



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 1, 2017 – 11:35 PM EDT

PDB ID : 5VHX  
EMDB ID: : EMD-8686  
Title : GluA2-1xGSG1L bound to ZK  
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.  
Deposited on : unknown  
Resolution : 8.30 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

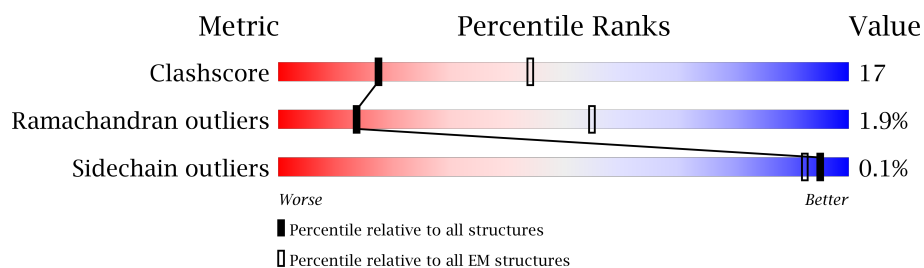
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


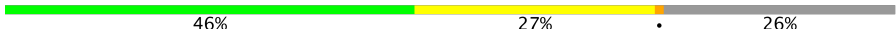



The reported resolution of this entry is 8.30 Å.

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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1057	 46% 27% • 26%
1	B	1057	 46% 27% • 26%
1	C	1057	 47% 26% • 26%
1	D	1057	 46% 28% • 26%
1	E	1057	 8% 9% 83%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26164 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamate receptor 2,Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	B	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	C	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	D	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	E	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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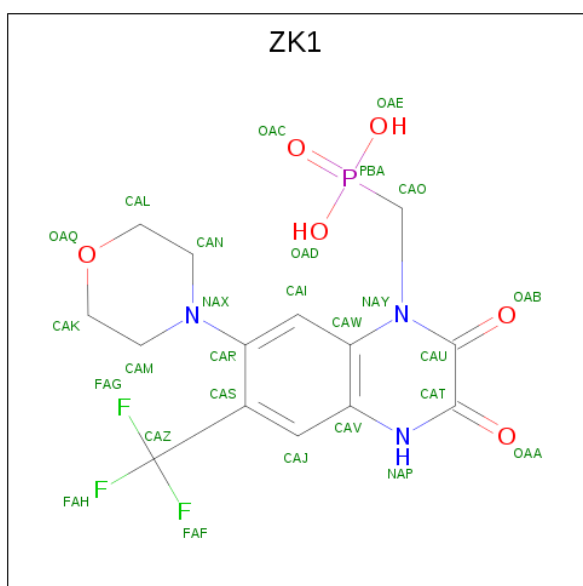
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
E	-588	GLU	ASN	conflict	UNP P19491
E	-447	LEU	VAL	conflict	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	THR	deletion	UNP P19491
E	?	-	GLU	deletion	UNP P19491
E	?	-	LEU	deletion	UNP P19491

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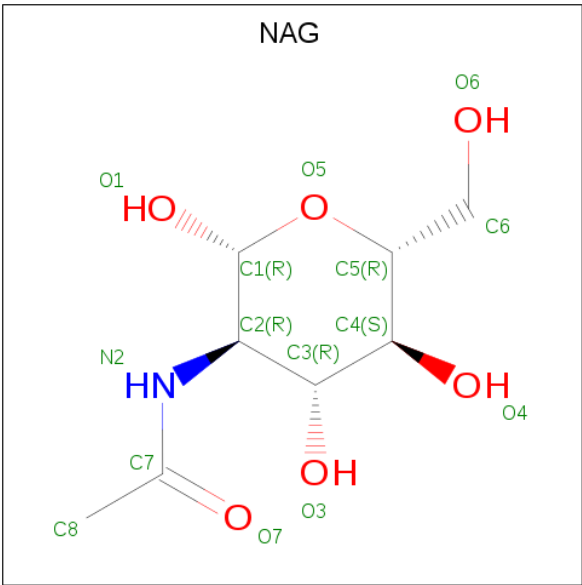
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	PRO	deletion	UNP P19491
E	?	-	SER	deletion	UNP P19491
E	-445	GLU	GLY	conflict	UNP P19491
E	-444	ASP	ASN	conflict	UNP P19491
E	-437	GLN	ASN	conflict	UNP P19491
E	-2	GLY	-	linker	UNP P19491
E	-1	THR	-	linker	UNP P19491
E	0	GLY	-	linker	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

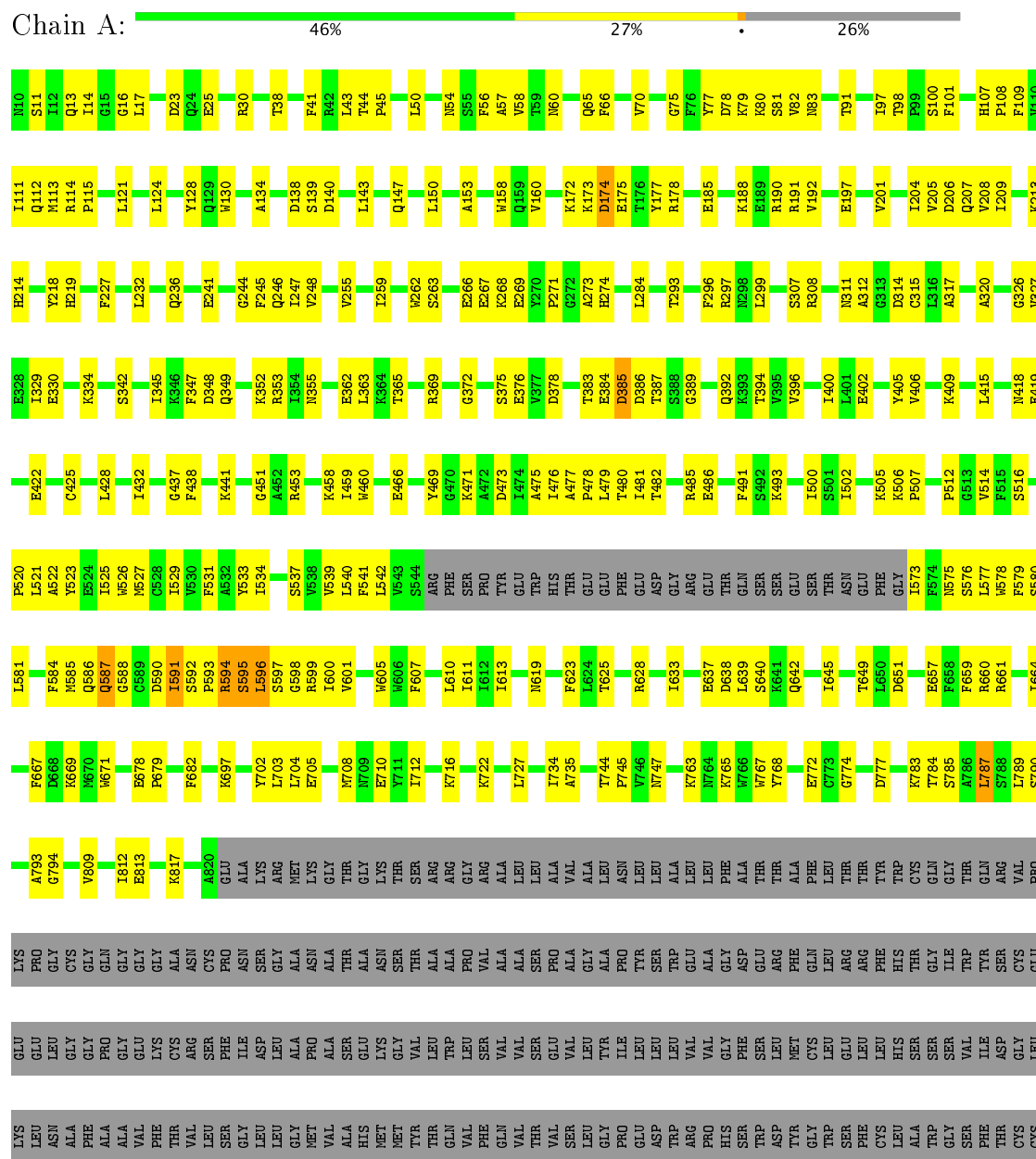


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein











K232	D157	F90	T29	SER	LYS	MET	LEU	GLU	ASP
THR	G188	H91	T30	ASN	GLY	TRP	ILE	TRP	PHE
VAL	L159	T92	K31	VAL	TYR	THR	ILE	HIS	SER
ILE	K160	G93	C32	ALA	ILE	THR	ILE	THR	LYS
GLU	L161	I94	Q33	GLY	ILE	MET	SER	GLU	PRO
PHE	N162	W95	G34	VAL	ALA	ARG	TYR	PHE	PHE
	A163	Y96	T35	PHE	THR	SER	THR	THR	MET
	F164	S97	Q36	TYR	PRO	ALA	ALA	GLU	SER
	A165	C98	K37	ILE	LYS	GLU	ALA	ASP	LEU
	A166	E99	V38	LEU	GLY	PRO	ASN	GLY	LEU
	V167	E100	P39	VAL	SER	SER	LEU	ARG	ILE
	F168	GLU	LYS	GLY	SER	VAL	ALA	GLU	SER
	T169	LEU	PRO	GLY	LEU	PHE	ALA	THR	ILE
	V170	GLY	GLY	LEU	GLY	VAL	PHE	GLN	MET
	L174	PRO	CYS	GLY	THR	ARG	THR	SER	ILE
		GLY	GLN	ALA	THR	THR	VAL	SER	LYS
		G106	GLY	MET	ALA	ALA	GLU	SER	PRO
		E107	GLY	LEU	ASN	GLY	ARG	THR	GLN
	K108	C109	GLY	VAL	LEU	GLY	MET	THR	LYS
	A179	R110	ALA	ALA	ALA	VAL	GLY	ASN	LYS
	H180	S111	ASN	LEU	LEU	VAL	VAL	GLU	SER
	M181	F112	CYS	ILE	LYS	ARG	ALA	PHE	LYS
	M182	I113	PRO	ILE	VAL	ARG	PRO	GLY	PRO
		D114	ASN	GLU	LEU	VAL	ILE	ILE	GLY
	Q185	L115	SER	PHE	SER	LYS	GLU	PHE	VAL
	V186	A116	GLY	CYS	GLU	ASN	SER	ASN	PHE
		P117	ALA	TYR	GLN	LYS	ALA	SER	SER
	V189	A118	ASN	SER	VAL	GLY	GLU	LEU	PHE
	T190	S119	ALA	ARG	LEU	LYS	ASP	TRP	LEU
		E120	ALA	ALA	LEU	TYR	SER	SER	PRO
	L193	K121	ALA	GLU	LYS	ALA	LYS	LEU	LEU
	G194	G122	ASN	ALA	LYS	TYR	GLN	GLY	ALA
	P195	V123	SER	LYS	LYS	ALA	THR	ALA	TYR
	E196	L124	THR	ARG	ASN	LEU	PHE	GLU	GLU
	D197	W125	ALA	MET	LYS	GLU	ILE	MET	ILE
	W198	L126	ALA	LYS	TRP	SER	ALA	GLN	TRP
	R199	S127	PRO	GLY	TRP	THR	TYR	GLN	MET
			VAL	THR	THR	GLY	TYR	GLY	CYS
	S202	S130	ALA	GLY	ASP	MET	GLY	CYS	ILE
	W203		ALA	ALA	LYS	ASN	THR	LEU	VAL
	D204	L133	SER	K1	GLY	TYR	ASP	ILE	PHE
	Y205	Y134	PRO	T2	GLY	ILE	SER	ASP	ALA
		I135	ALA	S3	CYS	GLU	GLY	PRO	ALA
	F209	L136	GLY	R4	GLY	GLN	SER	ARG	TYR
		L137	ALA	R5	ALA	THR	ARG	ILE	ILE
	W213	L138	PRO	G6	LYS	LYS	LEU	GLY	GLY
	G214		TYR	R7	ASP	PRO	SER	SER	VAL
	S215		SER	A8	CYS	GLY	PHE	GLY	SER
	F216	L144	TRP	L9	GLY	ASP	PHE	VAL	VAL
	T217	W145	TRP		GLY	THR	ARG	VAL	VAL
		C146	GLU	V12	SER	THR	ARG	ILE	LEU
	W220	E147	ALA		LYS	MET	ARG	VAL	PHE
		E148	GLY	A18	GLY	LYS	GLY	GLY	LEU
	S223	L149	ASP		LYS	VAL	LYS	VAL	VAL
	V224		GLU	F21	THR	GLY	ILE	VAL	SER
		S152	ARG	A22	SER	GLY	ALA	TRP	ARG
	L227	S153	F85	T23	ALA	ASN	VAL	TRP	PHE
		SER	Q86		LEU	LEU	PHE	TRP	SER
	Y230	VAL	L87	L27	SER	ASP	ASP	PHE	PRO
	T231	ILE		T28	LEU	SER	LYS	THR	TYR

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZK1

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.32	0/6287	0.46	0/8493
1	B	0.32	0/6265	0.45	0/8464
1	C	0.32	0/6287	0.45	0/8493
1	D	0.32	0/6265	0.45	0/8464
1	E	0.29	0/1443	0.46	0/1959
All	All	0.32	0/26547	0.45	0/35873

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6159	0	6155	221	0
1	B	6137	0	6132	224	0
1	C	6159	0	6155	215	0
1	D	6137	0	6132	231	0
1	E	1408	0	1406	78	0
2	A	27	0	13	3	0
2	B	27	0	13	2	0
2	C	27	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	13	1	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	2	0
3	D	14	0	13	3	0
All	All	26164	0	26084	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 17.

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:E:205:TYR:OH	1:E:209:PHE:CE2	2.14	1.00
1:A:531:PHE:HE2	1:E:213:TRP:CD2	1.84	0.94
1:E:205:TYR:HH	1:E:209:PHE:HE2	1.15	0.88
1:E:98:CYS:HA	1:E:109:CYS:HA	1.55	0.88
1:C:337:GLN:HG3	1:C:346:LYS:HG2	1.58	0.85
1:E:148:GLU:HG3	1:E:162:ASN:HD21	1.43	0.84
1:A:190:ARG:HE	1:A:469:TYR:HB3	1.46	0.81
1:A:188:LYS:HD2	1:A:190:ARG:HH22	1.46	0.80
1:B:790:SER:CB	1:E:185:GLN:HE22	1.95	0.80
1:D:247:ILE:HG23	1:D:248:VAL:HG23	1.64	0.80
1:D:595:SER:HA	1:D:599:ARG:HB3	1.64	0.79
1:B:595:SER:HA	1:B:599:ARG:HB2	1.63	0.78
1:B:790:SER:OG	1:E:185:GLN:NE2	2.16	0.78
1:B:209:ILE:HA	1:B:214:HIS:HD2	1.46	0.77
1:B:246:GLN:HE21	1:B:248:VAL:H	1.33	0.76
1:A:77:TYR:HE2	1:A:98:THR:HG21	1.49	0.76
1:D:308:ARG:NH2	1:D:325:GLN:OE1	2.19	0.76
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.52	0.75
1:A:451:GLY:O	1:A:485:ARG:NH2	2.20	0.75
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.69	0.74
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.69	0.74
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.69	0.73
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.70	0.73
1:C:344:ASN:HD21	1:C:346:LYS:HE3	1.51	0.73
1:D:355:ASN:N	1:D:376:GLU:OE2	2.19	0.73
1:B:247:ILE:HG23	1:B:248:VAL:HG23	1.69	0.73
1:A:600:ILE:HA	1:B:581:LEU:HD21	1.72	0.72
1:D:523:TYR:HA	1:D:526:TRP:HD1	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLY:H	1:B:65:GLN:HE22	1.38	0.71
1:A:661:ARG:NH1	1:D:755:GLU:O	2.24	0.71
1:D:77:TYR:OH	1:D:101:PHE:O	2.09	0.71
1:B:376:GLU:HG2	1:B:377:VAL:HG13	1.73	0.71
1:E:31:TRP:N	1:E:92:THR:O	2.24	0.71
1:E:93:GLY:H	1:E:97:SER:HA	1.56	0.70
1:A:512:PRO:HB2	1:A:516:SER:HB3	1.74	0.70
1:B:77:TYR:OH	1:B:101:PHE:O	2.06	0.70
1:B:375:SER:HB3	1:B:378:ASP:HB2	1.74	0.70
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.72	0.70
1:C:451:GLY:O	1:C:485:ARG:NH2	2.22	0.70
1:A:531:PHE:HE2	1:E:213:TRP:CE3	2.09	0.70
1:B:523:TYR:HA	1:B:526:TRP:HD1	1.57	0.70
1:E:21:PHE:HB2	1:E:215:SER:HB3	1.74	0.69
1:A:236:GLN:NE2	1:A:365:THR:O	2.26	0.69
1:D:16:GLY:H	1:D:65:GLN:HE22	1.40	0.69
1:E:205:TYR:OH	1:E:209:PHE:HE2	1.60	0.69
1:D:592:SER:HB3	1:D:599:ARG:HB2	1.73	0.69
1:B:209:ILE:HA	1:B:214:HIS:CD2	2.27	0.69
1:D:309:ARG:HG2	1:D:311:ASN:H	1.57	0.69
1:C:600:ILE:HA	1:D:581:LEU:HD21	1.73	0.69
1:A:586:GLN:HA	1:D:587:GLN:HE21	1.57	0.69
1:A:147:GLN:HE21	1:B:143:LEU:HD21	1.58	0.69
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.75	0.69
1:C:13:GLN:HB3	1:C:70:VAL:HG12	1.75	0.68
1:C:599:ARG:NH1	1:D:578:TRP:O	2.24	0.68
1:D:592:SER:O	1:D:599:ARG:NH2	2.26	0.68
1:D:716:LYS:HG3	1:D:772:GLU:HB3	1.76	0.68
1:A:531:PHE:CE2	1:E:213:TRP:CD2	2.75	0.68
1:D:246:GLN:HE21	1:D:248:VAL:H	1.38	0.68
1:A:246:GLN:HE21	1:A:248:VAL:H	1.41	0.68
1:A:263:SER:O	1:A:274:HIS:ND1	2.28	0.67
1:A:355:ASN:ND2	3:A:1102:NAG:O6	2.26	0.67
1:C:307:SER:O	1:C:308:ARG:NH1	2.25	0.67
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.76	0.67
1:B:537:SER:O	1:B:576:SER:OG	2.12	0.67
1:B:579:PHE:HZ	1:B:590:ASP:H	1.41	0.67
1:D:537:SER:O	1:D:576:SER:OG	2.12	0.67
1:A:11:SER:OG	1:A:44:THR:OG1	2.12	0.67
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.60	0.67
1:D:78:ASP:OD1	1:D:79:LYS:N	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLN:HE21	1:D:278:ILE:HG13	1.60	0.66
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.76	0.66
1:B:346:LYS:HD3	1:B:355:ASN:HD22	1.60	0.66
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.78	0.66
1:C:716:LYS:N	1:C:772:GLU:OE1	2.29	0.66
1:D:51:GLU:HG3	1:D:53:ALA:H	1.60	0.66
1:A:307:SER:O	1:A:308:ARG:NH1	2.29	0.66
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.78	0.66
1:C:143:LEU:HD21	1:D:147:GLN:HE21	1.61	0.66
1:B:309:ARG:HG2	1:B:311:ASN:H	1.60	0.65
1:D:583:ALA:HA	1:D:589:CYS:H	1.61	0.65
1:A:716:LYS:N	1:A:772:GLU:OE1	2.28	0.65
1:B:24:GLN:HE21	1:B:278:ILE:HG13	1.60	0.65
1:B:628:ARG:HG2	1:C:628:ARG:HH12	1.59	0.65
1:B:308:ARG:HH21	1:B:325:GLN:H	1.42	0.65
1:C:592:SER:HB3	1:C:599:ARG:HD3	1.79	0.65
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.60	0.65
1:A:143:LEU:HD21	1:B:147:GLN:HE21	1.62	0.65
1:C:355:ASN:N	1:C:376:GLU:OE2	2.24	0.65
1:C:476:ILE:HG12	1:C:734:ILE:HD12	1.78	0.65
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.78	0.65
1:C:633:ILE:HG23	1:C:638:ASP:HB2	1.79	0.65
1:B:263:SER:O	1:B:274:HIS:ND1	2.28	0.65
1:C:246:GLN:HE21	1:C:248:VAL:H	1.45	0.65
1:D:348:ASP:OD1	1:D:352:LYS:N	2.30	0.65
1:D:427:ASP:OD2	1:D:766:TRP:NE1	2.29	0.65
1:D:375:SER:HB3	1:D:378:ASP:HB2	1.78	0.65
1:E:2:THR:HG22	1:E:5:ARG:HH12	1.60	0.64
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.78	0.64
1:B:716:LYS:HG3	1:B:772:GLU:HB3	1.80	0.64
1:D:590:ASP:O	1:D:592:SER:N	2.23	0.64
1:B:305:GLU:O	1:B:325:GLN:NE2	2.30	0.64
1:B:334:LYS:NZ	1:B:349:GLN:O	2.21	0.64
1:B:78:ASP:OD1	1:B:79:LYS:N	2.30	0.64
1:C:263:SER:O	1:C:274:HIS:ND1	2.31	0.64
1:C:539:VAL:HA	1:C:542:LEU:HD12	1.80	0.64
1:C:590:ASP:O	1:C:592:SER:N	2.26	0.64
1:D:372:GLY:HA2	1:D:383:THR:HG23	1.78	0.64
1:C:337:GLN:HE21	1:C:346:LYS:HE2	1.63	0.64
1:C:520:PRO:O	1:C:619:ASN:ND2	2.31	0.64
1:C:78:ASP:OD1	1:C:79:LYS:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLN:HA	1:B:44:THR:HB	1.79	0.64
1:D:134:ALA:HB3	1:D:192:VAL:HG22	1.80	0.63
1:C:11:SER:OG	1:C:44:THR:OG1	2.17	0.63
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.80	0.63
1:C:259:ILE:HA	1:C:262:TRP:HB3	1.79	0.63
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.80	0.63
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.80	0.63
1:B:348:ASP:OD1	1:B:352:LYS:N	2.32	0.63
1:D:579:PHE:HZ	1:D:590:ASP:H	1.44	0.63
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.30	0.62
1:E:144:LEU:HD22	1:E:161:LEU:HD11	1.81	0.62
1:A:13:GLN:HB3	1:A:70:VAL:HG12	1.80	0.62
1:A:355:ASN:N	1:A:376:GLU:OE2	2.25	0.62
1:C:355:ASN:HD21	3:C:1102:NAG:H4	1.64	0.62
1:C:594:ARG:HB3	1:D:578:TRP:HE3	1.65	0.62
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.34	0.62
1:A:628:ARG:NH1	1:D:622:ALA:O	2.33	0.62
1:E:31:TRP:H	1:E:93:GLY:HA2	1.62	0.62
1:A:334:LYS:HD3	1:A:349:GLN:HA	1.81	0.62
1:A:514:VAL:HA	1:A:794:GLY:HA3	1.82	0.62
1:B:164:ASN:OD1	1:B:165:VAL:N	2.33	0.62
1:A:623:PHE:HE1	1:B:785:SER:HB2	1.65	0.62
1:B:493:LYS:HD3	1:C:493:LYS:HD3	1.82	0.61
1:C:527:MET:O	1:C:531:PHE:CD1	2.53	0.61
1:D:692:ARG:O	1:D:696:SER:OG	2.11	0.61
1:D:164:ASN:OD1	1:D:165:VAL:N	2.33	0.61
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.34	0.61
1:D:13:GLN:HA	1:D:44:THR:HB	1.81	0.61
1:A:573:ILE:HA	1:E:224:VAL:HB	1.81	0.61
1:B:35:GLN:OE1	1:B:261:ARG:NH2	2.34	0.61
1:C:347:PHE:HE1	1:C:353:ARG:HG2	1.65	0.61
1:B:600:ILE:HG22	1:C:581:LEU:HD11	1.82	0.61
1:B:436:CYS:HB2	1:B:438:PHE:HE2	1.66	0.61
1:B:520:PRO:O	1:B:619:ASN:ND2	2.33	0.61
1:A:476:ILE:HG12	1:A:734:ILE:HD12	1.81	0.60
1:B:396:VAL:N	1:B:473:ASP:OD2	2.34	0.60
1:D:480:THR:O	1:D:485:ARG:NH1	2.32	0.60
1:B:692:ARG:O	1:B:696:SER:OG	2.12	0.60
1:C:493:LYS:HG2	1:C:747:ASN:HD21	1.65	0.60
1:C:308:ARG:HB3	1:C:311:ASN:HD22	1.66	0.60
1:C:334:LYS:HD3	1:C:349:GLN:HA	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:PHE:CE2	1:E:213:TRP:CE3	2.89	0.60
1:A:78:ASP:OD1	1:A:79:LYS:N	2.34	0.60
1:A:493:LYS:HD3	1:D:493:LYS:HD3	1.81	0.60
1:B:372:GLY:HA2	1:B:383:THR:HG23	1.83	0.60
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.83	0.60
1:B:705:GLU:OE1	2:B:1101:ZK1:FAF	2.09	0.60
1:C:236:GLN:NE2	1:C:365:THR:O	2.34	0.60
1:A:50:LEU:HD23	1:A:57:ALA:HB1	1.82	0.60
1:A:539:VAL:HA	1:A:542:LEU:HD12	1.84	0.60
1:A:396:VAL:HB	1:A:473:ASP:H	1.67	0.60
1:D:513:GLY:O	1:D:515:PHE:N	2.35	0.60
1:C:262:TRP:CZ2	1:C:273:ALA:HA	2.36	0.59
1:A:209:ILE:HA	1:A:214:HIS:HD2	1.67	0.59
1:B:25:GLU:HG2	1:B:76:PHE:HZ	1.67	0.59
1:C:50:LEU:HD23	1:C:57:ALA:HB1	1.84	0.59
1:D:263:SER:O	1:D:274:HIS:ND1	2.31	0.59
1:C:130:TRP:CD2	1:C:191:ARG:HD3	2.37	0.59
1:A:308:ARG:HB3	1:A:311:ASN:HD22	1.67	0.59
1:B:483:LEU:N	1:C:755:GLU:OE2	2.30	0.59
1:D:586:GLN:O	1:D:588:GLY:N	2.36	0.59
1:A:266:GLU:HG2	1:A:268:LYS:H	1.67	0.59
1:A:520:PRO:O	1:A:619:ASN:ND2	2.36	0.59
1:C:523:TYR:HA	1:C:526:TRP:HD1	1.68	0.59
1:D:711:TYR:HB2	1:D:767:TRP:HE1	1.68	0.59
1:A:593:PRO:HD2	1:A:596:LEU:HD22	1.85	0.59
1:B:250:TYR:HA	1:B:255:VAL:HG11	1.83	0.59
1:D:411:ASN:HB2	1:D:414:MET:HB2	1.84	0.59
1:D:593:PRO:HD2	1:D:596:LEU:HD23	1.85	0.59
1:D:161:THR:OG1	1:D:187:LYS:NZ	2.35	0.58
1:A:541:PHE:HE2	1:E:227:LEU:HB3	1.66	0.58
1:C:13:GLN:HA	1:C:44:THR:HB	1.85	0.58
1:D:225:LEU:HD22	1:D:247:ILE:HB	1.85	0.58
1:D:152:SER:O	1:D:156:LYS:N	2.35	0.58
1:E:180:HIS:HB3	1:E:209:PHE:HE1	1.69	0.58
1:A:262:TRP:CZ2	1:A:273:ALA:HA	2.38	0.58
1:C:77:TYR:OH	1:C:101:PHE:O	2.13	0.58
1:A:787:LEU:HD12	1:D:521:LEU:HA	1.85	0.58
1:C:38:THR:HG21	1:C:297:ARG:HH21	1.68	0.58
1:C:396:VAL:HB	1:C:473:ASP:H	1.69	0.58
1:D:25:GLU:HG2	1:D:76:PHE:HZ	1.68	0.58
1:A:493:LYS:HG2	1:A:747:ASN:HD21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.86	0.58
1:B:579:PHE:HZ	1:B:590:ASP:N	2.01	0.58
1:D:344:ASN:HD22	3:D:1102:NAG:H4	1.69	0.58
1:D:705:GLU:OE1	2:D:1101:ZK1:FAF	2.11	0.58
1:A:16:GLY:H	1:A:65:GLN:HE22	1.50	0.57
1:E:204:ASP:O	1:E:205:TYR:HB2	2.04	0.57
1:A:247:ILE:HG23	1:A:248:VAL:HG23	1.86	0.57
1:C:211:ILE:HG13	1:C:213:LYS:H	1.69	0.57
1:C:409:LYS:HG3	1:C:415:LEU:HD12	1.85	0.57
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.86	0.57
1:C:774:GLY:N	1:C:777:ASP:OD2	2.38	0.57
1:A:633:ILE:HG23	1:A:638:ASP:HB2	1.86	0.57
1:A:25:GLU:N	1:A:25:GLU:OE1	2.35	0.57
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.87	0.57
1:A:347:PHE:HE1	1:A:353:ARG:HG2	1.69	0.57
1:A:348:ASP:OD1	1:A:352:LYS:N	2.38	0.57
1:A:78:ASP:N	1:A:81:SER:OG	2.38	0.57
1:C:531:PHE:N	1:C:531:PHE:CD1	2.73	0.57
1:C:78:ASP:N	1:C:81:SER:OG	2.37	0.57
1:D:540:LEU:HD13	1:D:579:PHE:HD2	1.70	0.57
1:E:159:LEU:HB3	1:E:230:TYR:HD1	1.68	0.57
1:A:134:ALA:HB3	1:A:192:VAL:HG22	1.87	0.57
1:E:121:LYS:HE2	1:E:125:TRP:HE1	1.69	0.57
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.85	0.57
1:A:415:LEU:HD13	1:A:419:GLU:HB3	1.86	0.56
1:B:261:ARG:O	1:B:264:THR:OG1	2.18	0.56
1:A:109:PHE:HZ	1:A:327:VAL:HG22	1.69	0.56
1:A:206:ASP:HA	1:A:209:ILE:HD12	1.88	0.56
1:B:236:GLN:NE2	1:B:364:LYS:O	2.38	0.56
1:B:225:LEU:HD22	1:B:247:ILE:HB	1.87	0.56
1:B:587:GLN:HE21	1:C:586:GLN:HA	1.70	0.56
1:C:345:ILE:HG12	1:C:353:ARG:NH2	2.20	0.56
1:D:684:ARG:N	1:D:688:GLU:OE1	2.37	0.56
1:B:684:ARG:N	1:B:688:GLU:OE1	2.38	0.56
1:D:396:VAL:N	1:D:473:ASP:OD2	2.34	0.56
1:B:642:GLN:NE2	1:B:645:ILE:HB	2.21	0.56
1:A:628:ARG:HH21	1:D:628:ARG:HG2	1.69	0.56
1:E:31:TRP:CH2	1:E:209:PHE:HB2	2.40	0.56
1:B:219:HIS:HD2	1:B:241:GLU:HB2	1.70	0.56
1:B:198:ARG:NH1	1:B:202:ASN:OD1	2.39	0.56
1:A:625:THR:HG23	1:D:625:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ARG:HD3	1:C:579:PHE:HB2	1.87	0.56
1:D:261:ARG:O	1:D:264:THR:OG1	2.17	0.56
1:D:642:GLN:NE2	1:D:645:ILE:HB	2.20	0.56
1:C:595:SER:H	1:C:599:ARG:HE	1.53	0.56
1:B:228:THR:OG1	1:B:246:GLN:OE1	2.15	0.55
1:D:299:LEU:HD23	1:D:306:ILE:HG21	1.87	0.55
1:A:172:LYS:O	1:A:174:ASP:N	2.39	0.55
1:A:30:ARG:NH1	1:A:269:GLU:O	2.39	0.55
1:B:711:TYR:HB2	1:B:767:TRP:HE1	1.72	0.55
1:B:813:GLU:HA	1:B:816:TYR:HD2	1.70	0.55
1:A:587:GLN:NE2	1:B:587:GLN:OE1	2.39	0.55
1:C:541:PHE:HB2	1:C:576:SER:HB3	1.86	0.55
1:C:587:GLN:NE2	1:D:587:GLN:OE1	2.40	0.55
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.41	0.55
1:B:12:ILE:O	1:B:44:THR:N	2.37	0.55
1:B:586:GLN:O	1:B:588:GLY:N	2.38	0.55
1:C:112:GLN:HE21	1:C:352:LYS:HA	1.71	0.55
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.89	0.55
1:A:586:GLN:O	1:A:588:GLY:N	2.40	0.55
1:B:610:LEU:HD21	1:C:613:ILE:HG21	1.87	0.55
1:C:178:ARG:NH1	1:C:211:ILE:HG22	2.22	0.55
1:E:178:VAL:O	1:E:182:MET:HG2	2.07	0.55
1:E:34:GLY:O	1:E:90:PHE:N	2.39	0.55
1:A:77:TYR:OH	1:A:101:PHE:O	2.16	0.55
1:A:330:GLU:HG2	1:A:334:LYS:HE3	1.89	0.55
1:A:453:ARG:HH21	1:A:458:LYS:HB3	1.72	0.55
1:A:13:GLN:HA	1:A:44:THR:HB	1.89	0.55
1:A:774:GLY:N	1:A:777:ASP:OD2	2.37	0.55
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.42	0.55
1:B:246:GLN:HE21	1:B:248:VAL:N	2.01	0.55
1:D:714:GLN:HE21	1:D:768:TYR:HA	1.71	0.55
1:A:355:ASN:ND2	3:A:1102:NAG:O5	2.40	0.54
1:A:531:PHE:N	1:A:531:PHE:CD1	2.73	0.54
1:D:246:GLN:HE21	1:D:248:VAL:N	2.05	0.54
1:E:157:ASP:HB3	1:E:160:LYS:HB2	1.89	0.54
1:B:146:LEU:O	1:B:149:VAL:HG22	2.06	0.54
1:D:130:TRP:CE2	1:D:191:ARG:HD3	2.42	0.54
1:D:597:SER:O	1:D:600:ILE:HG12	2.06	0.54
1:B:608:PHE:CZ	1:B:612:ILE:HD11	2.43	0.54
1:E:18:ALA:HA	1:E:21:PHE:HD2	1.72	0.54
1:E:189:VAL:O	1:E:193:LEU:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:HIS:HB3	1:E:209:PHE:CE1	2.42	0.54
1:B:592:SER:O	1:B:599:ARG:NH2	2.41	0.54
1:C:531:PHE:N	1:C:531:PHE:HD1	2.05	0.54
1:D:791:ASN:OD1	1:D:792:VAL:HG23	2.08	0.54
1:A:402:GLU:H	1:A:406:VAL:HB	1.73	0.54
1:D:146:LEU:O	1:D:149:VAL:HG22	2.08	0.54
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.43	0.54
1:A:405:TYR:HB3	1:A:425:CYS:SG	2.48	0.54
1:C:514:VAL:HG22	1:C:794:GLY:HA2	1.88	0.54
1:E:205:TYR:OH	1:E:209:PHE:CD2	2.52	0.54
1:A:66:PHE:CZ	1:A:312:ALA:HB1	2.42	0.53
1:A:79:LYS:NZ	1:A:140:ASP:HA	2.23	0.53
1:B:27:SER:HB3	1:B:270:TYR:HB3	1.90	0.53
1:B:480:THR:O	1:B:485:ARG:NH1	2.40	0.53
1:C:586:GLN:O	1:C:588:GLY:N	2.41	0.53
1:D:219:HIS:HD2	1:D:241:GLU:HB2	1.73	0.53
1:D:76:PHE:HE1	1:D:99:PRO:HG2	1.72	0.53
1:C:25:GLU:OE1	1:C:25:GLU:N	2.36	0.53
1:C:402:GLU:O	1:C:406:VAL:N	2.35	0.53
1:C:642:GLN:NE2	1:C:645:ILE:HB	2.24	0.53
1:B:696:SER:OG	1:B:700:TYR:HB3	2.08	0.53
1:B:710:GLU:OE2	1:B:722:LYS:NZ	2.31	0.53
1:C:291:VAL:HG13	1:C:336:VAL:HG11	1.91	0.53
1:C:66:PHE:CZ	1:C:312:ALA:HB1	2.44	0.53
1:D:481:ILE:HD11	1:D:733:GLY:HA3	1.90	0.53
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.74	0.53
1:C:402:GLU:H	1:C:406:VAL:HB	1.72	0.53
1:D:637:GLU:O	1:D:640:SER:OG	2.21	0.53
1:C:453:ARG:HH21	1:C:458:LYS:HB3	1.73	0.53
1:E:149:LEU:HA	1:E:152:SER:HB3	1.90	0.53
1:B:625:THR:HG21	1:C:625:THR:HG23	1.91	0.53
1:C:513:GLY:O	1:C:516:SER:OG	2.16	0.53
1:D:436:CYS:HB2	1:D:438:PHE:HE2	1.73	0.53
1:C:172:LYS:O	1:C:174:ASP:N	2.42	0.53
1:C:477:ALA:O	1:C:479:LEU:N	2.41	0.53
1:D:330:GLU:HA	1:D:333:LEU:HD12	1.90	0.53
1:E:195:PRO:O	1:E:197:ASP:N	2.41	0.53
1:E:30:TYR:HA	1:E:93:GLY:HA2	1.91	0.53
1:A:17:LEU:HB2	1:A:75:GLY:HA3	1.91	0.52
1:A:30:ARG:NH2	1:A:269:GLU:OE2	2.35	0.52
1:B:161:THR:OG1	1:B:187:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:LYS:HD2	1:C:355:ASN:HD22	1.74	0.52
1:D:348:ASP:OD1	1:D:351:GLY:N	2.42	0.52
1:B:436:CYS:HB2	1:B:438:PHE:CE2	2.45	0.52
1:C:134:ALA:HB3	1:C:192:VAL:HG22	1.90	0.52
1:C:405:TYR:HB3	1:C:425:CYS:SG	2.49	0.52
1:A:613:ILE:HG21	1:D:610:LEU:HD21	1.91	0.52
1:B:328:GLU:OE2	1:B:331:ARG:NH1	2.22	0.52
1:B:453:ARG:HB2	1:B:460:TRP:CD2	2.44	0.52
1:C:138:ASP:OD1	1:C:139:SER:N	2.43	0.52
1:A:477:ALA:O	1:A:479:LEU:N	2.41	0.52
1:B:152:SER:O	1:B:156:LYS:N	2.39	0.52
1:B:628:ARG:HG2	1:C:628:ARG:NH1	2.24	0.52
1:D:236:GLN:NE2	1:D:364:LYS:O	2.38	0.52
1:A:402:GLU:O	1:A:406:VAL:N	2.34	0.52
1:A:113:MET:HB3	1:A:284:LEU:HD22	1.90	0.52
1:D:711:TYR:O	1:D:715:ARG:HG2	2.09	0.52
1:B:50:LEU:HD23	1:B:57:ALA:HB1	1.92	0.52
1:C:267:GLU:HG3	1:C:271:PRO:HA	1.91	0.52
1:D:12:ILE:O	1:D:44:THR:N	2.42	0.52
1:C:15:GLY:HA3	1:C:73:ILE:HA	1.91	0.52
1:D:412:HIS:CE1	1:D:413:GLU:HG3	2.44	0.52
1:D:77:TYR:HE2	1:D:98:THR:HG21	1.74	0.52
1:E:185:GLN:O	1:E:189:VAL:HG23	2.09	0.52
1:E:23:THR:O	1:E:27:LEU:N	2.43	0.52
1:B:20:ARG:NE	1:B:49:ASN:O	2.41	0.52
1:D:250:TYR:HA	1:D:255:VAL:HG11	1.92	0.52
1:B:190:ARG:HD3	1:B:218:TYR:CE1	2.45	0.51
1:C:637:GLU:O	1:C:641:LYS:HG2	2.10	0.51
1:D:595:SER:O	1:D:597:SER:N	2.43	0.51
1:B:99:PRO:HA	1:B:113:MET:HB2	1.92	0.51
1:B:330:GLU:HA	1:B:333:LEU:HD12	1.92	0.51
1:B:579:PHE:CZ	1:B:591:ILE:HG22	2.45	0.51
1:A:362:GLU:O	1:A:369:ARG:N	2.44	0.51
1:A:595:SER:N	1:A:599:ARG:HE	2.08	0.51
1:C:226:GLY:HA2	1:C:246:GLN:HE22	1.75	0.51
1:D:10:ASN:O	1:D:42:ARG:N	2.42	0.51
1:A:581:LEU:HD21	1:D:600:ILE:HA	1.92	0.51
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.46	0.51
1:C:80:LYS:HA	1:D:83:ASN:ND2	2.25	0.51
1:A:642:GLN:NE2	1:A:645:ILE:HB	2.26	0.51
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.92	0.51
1:B:476:ILE:HG12	1:B:734:ILE:HD12	1.93	0.51
1:A:597:SER:O	1:A:600:ILE:HG12	2.11	0.51
1:B:185:GLU:OE2	1:B:213:LYS:NZ	2.37	0.51
1:B:46:HIS:HD2	1:B:68:ARG:NH1	2.09	0.51
1:C:308:ARG:HB3	1:C:311:ASN:ND2	2.25	0.51
1:C:480:THR:N	2:C:1101:ZK1:OAA	2.43	0.51
1:A:369:ARG:NH1	1:A:387:THR:HG23	2.25	0.51
1:B:174:ASP:CG	1:B:178:ARG:HH12	2.14	0.51
1:C:330:GLU:HG2	1:C:334:LYS:HE3	1.93	0.51
1:C:595:SER:N	1:C:599:ARG:HE	2.08	0.51
1:C:77:TYR:CE2	1:C:100:SER:HB2	2.46	0.51
1:D:309:ARG:HD3	1:D:311:ASN:HB2	1.93	0.51
1:D:529:ILE:HD12	1:D:612:ILE:HD13	1.92	0.51
1:A:97:ILE:HG13	1:A:111:ILE:HB	1.92	0.50
1:B:219:HIS:CD2	1:B:241:GLU:HB2	2.46	0.50
1:B:348:ASP:OD1	1:B:351:GLY:N	2.44	0.50
1:A:308:ARG:HB3	1:A:311:ASN:ND2	2.27	0.50
1:A:38:THR:HG21	1:A:297:ARG:HD3	1.94	0.50
1:B:505:LYS:HG3	1:B:719:ASP:HB2	1.93	0.50
1:B:595:SER:HB3	1:C:578:TRP:CG	2.46	0.50
1:D:405:TYR:HB3	1:D:425:CYS:SG	2.51	0.50
1:E:133:LEU:HD23	1:E:136:LEU:HD12	1.93	0.50
1:C:389:GLY:O	1:C:391:GLU:N	2.44	0.50
1:A:577:LEU:O	1:A:580:SER:OG	2.20	0.50
1:A:594:ARG:O	1:A:596:LEU:N	2.43	0.50
1:B:198:ARG:CZ	1:B:230:GLY:HA2	2.42	0.50
1:B:453:ARG:HA	1:B:460:TRP:HA	1.93	0.50
1:C:12:ILE:O	1:C:44:THR:N	2.43	0.50
1:C:364:LYS:HG3	1:C:369:ARG:NH2	2.26	0.50
1:A:542:LEU:HD11	1:E:170:VAL:HG21	1.94	0.50
1:D:345:ILE:HG12	1:D:353:ARG:NH2	2.26	0.50
1:D:714:GLN:NE2	1:D:768:TYR:HA	2.25	0.50
1:E:99:GLU:O	1:E:108:LYS:N	2.43	0.50
1:B:177:TYR:CD2	1:B:207:GLN:HG3	2.45	0.50
1:C:185:GLU:HA	1:C:188:LYS:HA	1.94	0.50
1:C:595:SER:H	1:C:599:ARG:HH11	1.59	0.50
1:A:409:LYS:HG2	1:A:422:GLU:CD	2.32	0.50
1:D:99:PRO:HA	1:D:113:MET:HB2	1.94	0.50
1:D:174:ASP:CG	1:D:178:ARG:HH12	2.16	0.50
1:E:127:SER:O	1:E:130:SER:OG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:HA	1:A:299:LEU:HD13	1.94	0.50
1:A:112:GLN:NE2	1:A:352:LYS:HG2	2.27	0.50
1:A:584:PHE:CZ	1:D:606:TRP:HZ3	2.28	0.50
1:C:534:ILE:O	1:C:537:SER:OG	2.23	0.50
1:D:190:ARG:HD3	1:D:218:TYR:CE1	2.46	0.50
1:C:93:HIS:HB3	1:C:327:VAL:HG22	1.94	0.49
1:D:608:PHE:CZ	1:D:612:ILE:HD11	2.46	0.49
1:A:83:ASN:ND2	1:B:80:LYS:HA	2.26	0.49
1:C:594:ARG:HD3	1:D:575:ASN:HB2	1.93	0.49
1:C:594:ARG:O	1:C:596:LEU:N	2.45	0.49
1:D:453:ARG:HB2	1:D:460:TRP:CD2	2.47	0.49
1:D:800:VAL:HA	1:D:803:LEU:HD12	1.94	0.49
1:A:590:ASP:OD1	1:A:591:ILE:N	2.39	0.49
1:A:594:ARG:HD3	1:B:575:ASN:HB2	1.94	0.49
1:A:657:GLU:HA	1:A:660:ARG:HG2	1.94	0.49
1:A:80:LYS:HA	1:B:83:ASN:ND2	2.27	0.49
1:B:15:GLY:N	1:B:72:ALA:O	2.40	0.49
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.76	0.49
1:A:581:LEU:HD11	1:D:600:ILE:HG22	1.95	0.49
1:A:14:ILE:HG13	1:A:45:PRO:HA	1.93	0.49
1:A:345:ILE:HG12	1:A:353:ARG:NH2	2.28	0.49
1:B:345:ILE:HG12	1:B:353:ARG:NH2	2.27	0.49
1:B:532:ALA:O	1:B:536:VAL:HG23	2.13	0.49
1:B:794:GLY:HA2	1:B:797:TYR:CD2	2.47	0.49
1:A:783:LYS:HD3	1:D:630:VAL:HG21	1.94	0.49
1:B:132:LYS:NZ	1:B:189:GLU:OE2	2.46	0.49
1:B:24:GLN:NE2	1:B:278:ILE:HG13	2.27	0.49
1:B:232:LEU:HB3	1:B:363:LEU:HD22	1.94	0.49
1:A:595:SER:H	1:A:599:ARG:HE	1.59	0.49
1:C:705:GLU:OE1	2:C:1101:ZK1:FAF	2.21	0.49
1:A:592:SER:HB3	1:A:599:ARG:HD3	1.95	0.49
1:B:308:ARG:HE	1:B:323:TRP:HE3	1.59	0.49
1:C:121:LEU:HA	1:C:245:PHE:CZ	2.48	0.49
1:A:79:LYS:O	1:A:82:VAL:HG12	2.13	0.49
1:B:428:LEU:O	1:B:432:ILE:HG12	2.13	0.49
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.77	0.49
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.94	0.49
1:A:23:ASP:HB3	1:A:271:PRO:HG2	1.95	0.49
1:B:411:ASN:HB2	1:B:414:MET:HB2	1.94	0.49
1:B:594:ARG:O	1:B:596:LEU:N	2.42	0.49
1:A:480:THR:N	2:A:1101:ZK1:OAA	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:OE2	1:A:213:LYS:NZ	2.38	0.48
1:D:536:VAL:O	1:D:540:LEU:HG	2.13	0.48
1:A:578:TRP:CG	1:D:595:SER:HB3	2.48	0.48
1:A:138:ASP:OD1	1:A:139:SER:N	2.45	0.48
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.77	0.48
1:C:211:ILE:HD12	1:C:213:LYS:HD2	1.95	0.48
1:D:219:HIS:CD2	1:D:241:GLU:HB2	2.48	0.48
1:A:188:LYS:HD2	1:A:190:ARG:NH2	2.22	0.48
1:A:705:GLU:OE1	2:A:1101:ZK1:FAF	2.21	0.48
1:B:755:GLU:O	1:C:661:ARG:NH1	2.47	0.48
1:D:325:GLN:O	1:D:329:ILE:HG13	2.11	0.48
1:D:454:ASP:O	1:D:458:LYS:HA	2.12	0.48
1:D:696:SER:OG	1:D:700:TYR:HB3	2.13	0.48
1:A:459:ILE:HG23	1:A:469:TYR:OH	2.13	0.48
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.52	0.48
1:B:412:HIS:CE1	1:B:413:GLU:HG3	2.48	0.48
1:B:795:VAL:HA	1:B:798:ILE:HG22	1.94	0.48
1:C:355:ASN:ND2	3:C:1102:NAG:H4	2.28	0.48
1:E:186:VAL:O	1:E:190:THR:HG23	2.14	0.48
1:A:594:ARG:HB3	1:B:578:TRP:HE3	1.79	0.48
1:A:651:ASP:HA	1:A:682:PHE:HB3	1.96	0.48
1:B:526:TRP:HA	1:B:529:ILE:HG22	1.96	0.48
1:C:169:ASN:HD21	1:C:172:LYS:HE3	1.77	0.48
1:C:744:THR:HB	1:C:745:PRO:HD3	1.96	0.48
1:D:594:ARG:O	1:D:596:LEU:N	2.47	0.48
1:A:236:GLN:HA	1:A:363:LEU:HD21	1.95	0.48
1:D:540:LEU:HD13	1:D:579:PHE:CD2	2.48	0.48
1:A:392:GLN:OE1	1:A:438:PHE:HA	2.13	0.48
1:B:400:ILE:HG21	1:B:450:TYR:CE1	2.49	0.48
1:B:800:VAL:HA	1:B:803:LEU:HD12	1.96	0.48
1:A:267:GLU:HB2	1:A:274:HIS:HB3	1.96	0.48
1:A:383:THR:HG22	1:A:385:ASP:H	1.78	0.48
1:C:189:GLU:O	1:C:190:ARG:NH1	2.44	0.48
1:D:435:HIS:CD2	1:D:753:LEU:HD21	2.49	0.48
1:E:36:GLN:NE2	1:E:199:ARG:H	2.11	0.48
1:A:77:TYR:CE2	1:A:100:SER:HB2	2.49	0.47
1:D:77:TYR:CE2	1:D:100:SER:HB2	2.49	0.47
1:D:409:LYS:NZ	1:D:419:GLU:OE1	2.43	0.47
1:E:166:ALA:O	1:E:169:THR:OG1	2.19	0.47
1:E:205:TYR:CZ	1:E:209:PHE:CD2	3.01	0.47
1:B:746:VAL:O	1:B:750:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HA	1:A:262:TRP:HB3	1.95	0.47
1:C:24:GLN:HE21	1:C:262:TRP:HZ2	1.63	0.47
1:D:453:ARG:HB2	1:D:460:TRP:CE3	2.49	0.47
1:A:708:MET:O	1:A:712:ILE:HG12	2.14	0.47
1:B:400:ILE:HG21	1:B:450:TYR:HE1	1.80	0.47
1:B:529:ILE:HD12	1:B:612:ILE:HD13	1.96	0.47
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.95	0.47
1:D:243:SER:OG	1:D:362:GLU:HG2	2.13	0.47
1:E:118:ALA:O	1:E:120:GLU:N	2.38	0.47
1:A:784:THR:OG1	1:A:785:SER:N	2.48	0.47
1:B:309:ARG:HD3	1:B:311:ASN:HB2	1.96	0.47
1:B:396:VAL:O	1:B:473:ASP:HB2	2.15	0.47
1:C:532:ALA:O	1:C:536:VAL:HG23	2.15	0.47
1:D:452:ALA:N	1:D:461:ASN:OD1	2.48	0.47
1:A:130:TRP:CZ3	1:A:191:ARG:HB3	2.49	0.47
1:A:121:LEU:HA	1:A:245:PHE:CZ	2.50	0.47
1:B:325:GLN:O	1:B:329:ILE:HG13	2.15	0.47
1:B:397:VAL:HB	1:B:442:LEU:HD23	1.97	0.47
1:C:30:ARG:NH2	1:C:269:GLU:OE2	2.47	0.47
1:D:355:ASN:ND2	3:D:1102:NAG:O5	2.37	0.47
1:D:744:THR:HB	1:D:745:PRO:HD3	1.97	0.47
1:B:347:PHE:HE1	1:B:353:ARG:HG2	1.80	0.47
1:C:363:LEU:HA	1:C:368:PRO:HA	1.95	0.47
1:D:396:VAL:O	1:D:473:ASP:HB2	2.14	0.47
1:E:29:THR:HG23	1:E:30:TYR:CD2	2.49	0.47
1:B:308:ARG:NE	1:B:323:TRP:HB2	2.29	0.47
1:B:76:PHE:HE1	1:B:99:PRO:HG2	1.79	0.47
1:A:246:GLN:HE21	1:A:248:VAL:N	2.11	0.47
1:A:744:THR:HB	1:A:745:PRO:HD3	1.96	0.47
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.97	0.47
1:C:599:ARG:HH22	1:D:581:LEU:C	2.18	0.47
1:A:664:ILE:HA	1:D:761:LYS:HZ3	1.80	0.47
1:A:428:LEU:O	1:A:432:ILE:HG12	2.15	0.47
1:B:702:TYR:CD2	1:B:704:LEU:HD23	2.49	0.47
1:C:428:LEU:O	1:C:432:ILE:HG12	2.14	0.47
1:D:231:ASP:HB3	1:D:234:LYS:HE3	1.97	0.47
1:D:215:VAL:HA	1:D:238:GLY:O	2.15	0.47
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.50	0.47
1:B:481:ILE:HG12	1:B:491:PHE:CD1	2.50	0.47
1:D:702:TYR:CD2	1:D:704:LEU:HD23	2.50	0.47
1:E:32:CYS:HB3	1:E:203:TRP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:SER:N	1:E:110:ARG:O	2.48	0.47
1:C:100:SER:C	1:C:114:ARG:HD3	2.34	0.46
1:C:177:TYR:HE2	1:C:204:ILE:HG12	1.80	0.46
1:C:415:LEU:HD13	1:C:419:GLU:HB3	1.96	0.46
1:C:522:ALA:H	1:C:525:ILE:HD12	1.79	0.46
1:D:428:LEU:O	1:D:432:ILE:HG12	2.14	0.46
1:E:216:PHE:O	1:E:220:MET:HG2	2.15	0.46
1:B:711:TYR:O	1:B:715:ARG:HG2	2.15	0.46
1:C:409:LYS:HG2	1:C:420:ARG:O	2.15	0.46
1:D:346:LYS:HD3	1:D:355:ASN:HD22	1.79	0.46
1:D:15:GLY:N	1:D:72:ALA:O	2.44	0.46
1:B:800:VAL:HG13	1:E:174:LEU:HB3	1.97	0.46
1:C:197:GLU:O	1:C:201:VAL:HG23	2.16	0.46
1:C:112:GLN:NE2	1:C:352:LYS:HG2	2.30	0.46
1:A:482:THR:O	1:A:486:GLU:N	2.48	0.46
1:A:628:ARG:HH12	1:D:623:PHE:HA	1.79	0.46
1:B:744:THR:HB	1:B:745:PRO:HD3	1.97	0.46
1:C:209:ILE:HA	1:C:214:HIS:HD2	1.81	0.46
1:C:219:HIS:HD2	1:C:241:GLU:OE1	1.98	0.46
1:D:334:LYS:NZ	1:D:349:GLN:O	2.24	0.46
1:D:464:VAL:O	1:D:468:VAL:HG23	2.16	0.46
1:D:481:ILE:HG12	1:D:491:PHE:CD1	2.51	0.46
1:D:746:VAL:O	1:D:750:VAL:HG23	2.16	0.46
1:B:266:GLU:HG2	1:B:268:LYS:H	1.80	0.46
1:C:323:TRP:CE3	1:C:325:GLN:HB2	2.51	0.46
1:E:177:MET:O	1:E:181:MET:HG2	2.16	0.46
1:A:255:VAL:O	1:A:259:ILE:HG12	2.15	0.46
1:B:243:SER:OG	1:B:362:GLU:HG2	2.15	0.46
1:B:464:VAL:O	1:B:468:VAL:HG23	2.15	0.46
1:C:789:LEU:HG	1:C:793:ALA:HB2	1.98	0.46
1:D:116:ASP:OD1	1:D:118:LYS:HG2	2.15	0.46
1:D:204:ILE:O	1:D:208:VAL:HG23	2.16	0.46
1:E:34:GLY:N	1:E:90:PHE:O	2.46	0.46
1:A:453:ARG:HB2	1:A:460:TRP:CE2	2.51	0.46
1:B:10:ASN:N	1:B:41:PHE:HA	2.31	0.46
1:D:397:VAL:HB	1:D:442:LEU:HD23	1.98	0.46
1:D:710:GLU:OE2	1:D:722:LYS:NZ	2.30	0.46
1:D:711:TYR:HB2	1:D:767:TRP:NE1	2.30	0.46
1:A:101:PHE:HA	1:A:114:ARG:HH11	1.80	0.46
1:B:427:ASP:O	1:B:431:GLU:HG2	2.16	0.46
1:B:651:ASP:HA	1:B:682:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:HA	1:C:158:TRP:HB2	1.98	0.46
1:D:197:GLU:O	1:D:201:VAL:HG23	2.16	0.46
1:C:255:VAL:O	1:C:259:ILE:HG12	2.16	0.46
1:D:232:LEU:HB3	1:D:363:LEU:HD22	1.98	0.46
1:D:27:SER:O	1:D:31:VAL:HG23	2.16	0.46
1:C:124:LEU:HD11	1:C:128:TYR:HE2	1.81	0.45
1:C:710:GLU:OE2	1:C:722:LYS:NZ	2.49	0.45
1:D:24:GLN:NE2	1:D:278:ILE:HG13	2.29	0.45
1:E:9:LEU:HA	1:E:12:VAL:HG22	1.96	0.45
1:A:124:LEU:HD11	1:A:128:TYR:HE1	1.81	0.45
1:A:481:ILE:HG12	1:A:491:PHE:CD1	2.51	0.45
1:B:141:ARG:HH22	1:B:196:CYS:N	2.13	0.45
1:C:348:ASP:OD1	1:C:352:LYS:N	2.49	0.45
1:A:369:ARG:HH12	1:A:386:ASP:C	2.20	0.45
1:A:526:TRP:HA	1:A:529:ILE:HG22	1.99	0.45
1:A:639:LEU:HA	1:A:642:GLN:HG2	1.98	0.45
1:B:77:TYR:CE2	1:B:100:SER:HB2	2.51	0.45
1:B:131:ASP:OD1	1:B:132:LYS:N	2.49	0.45
1:B:250:TYR:OH	1:B:277:THR:HB	2.16	0.45
1:C:116:ASP:OD1	1:C:118:LYS:HG2	2.17	0.45
1:C:453:ARG:HB2	1:C:460:TRP:CE2	2.52	0.45
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.98	0.45
1:D:590:ASP:OD1	1:D:599:ARG:NH2	2.49	0.45
1:E:124:LEU:HD21	1:E:186:VAL:HG11	1.97	0.45
1:A:500:ILE:HB	1:A:727:LEU:HB2	1.98	0.45
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.81	0.45
1:B:128:TYR:HB3	1:B:130:TRP:NE1	2.31	0.45
1:B:309:ARG:HG2	1:B:311:ASN:N	2.29	0.45
1:C:227:PHE:N	1:C:246:GLN:OE1	2.49	0.45
1:A:533:TYR:CE1	1:A:584:PHE:HB2	2.52	0.45
1:B:600:ILE:HA	1:C:581:LEU:HD21	1.99	0.45
1:C:708:MET:O	1:C:712:ILE:HG12	2.17	0.45
1:D:436:CYS:HB2	1:D:438:PHE:CE2	2.50	0.45
1:D:466:GLU:HA	1:D:471:LYS:HB2	1.99	0.45
1:D:50:LEU:HD22	1:D:61:ALA:HB2	1.98	0.45
1:A:628:ARG:NH1	1:D:623:PHE:HA	2.32	0.45
2:B:1101:ZK1:HAOA	2:B:1101:ZK1:HAI	1.73	0.45
1:E:165:ALA:O	1:E:169:THR:HG23	2.16	0.45
1:A:453:ARG:HB2	1:A:460:TRP:CD2	2.52	0.45
1:B:100:SER:HA	1:B:114:ARG:NH2	2.32	0.45
1:B:15:GLY:HA3	1:B:73:ILE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:SER:HB2	1:B:578:TRP:CG	2.51	0.45
1:D:374:TRP:CH2	1:D:376:GLU:HA	2.51	0.45
1:D:595:SER:CA	1:D:599:ARG:HB3	2.42	0.45
1:C:250:TYR:HA	1:C:255:VAL:HG11	1.98	0.45
1:C:813:GLU:O	1:C:817:LYS:HG3	2.17	0.45
1:A:534:ILE:O	1:A:537:SER:OG	2.24	0.45
1:B:657:GLU:HG2	1:B:660:ARG:NH1	2.31	0.45
1:C:598:GLY:O	1:C:601:VAL:HB	2.17	0.45
1:D:526:TRP:HA	1:D:529:ILE:HG22	1.98	0.45
1:D:607:PHE:O	1:D:611:ILE:HG12	2.17	0.45
1:E:37:ARG:HA	1:E:87:LEU:HA	1.99	0.45
1:A:296:PHE:CD1	1:A:299:LEU:HD22	2.52	0.44
1:B:11:SER:OG	1:B:44:THR:OG1	2.26	0.44
1:B:329:ILE:O	1:B:333:LEU:HG	2.17	0.44
1:D:704:LEU:HD12	1:D:705:GLU:O	2.17	0.44
1:A:400:ILE:HG12	1:A:402:GLU:HG2	1.99	0.44
1:B:704:LEU:HD12	1:B:705:GLU:O	2.17	0.44
1:D:344:ASN:ND2	3:D:1102:NAG:H4	2.31	0.44
1:D:332:ALA:O	1:D:336:VAL:HG23	2.16	0.44
1:D:347:PHE:HE1	1:D:353:ARG:HG2	1.81	0.44
1:D:598:GLY:O	1:D:601:VAL:HB	2.17	0.44
1:D:637:GLU:HG2	1:D:666:VAL:HG21	1.98	0.44
1:E:123:VAL:HG13	1:E:182:MET:HE3	2.00	0.44
1:B:650:LEU:HD12	1:B:683:VAL:O	2.17	0.44
1:C:330:GLU:HA	1:C:333:LEU:HD12	1.98	0.44
1:D:100:SER:HA	1:D:114:ARG:NH2	2.33	0.44
1:A:107:HIS:HA	1:A:108:PRO:HD3	1.82	0.44
1:D:10:ASN:N	1:D:41:PHE:HA	2.32	0.44
1:D:177:TYR:CD2	1:D:207:GLN:HG3	2.52	0.44
1:A:219:HIS:HD2	1:A:241:GLU:OE1	2.01	0.44
1:A:531:PHE:HE2	1:E:213:TRP:CE2	2.34	0.44
1:A:540:LEU:HD12	1:A:580:SER:HB3	1.98	0.44
1:B:27:SER:O	1:B:31:VAL:HG23	2.17	0.44
1:C:526:TRP:HA	1:C:529:ILE:HG22	2.00	0.44
1:D:128:TYR:HB3	1:D:130:TRP:NE1	2.33	0.44
1:E:204:ASP:O	1:E:205:TYR:CB	2.66	0.44
1:C:511:LYS:HA	1:C:512:PRO:HD3	1.87	0.44
1:C:595:SER:H	1:C:599:ARG:NE	2.15	0.44
1:D:231:ASP:OD1	1:D:232:LEU:N	2.51	0.44
1:A:502:ILE:O	1:A:722:LYS:HA	2.17	0.44
1:A:598:GLY:O	1:A:601:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:O	1:B:301:LYS:HG2	2.18	0.44
1:B:35:GLN:HG2	1:B:286:TYR:OH	2.17	0.44
1:D:122:LEU:O	1:D:126:GLU:HG3	2.18	0.44
1:D:250:TYR:OH	1:D:277:THR:HB	2.17	0.44
1:D:532:ALA:O	1:D:536:VAL:HG23	2.18	0.44
1:D:787:LEU:HD11	1:D:791:ASN:HD21	1.83	0.44
1:E:37:ARG:NH1	1:E:87:LEU:HB2	2.33	0.44
1:B:197:GLU:O	1:B:201:VAL:HG23	2.17	0.44
1:B:453:ARG:HB2	1:B:460:TRP:CE2	2.52	0.44
1:B:62:PHE:CE2	1:B:88:PHE:HB3	2.53	0.44
1:C:506:LYS:HA	1:C:507:PRO:HD3	1.70	0.44
1:A:585:MET:HG3	1:D:603:GLY:HA2	2.00	0.44
1:E:163:ALA:O	1:E:167:VAL:HG23	2.18	0.44
1:A:527:MET:O	1:A:531:PHE:CD1	2.71	0.44
1:A:813:GLU:O	1:A:817:LYS:HG3	2.18	0.44
1:B:711:TYR:HB2	1:B:767:TRP:NE1	2.31	0.44
1:C:592:SER:HA	1:C:593:PRO:HD3	1.83	0.44
1:D:329:ILE:O	1:D:333:LEU:HG	2.17	0.44
1:D:78:ASP:N	1:D:81:SER:OG	2.50	0.44
1:A:790:SER:HA	1:A:793:ALA:HB3	2.00	0.43
1:B:648:GLY:HA3	1:B:681:VAL:HB	1.99	0.43
1:A:314:ASP:OD1	1:A:315:CYS:N	2.51	0.43
1:B:606:TRP:HZ3	1:C:584:PHE:CZ	2.35	0.43
1:C:26:TYR:CE2	1:C:30:ARG:HD2	2.53	0.43
1:C:453:ARG:HB2	1:C:460:TRP:CD2	2.53	0.43
1:D:227:PHE:CG	1:D:244:GLY:HA3	2.53	0.43
1:D:685:THR:OG1	1:D:688:GLU:HG3	2.18	0.43
1:C:619:ASN:ND2	1:D:787:LEU:HB2	2.33	0.43
1:A:763:LYS:HA	1:A:767:TRP:CE3	2.53	0.43
1:C:595:SER:N	1:C:599:ARG:HH11	2.15	0.43
1:D:287:ASP:CG	1:D:341:LEU:H	2.22	0.43
1:D:592:SER:OG	1:D:596:LEU:HB3	2.19	0.43
1:D:57:ALA:HA	1:D:60:ASN:ND2	2.33	0.43
1:A:201:VAL:O	1:A:205:VAL:HG23	2.18	0.43
1:A:190:ARG:HD3	1:A:218:TYR:CE1	2.53	0.43
1:B:493:LYS:HA	1:B:494:PRO:HD3	1.91	0.43
1:B:52:VAL:HG21	1:B:78:ASP:H	1.82	0.43
1:B:619:ASN:ND2	1:C:787:LEU:HB2	2.33	0.43
1:B:481:ILE:HD11	1:B:733:GLY:HA3	1.99	0.43
1:B:95:SER:HA	1:B:109:PHE:HB3	1.99	0.43
1:D:130:TRP:CD2	1:D:191:ARG:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:LYS:HA	1:D:494:PRO:HD3	1.91	0.43
1:E:99:GLU:N	1:E:108:LYS:O	2.51	0.43
1:A:637:GLU:OE1	1:D:776:LYS:NZ	2.39	0.43
1:B:116:ASP:OD1	1:B:118:LYS:HG2	2.17	0.43
1:B:262:TRP:CZ2	1:B:273:ALA:HA	2.54	0.43
1:B:112:GLN:HE21	1:B:352:LYS:HG3	1.84	0.43
1:C:267:GLU:CG	1:C:271:PRO:HA	2.48	0.43
1:C:763:LYS:HA	1:C:767:TRP:CE3	2.54	0.43
1:D:99:PRO:O	1:D:114:ARG:HB2	2.17	0.43
1:D:124:LEU:HD11	1:D:128:TYR:HE1	1.84	0.43
1:D:131:ASP:OD1	1:D:132:LYS:N	2.51	0.43
1:A:640:SER:HB2	1:A:669:LYS:HD2	2.01	0.43
1:B:541:PHE:HB2	1:B:576:SER:HB2	1.99	0.43
1:C:599:ARG:HH22	1:D:582:GLY:N	2.17	0.43
1:C:809:VAL:HA	1:C:812:ILE:HG12	2.00	0.43
1:A:150:LEU:HD23	1:A:160:VAL:HG21	2.01	0.43
1:A:584:PHE:HD1	1:A:605:TRP:HZ2	1.66	0.43
1:B:466:GLU:O	1:B:471:LYS:N	2.52	0.43
1:A:599:ARG:NH1	1:B:578:TRP:O	2.52	0.43
1:D:246:GLN:HG3	1:D:248:VAL:H	1.82	0.43
1:D:35:GLN:HG2	1:D:286:TYR:OH	2.17	0.43
1:D:451:GLY:HA2	1:D:461:ASN:O	2.19	0.43
1:A:479:LEU:HD12	2:A:1101:ZK1:OAA	2.19	0.43
1:A:607:PHE:O	1:A:611:ILE:HG12	2.18	0.43
1:B:130:TRP:CD2	1:B:191:ARG:HD3	2.54	0.43
1:B:24:GLN:NE2	1:B:279:LYS:H	2.17	0.43
1:B:462:GLY:O	1:B:466:GLU:HG3	2.18	0.43
1:D:407:MET:N	1:D:422:GLU:O	2.49	0.43
1:C:619:ASN:HD22	1:D:787:LEU:HD22	1.82	0.43
1:D:95:SER:HA	1:D:109:PHE:HB3	2.00	0.43
1:E:202:SER:OG	1:E:203:TRP:N	2.50	0.43
1:A:247:ILE:HG13	1:A:342:SER:HB2	2.01	0.43
1:A:702:TYR:CE2	1:A:704:LEU:HD23	2.54	0.43
1:B:204:ILE:O	1:B:208:VAL:HG23	2.18	0.43
1:B:215:VAL:HA	1:B:238:GLY:O	2.18	0.43
1:B:287:ASP:CG	1:B:341:LEU:H	2.22	0.43
1:B:348:ASP:OD2	1:B:350:ASN:HB2	2.18	0.43
1:B:120:ALA:HA	1:B:374:TRP:CD1	2.54	0.43
1:C:370:LYS:HG2	1:C:372:GLY:H	1.82	0.43
1:C:619:ASN:HD21	1:D:787:LEU:HB2	1.83	0.43
1:C:672:THR:HG23	1:C:675:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:TYR:CD2	1:C:704:LEU:HD23	2.54	0.43
1:D:462:GLY:O	1:D:466:GLU:HG3	2.19	0.43
1:D:71:TYR:HE1	1:D:308:ARG:HB3	1.84	0.43
1:C:525:ILE:HG12	1:D:789:LEU:HB2	2.01	0.43
1:A:317:ALA:O	1:A:320:ALA:N	2.52	0.43
1:A:702:TYR:CD2	1:A:704:LEU:HD23	2.54	0.43
1:B:172:LYS:O	1:B:174:ASP:N	2.52	0.43
1:B:637:GLU:O	1:B:640:SER:OG	2.20	0.43
1:C:180:LEU:O	1:C:183:ASP:HB2	2.18	0.43
1:C:130:TRP:CZ3	1:C:191:ARG:HB3	2.53	0.43
1:C:540:LEU:HD12	1:C:580:SER:HB3	2.00	0.43
1:C:79:LYS:O	1:C:82:VAL:HG12	2.19	0.43
1:D:201:VAL:O	1:D:205:VAL:HG23	2.19	0.43
1:D:309:ARG:HG2	1:D:311:ASN:N	2.30	0.43
1:E:134:TYR:O	1:E:138:LEU:HG	2.19	0.43
1:A:41:PHE:CE2	1:A:297:ARG:HD2	2.54	0.42
1:A:91:THR:HG21	1:B:56:PHE:CD2	2.54	0.42
1:B:190:ARG:HA	1:B:218:TYR:CD1	2.54	0.42
1:B:534:ILE:O	1:B:537:SER:OG	2.24	0.42
1:C:97:ILE:HA	1:C:111:ILE:HB	2.00	0.42
1:E:94:ILE:O	1:E:95:TRP:HD1	2.01	0.42
1:C:113:MET:O	1:C:115:PRO:HD3	2.18	0.42
1:E:38:VAL:O	1:E:86:GLN:HB3	2.20	0.42
1:A:592:SER:HA	1:A:593:PRO:HD3	1.85	0.42
1:A:678:GLU:HA	1:A:679:PRO:C	2.38	0.42
1:C:132:LYS:HD3	1:C:159:GLN:OE1	2.19	0.42
1:C:190:ARG:HD3	1:C:218:TYR:CE1	2.55	0.42
1:C:227:PHE:CZ	1:C:232:LEU:HD21	2.54	0.42
1:C:607:PHE:O	1:C:611:ILE:HG12	2.19	0.42
1:D:24:GLN:NE2	1:D:279:LYS:H	2.17	0.42
1:A:197:GLU:O	1:A:201:VAL:HG23	2.18	0.42
1:B:105:GLY:O	1:B:107:HIS:ND1	2.50	0.42
1:B:190:ARG:HD3	1:B:218:TYR:HE1	1.83	0.42
1:D:592:SER:O	1:D:594:ARG:N	2.52	0.42
1:A:628:ARG:NH2	1:D:628:ARG:HG2	2.32	0.42
1:A:113:MET:O	1:A:115:PRO:HD3	2.20	0.42
1:A:466:GLU:HA	1:A:471:LYS:HB3	2.01	0.42
1:B:124:LEU:HD11	1:B:128:TYR:HE1	1.85	0.42
1:B:16:GLY:H	1:B:65:GLN:NE2	2.11	0.42
1:C:321:VAL:HA	1:C:322:PRO:HD3	1.89	0.42
1:C:54:ASN:O	1:C:58:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ASP:OD2	1:D:350:ASN:HB2	2.20	0.42
1:D:402:GLU:O	1:D:405:TYR:N	2.52	0.42
1:A:521:LEU:HD21	1:A:525:ILE:HB	2.01	0.42
1:B:453:ARG:HB2	1:B:460:TRP:CE3	2.54	0.42
1:C:232:LEU:HD23	1:C:363:LEU:HD13	2.00	0.42
1:C:387:THR:C	1:C:389:GLY:H	2.23	0.42
1:C:409:LYS:HD2	1:C:422:GLU:CD	2.40	0.42
1:C:590:ASP:CG	1:C:591:ILE:H	2.22	0.42
1:D:445:VAL:HG23	1:D:466:GLU:OE2	2.19	0.42
1:C:595:SER:HB2	1:D:578:TRP:CG	2.55	0.42
1:A:369:ARG:NH1	1:A:385:ASP:OD1	2.45	0.42
1:A:664:ILE:HA	1:D:761:LYS:NZ	2.34	0.42
1:A:505:LYS:HD3	1:A:697:LYS:HA	2.01	0.42
1:B:57:ALA:HA	1:B:60:ASN:ND2	2.34	0.42
1:C:480:THR:H	2:C:1101:ZK1:CAT	2.32	0.42
1:C:597:SER:O	1:C:600:ILE:HG12	2.19	0.42
1:C:637:GLU:O	1:C:640:SER:OG	2.23	0.42
1:E:166:ALA:HB1	1:E:223:SER:OG	2.20	0.42
1:A:522:ALA:H	1:A:525:ILE:HD12	1.85	0.42
1:A:54:ASN:O	1:A:58:VAL:HG23	2.19	0.42
1:B:308:ARG:NH2	1:B:325:GLN:H	2.14	0.42
1:B:363:LEU:HA	1:B:368:PRO:HA	2.02	0.42
1:B:505:LYS:NZ	1:B:697:LYS:HA	2.35	0.42
1:B:540:LEU:HB2	1:B:576:SER:OG	2.19	0.42
1:B:708:MET:O	1:B:712:ILE:HG12	2.20	0.42
1:C:521:LEU:O	1:C:526:TRP:NE1	2.53	0.42
1:C:76:PHE:CD1	1:C:99:PRO:HD2	2.54	0.42
1:D:16:GLY:H	1:D:65:GLN:NE2	2.12	0.42
1:A:91:THR:HG21	1:B:56:PHE:CE2	2.55	0.42
1:C:17:LEU:HB2	1:C:75:GLY:HA3	2.02	0.42
1:C:590:ASP:C	1:C:592:SER:H	2.20	0.42
1:C:651:ASP:HA	1:C:682:PHE:HB3	2.01	0.42
1:E:3:SER:HB2	1:E:7:ARG:HH12	1.85	0.42
1:A:576:SER:HA	1:A:579:PHE:HB3	2.02	0.41
1:A:590:ASP:O	1:A:591:ILE:HG22	2.20	0.41
1:A:667:PHE:HE1	1:A:727:LEU:HD13	1.84	0.41
1:B:79:LYS:O	1:B:82:VAL:HG12	2.20	0.41
1:D:323:TRP:CZ3	1:D:325:GLN:HB2	2.54	0.41
1:D:651:ASP:HA	1:D:682:PHE:CD1	2.55	0.41
1:C:651:ASP:HA	1:C:682:PHE:CD1	2.55	0.41
1:D:141:ARG:HH22	1:D:196:CYS:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ASP:O	1:D:431:GLU:HG2	2.19	0.41
1:E:177:MET:HE3	1:E:216:PHE:HB2	2.00	0.41
1:B:523:TYR:HA	1:B:526:TRP:CD1	2.47	0.41
1:B:742:LEU:O	1:B:746:VAL:HG23	2.20	0.41
1:B:99:PRO:O	1:B:114:ARG:HB2	2.20	0.41
1:C:702:TYR:CE2	1:C:704:LEU:HD23	2.55	0.41
1:D:211:ILE:HD12	1:D:213:LYS:HD2	2.02	0.41
1:D:42:ARG:HG2	1:D:43:LEU:O	2.21	0.41
1:D:398:THR:HA	1:D:443:THR:O	2.20	0.41
1:D:54:ASN:OD1	1:D:56:PHE:HB3	2.20	0.41
1:D:505:LYS:NZ	1:D:697:LYS:HA	2.35	0.41
1:E:159:LEU:HB3	1:E:230:TYR:CD1	2.53	0.41
1:B:403:SER:HA	1:B:404:PRO:HA	1.83	0.41
1:C:115:PRO:HB3	1:C:356:TYR:CG	2.56	0.41
1:D:112:GLN:HE21	1:D:352:LYS:HA	1.85	0.41
1:D:742:LEU:O	1:D:746:VAL:HG23	2.21	0.41
1:E:146:CYS:HA	1:E:149:LEU:HD12	2.02	0.41
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.55	0.41
1:A:204:ILE:O	1:A:208:VAL:HG23	2.20	0.41
1:A:56:PHE:CE2	1:B:91:THR:HG21	2.56	0.41
1:A:57:ALA:HA	1:A:60:ASN:ND2	2.35	0.41
1:C:287:ASP:O	1:C:291:VAL:HG23	2.20	0.41
1:C:314:ASP:OD1	1:C:315:CYS:N	2.53	0.41
1:C:374:TRP:CH2	1:C:376:GLU:HA	2.56	0.41
1:D:255:VAL:O	1:D:259:ILE:HG12	2.21	0.41
1:D:394:THR:HA	1:D:439:LYS:HB2	2.03	0.41
1:D:451:GLY:HA3	1:D:464:VAL:HG23	2.02	0.41
1:A:763:LYS:O	1:A:767:TRP:HB2	2.21	0.41
1:B:122:LEU:O	1:B:126:GLU:HG3	2.19	0.41
1:B:255:VAL:O	1:B:259:ILE:HG12	2.21	0.41
1:C:407:MET:N	1:C:422:GLU:O	2.50	0.41
1:C:460:TRP:CE3	1:C:464:VAL:HG11	2.56	0.41
1:C:651:ASP:OD2	1:C:684:ARG:HA	2.21	0.41
1:D:708:MET:O	1:D:712:ILE:HG12	2.20	0.41
1:E:214:GLY:HA2	1:E:217:THR:HG22	2.01	0.41
1:A:595:SER:HA	1:A:599:ARG:HH11	1.86	0.41
1:C:93:HIS:ND1	1:C:322:PRO:HG2	2.35	0.41
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.86	0.41
1:C:744:THR:O	1:C:748:LEU:HG	2.20	0.41
1:D:105:GLY:O	1:D:107:HIS:ND1	2.53	0.41
1:C:91:THR:HG21	1:D:56:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:ALA:HB2	1:E:190:THR:HG22	2.02	0.41
1:A:175:GLU:HA	1:A:178:ARG:HH11	1.85	0.41
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.56	0.41
1:A:372:GLY:HA2	1:A:383:THR:OG1	2.20	0.41
1:A:506:LYS:HA	1:A:507:PRO:HD3	1.68	0.41
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.86	0.41
1:C:348:ASP:OD2	1:C:350:ASN:HB2	2.21	0.41
1:D:505:LYS:HA	1:D:720:THR:HG22	2.03	0.41
1:A:710:GLU:OE2	1:A:768:TYR:OH	2.33	0.41
1:A:809:VAL:HA	1:A:812:ILE:HG12	2.02	0.41
1:C:231:ASP:O	1:C:234:LYS:HG2	2.21	0.41
1:C:418:ASN:ND2	1:C:440:TYR:O	2.46	0.41
1:D:24:GLN:HE22	1:D:279:LYS:H	1.68	0.41
1:E:115:LEU:HB3	1:E:116:ALA:H	1.80	0.41
1:E:34:GLY:HA3	1:E:90:PHE:HB2	2.03	0.41
1:A:153:ALA:HA	1:A:158:TRP:HB2	2.02	0.41
1:A:418:ASN:HD21	1:A:441:LYS:HA	1.85	0.41
1:B:141:ARG:HH12	1:B:196:CYS:C	2.25	0.41
1:B:207:GLN:O	1:B:211:ILE:HG12	2.21	0.41
1:C:91:THR:HG21	1:D:56:PHE:CE2	2.55	0.41
1:A:227:PHE:CZ	1:A:232:LEU:HD21	2.56	0.40
1:A:293:THR:O	1:A:297:ARG:HG2	2.21	0.40
1:A:384:GLU:O	1:A:386:ASP:N	2.54	0.40
1:C:121:LEU:HA	1:C:245:PHE:HZ	1.87	0.40
1:C:651:ASP:OD1	1:C:652:SER:N	2.54	0.40
1:A:789:LEU:HA	1:D:525:ILE:HG12	2.03	0.40
1:D:648:GLY:HA3	1:D:681:VAL:HB	2.03	0.40
1:B:41:PHE:HZ	1:B:297:ARG:HG3	1.86	0.40
1:B:453:ARG:HD2	1:B:460:TRP:CE2	2.57	0.40
1:B:13:GLN:HB3	1:B:70:VAL:HG12	2.02	0.40
1:C:57:ALA:HA	1:C:60:ASN:ND2	2.36	0.40
1:B:101:PHE:HA	1:B:102:PRO:HD3	1.92	0.40
1:B:595:SER:H	1:B:599:ARG:HG3	1.86	0.40
1:C:466:GLU:O	1:C:472:ALA:N	2.50	0.40
1:D:400:ILE:HD13	1:D:450:TYR:CE1	2.56	0.40
1:D:475:ALA:HB3	1:D:735:ALA:HB3	2.03	0.40
1:E:182:MET:O	1:E:186:VAL:HG23	2.21	0.40
1:E:94:ILE:HG12	1:E:95:TRP:CD1	2.56	0.40
1:A:610:LEU:HD21	1:B:613:ILE:HG21	2.04	0.40
1:B:321:VAL:HA	1:B:322:PRO:HD3	1.97	0.40
1:D:650:LEU:HD12	1:D:683:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ALA:HA	1:E:168:PHE:HD2	1.86	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 PDB entries followed by that with respect to all EM entries.

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	779/1057 (74%)	729 (94%)	35 (4%)	15 (2%)	9	47
1	B	776/1057 (73%)	728 (94%)	37 (5%)	11 (1%)	13	54
1	C	779/1057 (74%)	726 (93%)	38 (5%)	15 (2%)	9	47
1	D	776/1057 (73%)	728 (94%)	35 (4%)	13 (2%)	11	50
1	E	171/1057 (16%)	150 (88%)	13 (8%)	8 (5%)	3	28
All	All	3281/5285 (62%)	3061 (93%)	158 (5%)	62 (2%)	14	47

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	591	ILE
1	B	395	VAL
1	B	512	PRO
1	C	591	ILE
1	D	395	VAL
1	D	590	ASP
1	D	591	ILE
1	E	117	PRO
1	A	587	GLN
1	B	587	GLN
1	B	590	ASP
1	B	595	SER

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Mol	Chain	Res	Type
1	B	785	SER
1	C	173	LYS
1	C	174	ASP
1	C	587	GLN
1	D	587	GLN
1	D	595	SER
1	D	596	LEU
1	E	113	ILE
1	E	196	GLU
1	A	174	ASP
1	A	394	THR
1	A	575	ASN
1	A	594	ARG
1	A	595	SER
1	A	596	LEU
1	B	173	LYS
1	B	174	ASP
1	B	437	GLY
1	C	437	GLY
1	C	590	ASP
1	C	594	ARG
1	C	595	SER
1	C	596	LEU
1	C	787	LEU
1	D	520	PRO
1	D	594	ARG
1	E	112	PHE
1	A	173	LYS
1	A	389	GLY
1	A	437	GLY
1	C	390	LEU
1	C	394	THR
1	E	205	TYR
1	A	765	LYS
1	B	591	ILE
1	C	765	LYS
1	D	514	VAL
1	A	787	LEU
1	B	478	PRO
1	C	574	PHE
1	D	174	ASP
1	D	512	PRO

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Mol	Chain	Res	Type
1	D	782	GLU
1	E	194	GLY
1	A	478	PRO
1	C	16	GLY
1	D	437	GLY
1	E	116	ALA
1	E	195	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 PDB entries followed by that with respect to all EM entries.

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	666/888 (75%)	666 (100%)	0	100	100
1	B	664/888 (75%)	664 (100%)	0	100	100
1	C	666/888 (75%)	666 (100%)	0	100	100
1	D	664/888 (75%)	664 (100%)	0	100	100
1	E	152/888 (17%)	150 (99%)	2 (1%)	73	87
All	All	2812/4440 (63%)	2810 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	87	LEU
1	E	205	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	35	GLN
1	A	65	GLN
1	A	147	GLN
1	A	214	HIS

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	311	ASN
1	A	355	ASN
1	A	412	HIS
1	A	587	GLN
1	A	619	ASN
1	A	642	GLN
1	A	756	GLN
1	B	24	GLN
1	B	46	HIS
1	B	65	GLN
1	B	83	ASN
1	B	147	GLN
1	B	214	HIS
1	B	337	GLN
1	B	355	ASN
1	B	412	HIS
1	B	587	GLN
1	B	619	ASN
1	B	642	GLN
1	C	24	GLN
1	C	65	GLN
1	C	83	ASN
1	C	112	GLN
1	C	147	GLN
1	C	311	ASN
1	C	325	GLN
1	C	337	GLN
1	C	344	ASN
1	C	355	ASN
1	C	587	GLN
1	C	619	ASN
1	C	642	GLN
1	C	756	GLN
1	D	24	GLN
1	D	65	GLN
1	D	147	GLN
1	D	344	ASN
1	D	412	HIS
1	D	435	HIS
1	D	587	GLN
1	D	619	ASN

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Mol	Chain	Res	Type
1	D	642	GLN
1	D	714	GLN
1	E	162	ASN
1	E	180	HIS
1	E	185	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	ZK1	A	1101	-	28,29,29	3.10	10 (35%)	36,45,45	1.66	7 (19%)
3	NAG	A	1102	-	14,14,15	0.26	0	15,19,21	0.39	0
2	ZK1	B	1101	-	28,29,29	3.14	11 (39%)	36,45,45	1.60	6 (16%)
3	NAG	B	1102	-	14,14,15	0.20	0	15,19,21	0.48	0
2	ZK1	C	1101	-	28,29,29	3.11	11 (39%)	36,45,45	1.65	7 (19%)
3	NAG	C	1102	-	14,14,15	0.19	0	15,19,21	0.49	0
2	ZK1	D	1101	-	28,29,29	3.15	11 (39%)	36,45,45	1.62	7 (19%)
3	NAG	D	1102	-	14,14,15	0.18	0	15,19,21	0.50	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	ZK1	A	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	A	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	B	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	B	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	C	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	C	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	D	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	D	1102	-	-	0/6/23/26	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	ZK1	PBA-OAD	-3.68	1.46	1.54
2	A	1101	ZK1	PBA-OAD	-3.68	1.46	1.54
2	B	1101	ZK1	PBA-OAD	-3.66	1.46	1.54
2	D	1101	ZK1	PBA-OAD	-3.63	1.46	1.54
2	C	1101	ZK1	CAU-NAY	-2.09	1.35	1.38
2	A	1101	ZK1	CAU-NAY	-2.05	1.35	1.38
2	B	1101	ZK1	CAR-NAX	2.02	1.45	1.41
2	D	1101	ZK1	CAV-NAP	2.08	1.38	1.35
2	C	1101	ZK1	CAV-NAP	2.08	1.38	1.35
2	D	1101	ZK1	CAR-NAX	2.08	1.45	1.41
2	B	1101	ZK1	CAV-NAP	2.18	1.38	1.35
2	C	1101	ZK1	CAI-CAR	2.35	1.41	1.37
2	A	1101	ZK1	CAI-CAR	2.39	1.41	1.37
2	D	1101	ZK1	CAI-CAR	2.42	1.41	1.37
2	B	1101	ZK1	CAI-CAR	2.44	1.42	1.37
2	C	1101	ZK1	CAW-NAY	4.07	1.45	1.40
2	A	1101	ZK1	CAW-NAY	4.09	1.45	1.40
2	B	1101	ZK1	CAW-NAY	4.21	1.46	1.40
2	C	1101	ZK1	CAJ-CAS	4.28	1.44	1.37
2	D	1101	ZK1	CAW-NAY	4.37	1.46	1.40
2	B	1101	ZK1	PBA-OAE	4.38	1.65	1.54
2	A	1101	ZK1	CAJ-CAS	4.38	1.44	1.37
2	C	1101	ZK1	PBA-OAE	4.40	1.65	1.54
2	D	1101	ZK1	CAJ-CAS	4.43	1.44	1.37
2	A	1101	ZK1	PBA-OAE	4.43	1.65	1.54
2	D	1101	ZK1	PBA-OAE	4.44	1.65	1.54
2	B	1101	ZK1	CAJ-CAS	4.48	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ZK1	CAT-NAP	5.77	1.43	1.33
2	C	1101	ZK1	CAT-NAP	5.88	1.43	1.33
2	D	1101	ZK1	CAT-NAP	5.99	1.43	1.33
2	B	1101	ZK1	CAT-NAP	6.08	1.44	1.33
2	B	1101	ZK1	OAB-CAU	6.44	1.40	1.24
2	A	1101	ZK1	OAB-CAU	6.47	1.40	1.24
2	C	1101	ZK1	OAB-CAU	6.47	1.40	1.24
2	D	1101	ZK1	OAB-CAU	6.49	1.40	1.24
2	A	1101	ZK1	OAA-CAT	6.50	1.40	1.24
2	D	1101	ZK1	OAA-CAT	6.56	1.41	1.24
2	C	1101	ZK1	OAA-CAT	6.57	1.41	1.24
2	B	1101	ZK1	OAA-CAT	6.58	1.41	1.24
2	A	1101	ZK1	PBA-OAC	6.84	1.65	1.50
2	B	1101	ZK1	PBA-OAC	6.86	1.65	1.50
2	C	1101	ZK1	PBA-OAC	6.89	1.65	1.50
2	D	1101	ZK1	PBA-OAC	6.90	1.65	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ZK1	CAI-CAR-NAX	-3.32	118.15	122.69
2	B	1101	ZK1	CAI-CAR-NAX	-3.14	118.40	122.69
2	A	1101	ZK1	CAI-CAR-NAX	-3.00	118.58	122.69
2	C	1101	ZK1	CAI-CAR-NAX	-2.93	118.69	122.69
2	C	1101	ZK1	FAG-CAZ-CAS	-2.42	108.33	112.69
2	B	1101	ZK1	FAG-CAZ-CAS	-2.40	108.37	112.69
2	A	1101	ZK1	FAG-CAZ-CAS	-2.39	108.38	112.69
2	D	1101	ZK1	FAG-CAZ-CAS	-2.34	108.48	112.69
2	C	1101	ZK1	CAM-NAX-CAR	2.02	120.99	116.33
2	D	1101	ZK1	CAM-NAX-CAR	2.07	121.12	116.33
2	A	1101	ZK1	CAM-NAX-CAR	2.10	121.17	116.33
2	B	1101	ZK1	CAO-NAY-CAU	2.18	120.42	117.79
2	D	1101	ZK1	CAO-NAY-CAU	2.29	120.55	117.79
2	A	1101	ZK1	CAO-NAY-CAU	2.74	121.10	117.79
2	C	1101	ZK1	CAO-NAY-CAU	2.76	121.12	117.79
2	A	1101	ZK1	CAV-CAW-NAY	3.51	120.27	117.66
2	C	1101	ZK1	CAV-CAW-NAY	3.55	120.30	117.66
2	B	1101	ZK1	CAV-CAW-NAY	3.58	120.31	117.66
2	D	1101	ZK1	CAV-CAW-NAY	3.69	120.40	117.66
2	D	1101	ZK1	CAN-NAX-CAM	3.69	119.40	111.57
2	B	1101	ZK1	CAN-NAX-CAM	3.70	119.41	111.57
2	C	1101	ZK1	CAN-NAX-CAM	3.82	119.66	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ZK1	CAN-NAX-CAM	3.86	119.74	111.57
2	D	1101	ZK1	CAT-NAP-CAV	3.87	119.45	116.42
2	B	1101	ZK1	CAT-NAP-CAV	4.06	119.60	116.42
2	C	1101	ZK1	CAT-NAP-CAV	4.23	119.73	116.42
2	A	1101	ZK1	CAT-NAP-CAV	4.29	119.78	116.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ZK1	3	0
3	A	1102	NAG	2	0
2	B	1101	ZK1	2	0
2	C	1101	ZK1	3	0
3	C	1102	NAG	2	0
2	D	1101	ZK1	1	0
3	D	1102	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.