.44
1:A:245:TYR:O	1:A:249:ALA:N	2.46	0.44
1:B:386:LEU:HD12	1:B:390:CYS:HB3	2.00	0.44
1:B:8:GLU:HB3	1:B:25:VAL:CG2	2.41	0.44
1:C:55:LYS:HD2	1:C:55:LYS:N	2.32	0.44
1:D:44:ILE:N	1:D:45:PRO:CD	2.81	0.44
1:A:402:GLU:O	1:A:405:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:285:LYS:HD3	1:B:347:ASP:CG	2.37	0.44
1:C:47:PHE:HA	1:C:155:ALA:HB1	1.99	0.44
1:A:244:GLU:O	1:A:248:LEU:HB2	2.17	0.43
1:A:111:ASN:CG	1:A:139:ASN:HB2	2.38	0.43
1:C:324:MET:HB2	1:D:409:ILE:CG2	2.48	0.43
1:D:49:ARG:NH2	4:D:490:HOH:O	2.48	0.43
1:A:158:SER:O	1:A:161:ILE:HB	2.18	0.43
1:A:117:ILE:O	1:A:121:LEU:HD23	2.18	0.43
1:B:49:ARG:HB3	1:B:49:ARG:HH11	1.82	0.43
1:C:181:PHE:O	1:C:184:ILE:N	2.50	0.43
1:A:430:ILE:HD13	1:A:430:ILE:HA	1.84	0.43
1:A:313:ASN:HB2	1:A:395:THR:OG1	2.17	0.43
1:D:54:VAL:HA	1:D:253:LEU:HD23	2.00	0.43
1:A:449:THR:HB	1:A:452:GLU:HG2	2.00	0.43
1:B:97:VAL:HG23	1:B:98:TYR:CD1	2.52	0.43
1:A:380:THR:O	1:A:383:CYS:HB2	2.19	0.43
1:A:421:HIS:H	1:A:421:HIS:CD2	2.36	0.43
1:A:246:SER:O	1:A:250:VAL:HG13	2.18	0.43
1:C:327:LYS:HD2	1:D:193:GLN:CB	2.48	0.43
1:A:179:VAL:O	1:A:182:GLN:HG2	2.19	0.43
1:B:306:ARG:O	1:B:306:ARG:HG3	2.18	0.43
1:A:321:SER:HB3	1:A:324:MET:HE3	2.00	0.43
1:D:49:ARG:HG3	1:D:90:MET:CE	2.47	0.43
1:B:57:ALA:HB2	1:B:253:LEU:HA	2.00	0.43
1:C:40:LYS:O	1:C:42:SER:N	2.51	0.43
1:C:86:ASN:OD1	1:C:88:LYS:HB2	2.18	0.43
1:D:332:VAL:HB	1:D:333:PRO:HD3	2.00	0.43
1:A:297:ASP:OD2	1:D:359:LEU:HD23	2.18	0.43
1:B:439:ARG:NH1	1:B:439:ARG:CG	2.81	0.43
1:A:259:PHE:HA	1:A:260:PRO:HD3	1.79	0.43
1:B:281:HIS:HB2	1:B:372:MET:CE	2.48	0.43
1:B:150:THR:CG2	1:B:253:LEU:HD21	2.48	0.43
1:C:84:LEU:O	1:C:86:ASN:N	2.51	0.43
1:A:185:LEU:HD23	1:A:405:VAL:HG21	1.99	0.43
1:B:92:GLN:O	1:B:94:PRO:HD3	2.19	0.43
1:C:6:ARG:HE	1:C:6:ARG:HB3	1.63	0.43
1:D:130:GLN:N	1:D:130:GLN:NE2	2.60	0.43
1:D:429:LYS:O	1:D:432:ALA:HB3	2.18	0.43
1:B:424:GLY:O	1:B:427:VAL:HB	2.19	0.43
1:A:271:THR:HG23	1:A:272:SER:H	1.82	0.43
1:A:62:ASN:OD1	1:A:245:TYR:HE1	2.02	0.43
1:A:17:VAL:HG23	1:A:18:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:PRO:HB2	1:A:373:PHE:HD2	1.83	0.43
1:C:302:SER:CB	1:C:314:LEU:HD13	2.48	0.43
1:D:152:PHE:CZ	1:D:369:GLY:HA2	2.53	0.43
1:A:163:LEU:HG	1:A:167:ILE:HD11	1.99	0.43
1:B:40:LYS:HD3	1:B:94:PRO:O	2.18	0.43
1:B:115:ALA:HB2	1:B:134:PRO:HB3	2.01	0.43
1:D:304:GLY:O	1:D:308:GLY:N	2.52	0.43
1:D:456:ILE:HG23	1:D:456:ILE:O	2.19	0.43
1:D:436:LYS:NZ	1:D:440:GLU:HB2	2.33	0.43
1:B:285:LYS:HG3	1:B:344:ILE:HA	2.01	0.43
1:C:63:LYS:O	1:C:65:LEU:N	2.42	0.43
1:A:322:SER:CA	1:B:429:LYS:NZ	2.81	0.43
1:A:196:VAL:CB	1:A:197:PRO:HD2	2.49	0.43
1:B:323:ILE:O	1:B:323:ILE:HG22	2.19	0.43
1:D:210:LEU:HD13	1:D:294:ILE:CD1	2.48	0.43
1:C:327:LYS:HD2	1:D:193:GLN:HB2	2.01	0.43
1:C:193:GLN:HG3	1:D:329:ASN:OD1	2.18	0.43
1:C:279:MET:CE	1:C:279:MET:HA	2.49	0.43
1:A:248:LEU:O	1:A:251:LYS:HB3	2.19	0.43
1:C:45:PRO:HG2	1:C:373:PHE:HD1	1.83	0.43
1:B:282:GLY:O	1:C:279:MET:HE3	2.18	0.43
1:B:169:GLN:HG2	1:B:384:TYR:HE1	1.84	0.43
1:C:204:PHE:O	1:C:207:PHE:HB2	2.18	0.43
1:A:243:LYS:O	1:A:244:GLU:C	2.56	0.42
1:D:110:THR:HG22	1:D:114:LEU:HD13	2.01	0.42
1:A:161:ILE:O	1:A:164:VAL:HG22	2.19	0.42
1:A:40:LYS:O	1:A:42:SER:N	2.45	0.42
1:C:145:ASN:O	1:C:271:THR:HB	2.18	0.42
1:A:65:LEU:HD21	1:A:245:TYR:HB2	2.01	0.42
1:A:65:LEU:HB3	1:A:67:THR:HG23	2.01	0.42
1:B:419:ILE:HG21	1:B:448:LEU:CD2	2.49	0.42
1:C:169:GLN:O	1:C:172:GLU:HB3	2.19	0.42
1:D:119:LEU:HD13	1:D:129:TYR:O	2.20	0.42
1:B:354:ALA:HB1	1:C:289:VAL:HG11	2.00	0.42
1:C:65:LEU:HD13	1:C:244:GLU:HB2	2.01	0.42
1:D:388:GLU:O	1:D:389:LYS:HD2	2.20	0.42
1:C:130:GLN:HE21	1:C:133:ASN:HA	1.84	0.42
1:A:56:LYS:HA	1:A:80:CYS:SG	2.59	0.42
1:C:44:ILE:N	1:C:45:PRO:HD2	2.31	0.42
1:C:272:SER:HB3	1:C:361:LEU:HA	2.01	0.42
1:A:70:LYS:NZ	1:A:74:ASN:HD21	2.17	0.42
1:B:336:VAL:O	1:B:339:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:139:ASN:HD22	1:C:142:GLN:HB2	1.84	0.42
1:C:265:GLU:HG3	1:C:265:GLU:H	1.49	0.42
1:A:144:THR:O	1:A:149:PRO:HD2	2.19	0.42
1:A:359:LEU:HD12	1:A:359:LEU:H	1.83	0.42
1:C:280:VAL:O	1:C:284:LEU:HD22	2.20	0.42
1:A:318:GLN:CG	1:A:319:ALA:N	2.75	0.42
1:D:103:GLY:HA3	1:D:148:TYR:CD2	2.55	0.42
1:B:370:GLN:OE1	1:D:342:LYS:HE2	2.19	0.42
1:C:62:ASN:HB3	1:C:67:THR:OG1	2.18	0.42
1:A:284:LEU:HD21	1:A:376:VAL:CG2	2.30	0.42
1:C:45:PRO:O	1:C:159:SER:OG	2.36	0.42
1:B:140:LYS:O	1:B:141:CYS:HB2	2.19	0.42
1:A:334:GLU:OE1	1:C:363:VAL:HB	2.19	0.42
1:C:332:VAL:O	1:C:336:VAL:HG23	2.19	0.42
1:B:103:GLY:HA3	1:B:148:TYR:CD2	2.54	0.42
1:D:272:SER:O	1:D:273:ASP:CB	2.68	0.42
1:C:304:GLY:HA2	1:C:305:PRO:HD3	1.84	0.42
1:D:170:LEU:HD11	1:D:386:LEU:HD23	2.01	0.42
1:D:439:ARG:CZ	1:D:453:LEU:HB3	2.48	0.42
1:D:264:ALA:C	1:D:266:ASP:N	2.72	0.42
1:B:124:HIS:CD2	1:B:131:TYR:CD1	3.07	0.42
1:D:18:PRO:HB2	1:D:21:ALA:HB2	2.00	0.42
1:B:415:LEU:HB3	1:B:419:ILE:HD13	2.01	0.42
1:A:304:GLY:HA2	1:A:305:PRO:HD2	1.94	0.42
1:C:378:ILE:HD13	1:C:379:LEU:N	2.34	0.42
1:D:453:LEU:HA	1:D:453:LEU:HD12	1.81	0.42
1:C:9:GLU:HA	1:C:14:THR:HG22	2.00	0.42
1:B:10:ASP:OD2	1:D:319:ALA:HB2	2.20	0.42
1:B:281:HIS:O	1:B:283:ALA:N	2.53	0.42
1:A:300:LEU:O	1:A:303:SER:HB3	2.20	0.42
1:A:56:LYS:CB	1:A:80:CYS:SG	3.06	0.42
1:C:241:THR:N	1:C:242:PRO:CD	2.83	0.42
1:C:313:ASN:OD1	1:C:397:ASN:ND2	2.53	0.42
1:A:5:ILE:HB	1:A:17:VAL:O	2.19	0.42
1:D:76:ILE:O	1:D:79:ALA:HB3	2.19	0.42
1:A:99:GLN:HG3	1:A:99:GLN:O	2.20	0.42
1:A:303:SER:HB2	1:B:192:LEU:HB3	2.02	0.42
1:B:150:THR:CG2	1:B:228:VAL:HB	2.50	0.42
1:B:365:GLU:O	1:B:368:ILE:HB	2.20	0.42
1:D:157:TYR:CD2	1:D:226:LEU:HD13	2.55	0.42
1:A:312:ILE:HA	1:A:396:ALA:HA	2.02	0.42
1:B:231:GLY:O	1:B:241:THR:HB	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:PHE:CA	1:A:109:ASN:HD21	2.29	0.42
1:A:44:ILE:N	1:A:45:PRO:CD	2.83	0.42
1:B:5:ILE:N	1:B:5:ILE:CD1	2.82	0.42
1:B:391:ILE:HG13	1:B:392:ASN:N	2.34	0.42
1:B:273:ASP:OD1	1:C:290:LYS:NZ	2.46	0.42
1:B:226:LEU:HA	1:B:226:LEU:HD12	1.87	0.42
1:A:400:VAL:HG12	1:A:401:CYS:N	2.34	0.42
1:B:198:MET:HG2	1:B:199:THR:N	2.35	0.41
1:C:175:GLU:HG2	1:C:208:SER:CB	2.49	0.41
1:C:101:GLY:O	1:C:103:GLY:N	2.53	0.41
1:A:374:GLU:O	1:A:378:ILE:HG12	2.20	0.41
1:B:100:GLY:HA3	1:D:331:VAL:O	2.20	0.41
1:A:194:ASP:H	1:B:305:PRO:HD2	1.85	0.41
1:D:277:TYR:HA	1:D:280:VAL:HG22	2.02	0.41
1:D:280:VAL:HG23	1:D:281:HIS:H	1.84	0.41
1:B:363:VAL:HG11	1:C:191:GLN:HG2	2.01	0.41
1:A:310:ASN:O	1:A:400:VAL:HG11	2.20	0.41
1:D:395:THR:HG22	1:D:396:ALA:H	1.85	0.41
1:C:96:ASP:HB3	1:C:98:TYR:O	2.19	0.41
1:D:213:GLU:HA	1:D:216:LYS:HD3	2.02	0.41
1:B:286:ARG:O	1:B:289:VAL:HG22	2.20	0.41
1:A:74:ASN:O	1:A:78:ALA:CB	2.68	0.41
1:A:36:ILE:HG21	1:A:98:TYR:CG	2.55	0.41
1:D:126:LYS:CB	1:D:126:LYS:NZ	2.83	0.41
1:B:445:ARG:CB	1:B:447:LEU:HD13	2.50	0.41
1:D:267:LEU:HG	1:D:268:ILE:HG23	2.02	0.41
1:A:153:ARG:NH2	1:A:274:CYS:SG	2.94	0.41
1:B:44:ILE:N	1:B:45:PRO:CD	2.79	0.41
1:B:46:GLU:CG	1:B:47:PHE:H	2.33	0.41
1:C:324:MET:HB2	1:D:409:ILE:HB	2.02	0.41
1:B:281:HIS:HA	1:B:284:LEU:HD22	2.02	0.41
1:C:235:ILE:CD1	1:C:236:GLY:N	2.81	0.41
1:A:27:THR:O	1:A:31:ILE:HG13	2.20	0.41
1:C:88:LYS:HG3	1:C:89:CYS:N	2.35	0.41
1:B:387:LEU:HA	1:B:391:ILE:HG12	2.02	0.41
1:D:226:LEU:CD2	1:D:260:PRO:HG2	2.49	0.41
1:D:403:GLY:O	1:D:407:ASN:HB2	2.19	0.41
1:D:203:GLU:O	1:D:206:ALA:HB3	2.20	0.41
1:C:190:THR:HG23	1:C:195:ALA:HB2	2.02	0.41
1:A:239:LEU:O	1:A:242:PRO:HD2	2.20	0.41
1:D:242:PRO:O	1:D:243:LYS:HB2	2.20	0.41
1:B:200:LEU:O	1:B:203:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:130:GLN:CA	1:D:130:GLN:NE2	2.78	0.41
1:D:172:GLU:O	1:D:176:ARG:HB2	2.19	0.41
1:D:295:CYS:SG	1:D:336:VAL:CB	3.09	0.41
1:A:315:PRO:HG3	1:A:390:CYS:O	2.21	0.41
1:B:97:VAL:HG23	1:B:98:TYR:N	2.35	0.41
1:A:415:LEU:O	1:A:419:ILE:N	2.47	0.41
1:C:63:LYS:NZ	1:C:63:LYS:HB3	2.35	0.41
1:C:146:ASP:C	1:C:149:PRO:HD2	2.41	0.41
1:B:331:VAL:CG1	1:B:332:VAL:N	2.84	0.41
1:C:6:ARG:NH1	1:C:127:GLY:HA3	2.34	0.41
1:D:127:GLY:C	1:D:129:TYR:N	2.74	0.41
1:D:414:TYR:O	1:D:418:PHE:CE2	2.74	0.41
1:B:340:CYS:O	1:B:343:VAL:HB	2.20	0.41
1:C:75:ALA:HB1	1:C:132:LEU:HD22	2.03	0.41
1:C:158:SER:HB3	1:C:259:PHE:CZ	2.56	0.41
1:C:390:CYS:O	1:C:394:ILE:HG13	2.21	0.41
1:A:1:MET:SD	1:A:2:SER:N	2.93	0.41
1:A:241:THR:O	1:A:245:TYR:HB3	2.20	0.41
1:A:23:TYR:O	1:A:23:TYR:CD2	2.74	0.41
1:A:405:VAL:CG2	1:A:406:TYR:H	2.34	0.41
1:C:312:ILE:HD12	1:C:394:ILE:HG21	2.02	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.79	0.41
1:A:322:SER:CA	1:B:429:LYS:HZ3	2.34	0.41
1:C:323:ILE:HB	1:C:324:MET:SD	2.61	0.41
1:B:87:GLY:O	1:B:89:CYS:N	2.54	0.41
1:A:199:THR:C	1:A:201:GLY:N	2.73	0.41
1:B:17:VAL:HG23	1:B:18:PRO:HD2	2.03	0.41
1:B:17:VAL:HA	1:B:18:PRO:HD3	1.90	0.41
1:D:186:LYS:O	1:D:197:PRO:HA	2.20	0.41
1:D:62:ASN:HB3	1:D:68:ILE:HG12	2.02	0.41
1:B:398:LYS:HG2	1:B:402:GLU:HG3	2.02	0.41
1:D:62:ASN:HB3	1:D:67:THR:HG1	1.86	0.41
1:C:320:GLY:O	1:C:322:SER:N	2.54	0.41
1:A:48:VAL:C	1:A:50:GLY:N	2.72	0.41
1:B:357:GLY:O	1:C:293:LYS:HG2	2.20	0.41
1:A:196:VAL:HB	1:A:197:PRO:HD2	2.02	0.41
1:A:303:SER:O	1:A:308:GLY:HA3	2.20	0.41
1:A:312:ILE:HB	1:A:394:ILE:HG21	2.03	0.41
1:A:312:ILE:HD12	1:A:394:ILE:HD13	2.03	0.41
1:A:35:TYR:O	1:C:381:ASN:HB3	2.20	0.41
1:D:100:GLY:C	1:D:102:ALA:H	2.24	0.41
1:A:323:ILE:HG12	1:B:425:ASP:CG	2.42	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:LYS:CG	1:A:244:GLU:N	2.84	0.40
1:D:54:VAL:CG1	1:D:55:LYS:N	2.84	0.40
1:C:272:SER:HA	1:C:362:ASN:H	1.85	0.40
1:C:163:LEU:O	1:C:167:ILE:HG13	2.21	0.40
1:C:130:GLN:NE2	1:C:132:LEU:O	2.54	0.40
1:D:243:LYS:HD3	1:D:244:GLU:H	1.86	0.40
1:A:89:CYS:HB3	1:A:117:ILE:HD13	2.03	0.40
1:C:414:TYR:O	1:C:417:PRO:HD2	2.21	0.40
1:C:93:PHE:HA	1:C:109:ASN:ND2	2.36	0.40
1:C:343:VAL:HG22	1:C:378:ILE:HD11	2.03	0.40
1:C:181:PHE:HZ	1:C:394:ILE:O	2.05	0.40
1:B:264:ALA:O	1:B:266:ASP:N	2.54	0.40
1:A:317:LEU:N	1:A:317:LEU:CD2	2.84	0.40
1:B:199:THR:HG22	1:B:202:GLN:CG	2.51	0.40
1:B:276:ALA:O	1:B:280:VAL:HG13	2.22	0.40
1:D:242:PRO:HA	1:D:246:SER:HG	1.85	0.40
1:D:414:TYR:O	1:D:414:TYR:CD1	2.75	0.40
1:A:303:SER:O	1:A:304:GLY:O	2.39	0.40
1:B:74:ASN:HA	1:B:77:ILE:HG12	2.03	0.40
1:B:6:ARG:HH21	1:B:126:LYS:HZ2	1.68	0.40
1:A:314:LEU:HG	1:A:390:CYS:SG	2.61	0.40
1:A:317:LEU:N	1:A:317:LEU:HD23	2.37	0.40
1:A:325:PRO:HG2	1:B:409:ILE:CD1	2.52	0.40
1:C:172:GLU:CB	1:C:176:ARG:HH21	2.22	0.40
1:A:164:VAL:HG23	1:A:165:ASP:N	2.37	0.40
1:D:168:ASN:HD22	1:D:168:ASN:HA	1.70	0.40
1:B:343:VAL:HG21	1:B:379:LEU:CD2	2.49	0.40
1:B:108:MET:HE2	1:B:111:ASN:ND2	2.37	0.40
1:C:124:HIS:CD2	1:C:131:TYR:CE1	3.10	0.40
1:B:287:LEU:CD1	1:B:291:MET:HG3	2.52	0.40
1:A:290:LYS:NZ	1:D:273:ASP:OD2	2.55	0.40
1:D:114:LEU:HD12	1:D:114:LEU:N	2.37	0.40
1:A:125:GLN:H	1:A:125:GLN:CD	2.25	0.40
1:C:177:LYS:O	1:C:180:GLU:HB3	2.22	0.40
1:A:387:LEU:O	1:A:392:ASN:HB2	2.22	0.40
1:D:25:VAL:HB	1:D:29:ARG:HH11	1.87	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	457/478 (96%)	341 (75%)	82 (18%)	34 (7%)	2	1
1	B	458/478 (96%)	352 (77%)	70 (15%)	36 (8%)	1	1
1	C	411/478 (86%)	295 (72%)	77 (19%)	39 (10%)	1	1
1	D	457/478 (96%)	356 (78%)	63 (14%)	38 (8%)	1	1
All	All	1783/1912 (93%)	1344 (75%)	292 (16%)	147 (8%)	1	1

All (147) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	25	VAL
1	A	84	LEU
1	A	88	LYS
1	A	232	ALA
1	A	235	ILE
1	A	242	PRO
1	A	244	GLU
1	A	245	TYR
1	A	267	LEU
1	A	304	GLY
1	A	319	ALA
1	A	328	VAL
1	A	456	ILE
1	A	457	PHE
1	B	41	ILE
1	B	46	GLU
1	B	85	ASN
1	B	237	THR
1	B	264	ALA
1	B	266	ASP
1	B	322	SER
1	B	328	VAL
1	B	459	VAL

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Mol	Chain	Res	Type
1	C	47	PHE
1	C	85	ASN
1	C	90	MET
1	C	91	ASP
1	C	182	GLN
1	C	237	THR
1	C	239	LEU
1	C	242	PRO
1	C	245	TYR
1	C	268	ILE
1	C	328	VAL
1	C	398	LYS
1	D	47	PHE
1	D	86	ASN
1	D	128	GLU
1	D	133	ASN
1	D	233	THR
1	D	239	LEU
1	D	243	LYS
1	D	273	ASP
1	D	303	SER
1	D	326	ALA
1	D	457	PHE
1	A	46	GLU
1	A	223	GLU
1	A	234	ALA
1	A	356	ALA
1	B	4	ASN
1	B	19	ALA
1	B	88	LYS
1	B	135	ASN
1	B	182	GLN
1	B	197	PRO
1	B	235	ILE
1	B	303	SER
1	B	307	ALA
1	B	309	LEU
1	B	325	PRO
1	B	364	MET
1	C	64	GLU
1	C	89	CYS
1	C	240	ASN

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Mol	Chain	Res	Type
1	C	304	GLY
1	C	309	LEU
1	C	321	SER
1	C	396	ALA
1	D	46	GLU
1	D	64	GLU
1	D	234	ALA
1	D	267	LEU
1	D	304	GLY
1	D	320	GLY
1	D	391	ILE
1	D	446	GLY
1	A	145	ASN
1	A	237	THR
1	A	398	LYS
1	B	102	ALA
1	B	234	ALA
1	B	243	LYS
1	B	270	ALA
1	C	102	ALA
1	C	236	GLY
1	C	270	ALA
1	C	359	LEU
1	C	397	ASN
1	D	85	ASN
1	D	186	LYS
1	D	390	CYS
1	D	398	LYS
1	A	4	ASN
1	A	33	ASN
1	A	89	CYS
1	A	128	GLU
1	A	143	SER
1	A	222	ALA
1	A	387	LEU
1	B	18	PRO
1	B	155	ALA
1	B	232	ALA
1	B	265	GLU
1	B	387	LEU
1	C	25	VAL
1	C	65	LEU

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Mol	Chain	Res	Type
1	C	318	GLN
1	C	387	LEU
1	D	237	THR
1	D	411	ILE
1	D	443	LEU
1	A	94	PRO
1	B	44	ILE
1	B	45	PRO
1	B	304	GLY
1	B	456	ILE
1	C	128	GLU
1	C	269	GLU
1	C	273	ASP
1	C	330	PRO
1	D	70	LYS
1	D	181	PHE
1	D	266	ASP
1	D	289	VAL
1	D	328	VAL
1	D	439	ARG
1	A	127	GLY
1	A	372	MET
1	B	90	MET
1	C	235	ILE
1	C	354	ALA
1	D	43	ASP
1	D	149	PRO
1	D	182	GLN
1	A	231	GLY
1	C	41	ILE
1	A	41	ILE
1	C	76	ILE
1	C	101	GLY
1	D	118	GLY
1	B	31	ILE
1	C	308	GLY
1	D	5	ILE
1	C	36	ILE
1	D	456	ILE



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	385/402 (96%)	345 (90%)	40 (10%)	10	23
1	B	386/402 (96%)	347 (90%)	39 (10%)	11	24
1	C	346/402 (86%)	306 (88%)	40 (12%)	8	18
1	D	385/402 (96%)	343 (89%)	42 (11%)	9	21
All	All	1502/1608 (93%)	1341 (89%)	161 (11%)	10	22

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	5	ILE
1	A	11	LEU
1	A	14	THR
1	A	15	ARG
1	A	20	ASP
1	A	32	GLU
1	A	35	TYR
1	A	65	LEU
1	A	77	ILE
1	A	86	ASN
1	A	94	PRO
1	A	107	ASN
1	A	125	GLN
1	A	145	ASN
1	A	186	LYS
1	A	189	ARG
1	A	212	LYS
1	A	221	THR
1	A	240	ASN
1	A	265	GLU
1	A	267	LEU
1	A	273	ASP
1	A	293	LYS
1	A	306	ARG

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Mol	Chain	Res	Type
1	A	309	LEU
1	A	314	LEU
1	A	317	LEU
1	A	318	GLN
1	A	324	MET
1	A	331	VAL
1	A	337	ASN
1	A	339	VAL
1	A	352	MET
1	A	360	GLN
1	A	385	ASN
1	A	392	ASN
1	A	422	HIS
1	A	448	LEU
1	B	5	ILE
1	B	43	ASP
1	B	46	GLU
1	B	47	PHE
1	B	49	ARG
1	B	125	GLN
1	B	136	ASP
1	B	145	ASN
1	B	162	LYS
1	B	165	ASP
1	B	168	ASN
1	B	169	GLN
1	B	172	GLU
1	B	194	ASP
1	B	197	PRO
1	B	212	LYS
1	B	219	GLN
1	B	226	LEU
1	B	237	THR
1	B	240	ASN
1	B	241	THR
1	B	243	LYS
1	B	246	SER
1	B	265	GLU
1	B	274	CYS
1	B	284	LEU
1	B	306	ARG
1	B	324	MET

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Mol	Chain	Res	Type
1	B	331	VAL
1	B	339	VAL
1	B	352	MET
1	B	355	GLU
1	B	361	LEU
1	B	370	GLN
1	B	385	ASN
1	B	404	TYR
1	B	425	ASP
1	B	439	ARG
1	B	459	VAL
1	C	5	ILE
1	C	6	ARG
1	C	15	ARG
1	C	16	GLU
1	C	17	VAL
1	C	20	ASP
1	C	39	ASN
1	C	52	VAL
1	C	55	LYS
1	C	64	GLU
1	C	88	LYS
1	C	95	VAL
1	C	107	ASN
1	C	128	GLU
1	C	139	ASN
1	C	146	ASP
1	C	154	ILE
1	C	172	GLU
1	C	185	LEU
1	C	189	ARG
1	C	196	VAL
1	C	210	LEU
1	C	219	GLN
1	C	237	THR
1	C	241	THR
1	C	242	PRO
1	C	265	GLU
1	C	266	ASP
1	C	267	LEU
1	C	268	ILE
1	C	269	GLU

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Mol	Chain	Res	Type
1	C	272	SER
1	C	284	LEU
1	C	321	SER
1	C	324	MET
1	C	370	GLN
1	C	378	ILE
1	C	385	ASN
1	C	397	ASN
1	C	411	ILE
1	D	4	ASN
1	D	5	ILE
1	D	25	VAL
1	D	34	PHE
1	D	52	VAL
1	D	77	ILE
1	D	89	CYS
1	D	91	ASP
1	D	96	ASP
1	D	119	LEU
1	D	125	GLN
1	D	129	TYR
1	D	130	GLN
1	D	158	SER
1	D	183	ASP
1	D	203	GLU
1	D	211	LEU
1	D	223	GLU
1	D	226	LEU
1	D	227	GLU
1	D	239	LEU
1	D	240	ASN
1	D	265	GLU
1	D	267	LEU
1	D	272	SER
1	D	316	GLU
1	D	323	ILE
1	D	324	MET
1	D	331	VAL
1	D	334	GLU
1	D	360	GLN
1	D	370	GLN
1	D	385	ASN

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Mol	Chain	Res	Type
1	D	395	THR
1	D	400	VAL
1	D	408	SER
1	D	413	THR
1	D	422	HIS
1	D	433	GLU
1	D	445	ARG
1	D	447	LEU
1	D	448	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	62	ASN
1	A	74	ASN
1	A	85	ASN
1	A	109	ASN
1	A	124	HIS
1	A	137	HIS
1	A	191	GLN
1	A	202	GLN
1	A	217	ASN
1	A	219	GLN
1	A	229	ASN
1	A	310	ASN
1	A	313	ASN
1	A	329	ASN
1	A	358	GLN
1	A	360	GLN
1	A	416	ASN
1	A	421	HIS
1	A	422	HIS
1	B	38	ASN
1	B	62	ASN
1	B	66	GLN
1	B	74	ASN
1	B	85	ASN
1	B	99	GLN
1	B	111	ASN
1	B	124	HIS
1	B	135	ASN

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Mol	Chain	Res	Type
1	B	142	GLN
1	B	145	ASN
1	B	168	ASN
1	B	191	GLN
1	B	193	GLN
1	B	281	HIS
1	B	346	ASN
1	B	360	GLN
1	B	377	HIS
1	B	421	HIS
1	C	62	ASN
1	C	107	ASN
1	C	109	ASN
1	C	111	ASN
1	C	124	HIS
1	C	125	GLN
1	C	130	GLN
1	C	137	HIS
1	C	139	ASN
1	C	168	ASN
1	C	219	GLN
1	C	313	ASN
1	C	329	ASN
1	C	338	GLN
1	C	346	ASN
1	C	397	ASN
1	C	407	ASN
1	C	416	ASN
1	D	4	ASN
1	D	26	HIS
1	D	62	ASN
1	D	130	GLN
1	D	168	ASN
1	D	310	ASN
1	D	313	ASN
1	D	338	GLN
1	D	362	ASN
1	D	370	GLN
1	D	377	HIS
1	D	397	ASN
1	D	423	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	A	601	-	12,12,12	0.51	0	17,17,17	0.80	1 (5%)
3	ACT	A	701	-	1,3,3	2.93	1 (100%)	0,3,3	0.00	-
2	BGC	B	701	-	12,12,12	0.21	0	17,17,17	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	601	-	-	0/2/22/22	0/1/1/1
3	ACT	A	701	-	-	0/0/0/0	0/0/0/0
2	BGC	B	701	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ACT	CH3-C	2.93	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	601	BGC	C1-C2-C3	-2.52	106.54	110.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	459/478 (96%)	0.34	30 (6%)	18 21	2, 23, 50, 79	0
1	B	460/478 (96%)	0.33	34 (7%)	14 15	4, 22, 50, 69	0
1	C	413/478 (86%)	0.41	32 (7%)	13 14	3, 23, 46, 81	0
1	D	459/478 (96%)	0.25	21 (4%)	31 35	4, 21, 49, 100	0
All	All	1791/1912 (93%)	0.33	117 (6%)	18 21	2, 22, 49, 100	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	87	GLY	11.7
1	A	87	GLY	7.6
1	C	413	THR	7.4
1	C	412	VAL	6.7
1	B	323	ILE	5.9
1	B	237	THR	5.5
1	C	324	MET	5.4
1	C	45	PRO	5.3
1	C	323	ILE	5.2
1	B	272	SER	5.2
1	C	326	ALA	5.0
1	D	326	ALA	5.0
1	B	44	ILE	4.9
1	C	44	ILE	4.8
1	A	272	SER	4.8
1	B	45	PRO	4.6
1	A	44	ILE	4.5
1	C	410	GLY	4.5
1	A	323	ILE	4.4
1	B	3	ASN	4.4
1	A	45	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	453	LEU	4.3
1	D	237	THR	4.2
1	D	2	SER	4.2
1	B	86	ASN	4.2
1	A	86	ASN	4.1
1	A	414	TYR	4.1
1	A	2	SER	4.0
1	D	1	MET	4.0
1	C	414	TYR	3.9
1	D	86	ASN	3.9
1	A	129	TYR	3.8
1	C	238	GLY	3.8
1	C	409	ILE	3.7
1	B	324	MET	3.6
1	C	417	PRO	3.6
1	C	416	ASN	3.5
1	A	273	ASP	3.4
1	C	237	THR	3.4
1	B	273	ASP	3.4
1	A	1	MET	3.3
1	C	76	ILE	3.3
1	A	185	LEU	3.3
1	C	73	ALA	3.3
1	D	325	PRO	3.2
1	C	242	PRO	3.2
1	C	241	THR	3.2
1	B	129	TYR	3.2
1	A	7	ILE	3.2
1	C	265	GLU	3.1
1	D	45	PRO	3.1
1	D	3	ASN	3.1
1	A	3	ASN	3.1
1	D	242	PRO	3.0
1	C	127	GLY	3.0
1	A	348	THR	3.0
1	A	117	ILE	3.0
1	A	237	THR	3.0
1	C	5	ILE	3.0
1	B	427	VAL	3.0
1	A	427	VAL	2.9
1	B	264	ALA	2.9
1	B	270	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	199	THR	2.8
1	B	271	THR	2.8
1	C	271	THR	2.8
1	B	2	SER	2.7
1	B	274	CYS	2.7
1	D	44	ILE	2.7
1	B	238	GLY	2.6
1	B	320	GLY	2.6
1	A	21	ALA	2.6
1	A	125	GLN	2.6
1	B	457	PHE	2.6
1	B	1	MET	2.6
1	B	319	ALA	2.6
1	C	391	ILE	2.5
1	A	5	ILE	2.5
1	A	234	ALA	2.5
1	D	323	ILE	2.5
1	D	88	LYS	2.4
1	B	241	THR	2.4
1	A	90	MET	2.4
1	C	234	ALA	2.4
1	A	131	TYR	2.4
1	B	4	ASN	2.4
1	B	326	ALA	2.4
1	D	234	ALA	2.3
1	C	185	LEU	2.3
1	A	347	ASP	2.3
1	B	235	ILE	2.3
1	A	236	GLY	2.3
1	D	271	THR	2.2
1	B	17	VAL	2.2
1	B	128	GLU	2.2
1	D	414	TYR	2.2
1	C	87	GLY	2.2
1	D	241	THR	2.2
1	D	58	ALA	2.2
1	A	248	LEU	2.2
1	A	438	VAL	2.2
1	C	273	ASP	2.2
1	C	348	THR	2.1
1	B	345	GLY	2.1
1	B	428	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	272	SER	2.1
1	D	418	PHE	2.1
1	B	85	ASN	2.1
1	D	345	GLY	2.1
1	C	179	VAL	2.1
1	A	23	TYR	2.1
1	B	87	GLY	2.1
1	C	356	ALA	2.1
1	A	83	VAL	2.1
1	B	304	GLY	2.0
1	B	245	TYR	2.0
1	B	228	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	B	701	12/12	0.24	1.46	43,43,43,43	0
2	BGC	A	601	12/12	0.19	0.51	43,43,43,43	0
3	ACT	A	701	4/4	0.15	-0.48	31,31,31,31	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.