



# Full wwPDB EM Model Validation Report ⓘ

Feb 25, 2020 – 12:27 PM EST

PDB ID : 6L6F  
EMDB ID : EMD-0839  
Title : GluK3 receptor complex with UBP301  
Authors : Kumar, J.; Kumari, J.; Burada, A.P.  
Deposited on : 2019-10-28  
Resolution : 10.60 Å (reported)  
Based on initial model : 6JFY

This is a Full wwPDB EM 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

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

with specific help available everywhere you see the ⓘ symbol.

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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  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.8

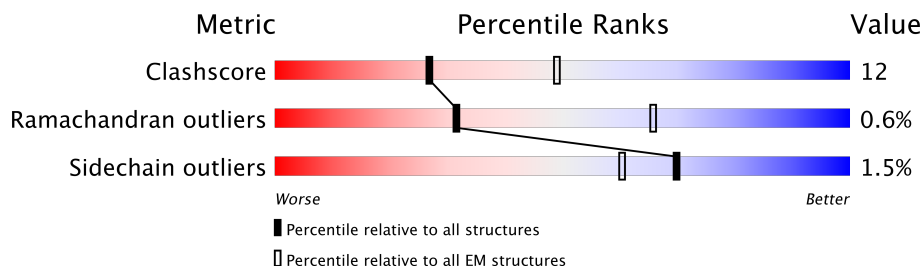
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*





The reported resolution of this entry is 10.60 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. 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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	832	
1	B	832	
1	C	832	
1	D	832	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22836 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 ionotropic, kainate 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		
1	B	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		
1	C	715	Total	C	N	O	S	0	0
			5706	3670	970	1036	30		
1	D	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		

There are 44 discrepancies between the modelled and reference sequences:

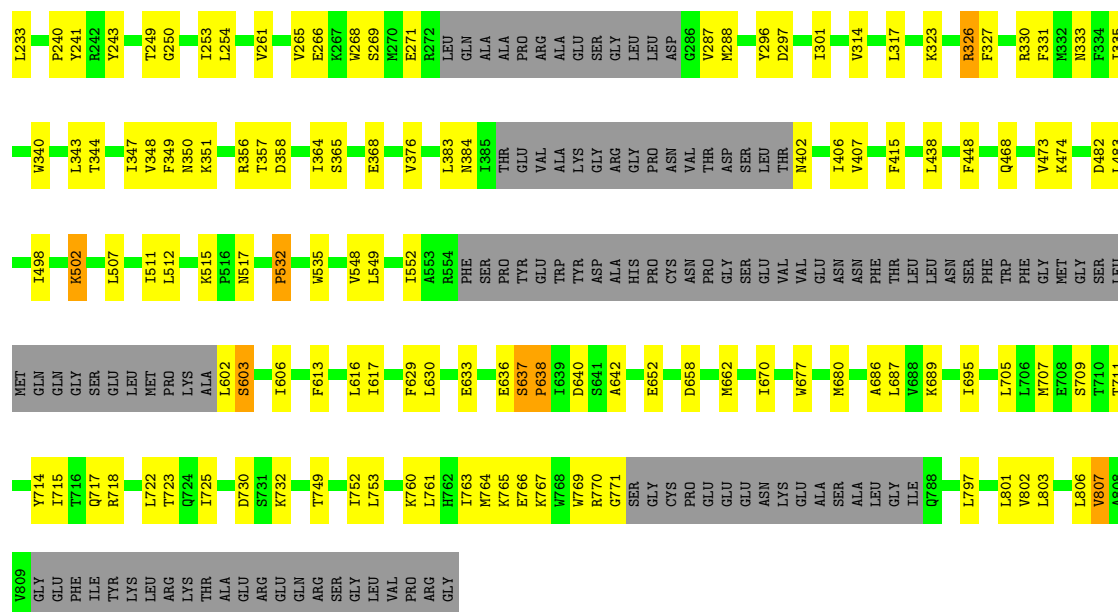
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	THR	CYS	engineered mutation	UNP G3V9I2
A	305	THR	CYS	engineered mutation	UNP G3V9I2
A	547	VAL	CYS	engineered mutation	UNP G3V9I2
A	825	ARG	-	expression tag	UNP G3V9I2
A	826	SER	-	expression tag	UNP G3V9I2
A	827	GLY	-	expression tag	UNP G3V9I2
A	828	LEU	-	expression tag	UNP G3V9I2
A	829	VAL	-	expression tag	UNP G3V9I2
A	830	PRO	-	expression tag	UNP G3V9I2
A	831	ARG	-	expression tag	UNP G3V9I2
A	832	GLY	-	expression tag	UNP G3V9I2
B	86	THR	CYS	engineered mutation	UNP G3V9I2
B	305	THR	CYS	engineered mutation	UNP G3V9I2
B	547	VAL	CYS	engineered mutation	UNP G3V9I2
B	825	ARG	-	expression tag	UNP G3V9I2
B	826	SER	-	expression tag	UNP G3V9I2
B	827	GLY	-	expression tag	UNP G3V9I2
B	828	LEU	-	expression tag	UNP G3V9I2
B	829	VAL	-	expression tag	UNP G3V9I2
B	830	PRO	-	expression tag	UNP G3V9I2
B	831	ARG	-	expression tag	UNP G3V9I2
B	832	GLY	-	expression tag	UNP G3V9I2

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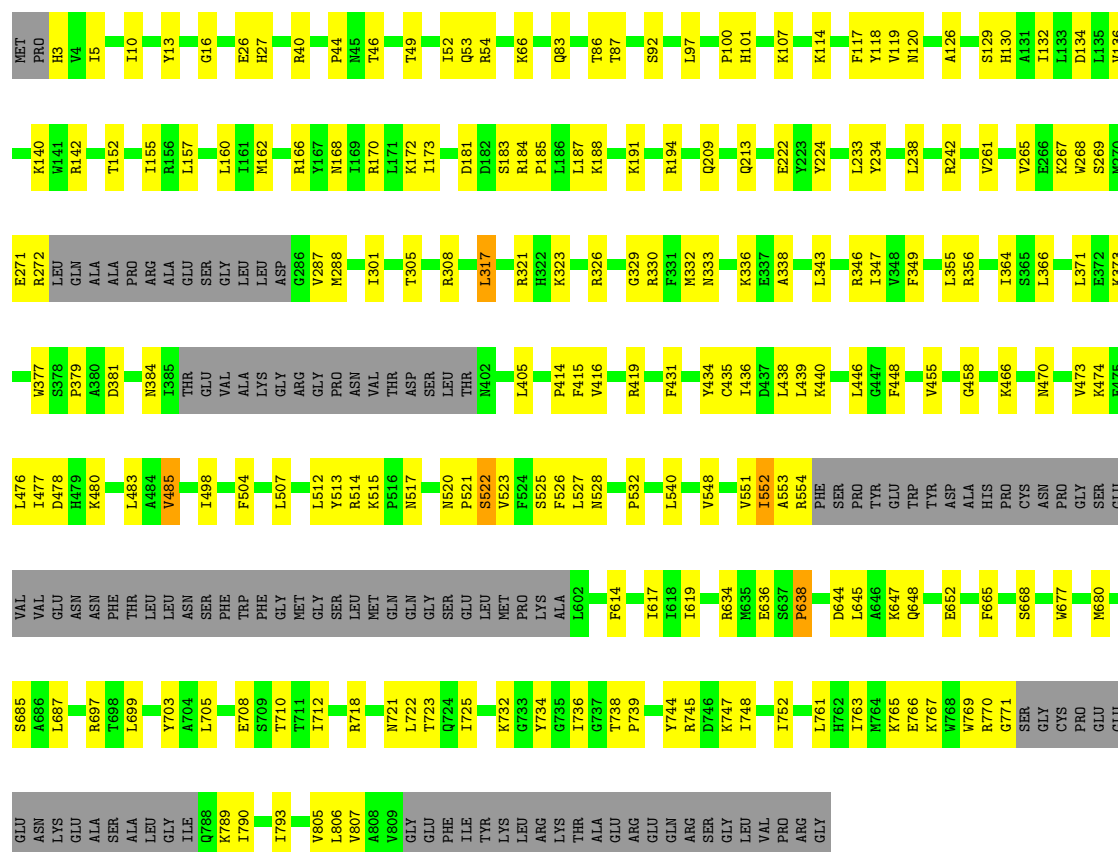
Chain	Residue	Modelled	Actual	Comment	Reference
C	86	THR	CYS	engineered mutation	UNP G3V9I2
C	305	THR	CYS	engineered mutation	UNP G3V9I2
C	547	VAL	CYS	engineered mutation	UNP G3V9I2
C	825	ARG	-	expression tag	UNP G3V9I2
C	826	SER	-	expression tag	UNP G3V9I2
C	827	GLY	-	expression tag	UNP G3V9I2
C	828	LEU	-	expression tag	UNP G3V9I2
C	829	VAL	-	expression tag	UNP G3V9I2
C	830	PRO	-	expression tag	UNP G3V9I2
C	831	ARG	-	expression tag	UNP G3V9I2
C	832	GLY	-	expression tag	UNP G3V9I2
D	86	THR	CYS	engineered mutation	UNP G3V9I2
D	305	THR	CYS	engineered mutation	UNP G3V9I2
D	547	VAL	CYS	engineered mutation	UNP G3V9I2
D	825	ARG	-	expression tag	UNP G3V9I2
D	826	SER	-	expression tag	UNP G3V9I2
D	827	GLY	-	expression tag	UNP G3V9I2
D	828	LEU	-	expression tag	UNP G3V9I2
D	829	VAL	-	expression tag	UNP G3V9I2
D	830	PRO	-	expression tag	UNP G3V9I2
D	831	ARG	-	expression tag	UNP G3V9I2
D	832	GLY	-	expression tag	UNP G3V9I2





- Molecule 1: Glutamate receptor ionotropic, kainate 3

Chain C: 62% 23% 14%



- Molecule 1: Glutamate receptor ionotropic, kainate 3

Chain D:  66% 19% 14%

MET	P185	Y304	THR	N523	T604	I752	PRO
PRO	L186	T305	H402	F524	R605	L753	ARG
H3	L187	R308	I406	L527	I606	Q754	GLY
G8	K188	Y407	Y407	P532	G609	L755	
A24	E189	S316	F415	P632	F613	D759	
H27	R192	R321	V416	D533	F629		
A28	F196	A324	G427	I534	E633	K764	
A33	R197	W325	R430	W535	E633	E766	
N34	F200	R326	Y434	R554	P638	K767	
I35	H204	F327	C435	PHE	I639	W768	
N39	Q209	Q328	TYR	SER	D640	W769	
L42	I210	M332	TRP	PRO	D643	K770	
L48	L211	I335	TVR	GLU	A646	G771	
D61	K212	Q339	ASP	ALA	K650	GLY	
I52	Q222	R346	ALA	HIS	K657	CYS	
Q53	H225	I347	PRO	PRO	K657	PRO	
F57	F226	Y348	ASN	CYS	M662	GLU	
H58	L233	F349	PRO	GLY	T672	ALA	
D59	E239	N350	SER	SER	M676	ALA	
K65	E247	L355	GLU	GLU	S685	LEU	
Q70	R242	D360	VAL	VAL	K689	GLY	
I78	Y243	L361	GLU	ASN	G694	PHE	
T87	N247	I364	ASN	ASN	I695	TLE	
V119	R252	E368	THR	PHE	G696	T715	
L133	V265	G370	LEU	LEU	R697	R718	
D134	W268	G375	ASN	ASN	T698	N719	
L135	R272	W377	SER	TRP	L699	ARG	
W141	LEU	L383	PHE	PHE	L705	LYS	
V146	GLN	N384	GLY	GLY	I715	THR	
D150	ALA	I385	MET	MET	R718	ALA	
S151	PRO	THR	GLY	GLY	N719	ARG	
T152	ARG	VAL	ALA	GLN	L722	GLY	
G153	ALA	LYS	LYS	GLN	I729	THR	
R156	GLU	ARG	S510	GLY	Y734	ALA	
R166	SER	GLY	I511	GLU	G735	GLU	
L171	LEU	PRO	W513	LEU	I736	GLN	
S183	ASP	ASN	R514	MET	K747	ARG	
R194	G286	VAL	T519	PRO	I750	SER	
	V287	THR	N520	LYS	A751	GLY	
	K288	ASP	P521	ALA		LEU	
	S303	LEU	S522	L602		VAL	
			S603				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	16.73	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/5834	0.64	0/7896
1	B	0.33	0/5834	0.69	8/7896 (0.1%)
1	C	0.33	0/5830	0.65	2/7891 (0.0%)
1	D	0.32	0/5834	0.63	1/7896 (0.0%)
All	All	0.33	0/23332	0.65	11/31579 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	LEU	CA-CB-CG	7.14	131.71	115.30
1	B	201	ASP	CB-CG-OD1	6.97	124.57	118.30
1	B	730	ASP	CB-CG-OD2	6.95	124.55	118.30
1	C	540	LEU	CA-CB-CG	6.59	130.45	115.30
1	B	51	ASP	CB-CG-OD1	5.89	123.61	118.30
1	B	797	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	630	LEU	CA-CB-CG	5.35	127.60	115.30
1	B	233	LEU	CA-CB-CG	5.29	127.46	115.30
1	D	211	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	222	GLU	CA-CB-CG	5.10	124.62	113.40
1	B	616	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5710	0	5741	140	0
1	B	5710	0	5741	159	0
1	C	5706	0	5736	145	0
1	D	5710	0	5741	121	0
All	All	22836	0	22959	546	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 12.

All (546) 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:C:548:VAL:CG1	1:C:552:ILE:HD11	1.35	1.54
1:C:548:VAL:HG12	1:C:552:ILE:CD1	1.46	1.45
1:B:803:LEU:O	1:B:807:VAL:CG1	1.67	1.42
1:C:268:TRP:CZ2	1:C:272:ARG:C	1.96	1.39
1:C:718:ARG:HG2	1:C:771:GLY:C	1.44	1.37
1:B:637:SER:CB	1:B:638:PRO:HD2	1.49	1.34
1:B:637:SER:CB	1:B:638:PRO:CD	2.06	1.33
1:B:717:GLN:HG3	1:B:771:GLY:O	1.30	1.25
1:B:803:LEU:O	1:B:807:VAL:HG12	1.40	1.17
1:A:433:GLY:HA2	1:A:768:TRP:CZ3	1.81	1.15
1:A:605:ARG:NH1	1:B:549:LEU:HD13	1.60	1.15
1:D:377:TRP:HD1	1:D:383:LEU:HB2	1.09	1.15
1:B:548:VAL:HG13	1:B:552:ILE:HD11	1.21	1.14
1:B:803:LEU:O	1:B:807:VAL:HG11	1.34	1.14
1:B:629:PHE:CZ	1:B:633:GLU:OE2	2.00	1.14
1:B:548:VAL:O	1:B:552:ILE:HG13	1.40	1.14
1:B:548:VAL:CG1	1:B:552:ILE:HD11	1.80	1.12
1:B:637:SER:HB2	1:B:638:PRO:CD	1.74	1.09
1:B:714:TYR:HB2	1:B:769:TRP:CD1	1.89	1.07
1:B:637:SER:HB3	1:B:638:PRO:CD	1.79	1.06
1:D:718:ARG:NH2	1:D:771:GLY:H	1.55	1.03
1:C:267:LYS:O	1:C:271:GLU:HG3	1.58	1.02
1:C:718:ARG:CG	1:C:771:GLY:C	2.29	1.01
1:A:433:GLY:CA	1:A:768:TRP:CH2	2.44	1.01
1:A:605:ARG:HH11	1:B:549:LEU:HD13	1.12	1.00
1:B:629:PHE:CE2	1:B:633:GLU:OE2	2.14	1.00
1:B:511:ILE:HD12	1:B:642:ALA:HB1	1.41	1.00
1:B:548:VAL:CG1	1:B:552:ILE:CD1	2.40	0.99
1:A:134:ASP:HB3	1:A:383:LEU:HD22	1.44	0.98
1:B:637:SER:HB3	1:B:638:PRO:HD3	1.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:C	1:A:768:TRP:CZ2	2.39	0.96
1:D:377:TRP:CD1	1:D:383:LEU:HB2	2.01	0.95
1:A:433:GLY:O	1:A:768:TRP:CZ2	2.19	0.95
1:A:433:GLY:HA2	1:A:768:TRP:CH2	2.03	0.94
1:A:522:SER:HB2	1:A:523:VAL:HA	1.49	0.93
1:D:629:PHE:CE2	1:D:633:GLU:OE2	2.21	0.93
1:B:717:GLN:HG3	1:B:771:GLY:C	1.88	0.93
1:B:717:GLN:CG	1:B:771:GLY:O	2.17	0.90
1:B:548:VAL:HG13	1:B:552:ILE:CD1	2.00	0.90
1:B:24:ALA:HA	1:B:268:TRP:HH2	1.36	0.90
1:B:714:TYR:HB2	1:B:769:TRP:HD1	1.35	0.90
1:D:802:VAL:O	1:D:806:LEU:HB3	1.71	0.89
1:B:548:VAL:HG12	1:B:552:ILE:HD12	1.54	0.89
1:D:718:ARG:NH2	1:D:771:GLY:N	2.21	0.89
1:D:522:SER:OG	1:D:524:PHE:CD2	2.25	0.89
1:B:548:VAL:O	1:B:552:ILE:CG1	2.22	0.87
1:A:605:ARG:NH1	1:B:549:LEU:CD1	2.37	0.86
1:B:511:ILE:CD1	1:B:642:ALA:HB1	2.06	0.86
1:B:548:VAL:HG12	1:B:552:ILE:CD1	2.06	0.85
1:D:522:SER:OG	1:D:524:PHE:HD2	1.59	0.85
1:B:637:SER:HB2	1:B:638:PRO:HD2	0.85	0.85
1:C:268:TRP:CH2	1:C:272:ARG:C	2.49	0.85
1:A:434:TYR:HA	1:A:768:TRP:NE1	1.93	0.84
1:C:268:TRP:CE2	1:C:272:ARG:C	2.50	0.84
1:D:375:GLY:HA2	1:D:385:ILE:HG22	1.59	0.84
1:D:718:ARG:NE	1:D:771:GLY:C	2.32	0.83
1:C:515:LYS:HG3	1:C:723:THR:HB	1.59	0.82
1:A:433:GLY:N	1:A:768:TRP:CH2	2.48	0.82
1:A:765:LYS:HD2	1:A:769:TRP:CE3	2.16	0.80
1:C:548:VAL:HA	1:C:551:VAL:HG12	1.63	0.80
1:D:602:LEU:HD23	1:D:606:ILE:HG23	1.62	0.79
1:D:718:ARG:CZ	1:D:771:GLY:H	1.96	0.79
1:A:134:ASP:CB	1:A:383:LEU:HD22	2.14	0.78
1:D:602:LEU:CD2	1:D:606:ILE:HG23	2.13	0.77
1:A:766:GLU:HA	1:A:770:ARG:HB2	1.67	0.76
1:C:268:TRP:CZ2	1:C:272:ARG:O	2.40	0.74
1:D:718:ARG:CZ	1:D:771:GLY:C	2.57	0.73
1:A:377:TRP:HD1	1:A:383:LEU:CD1	2.02	0.73
1:B:714:TYR:CB	1:B:769:TRP:HD1	2.02	0.73
1:C:515:LYS:CG	1:C:723:THR:HB	2.19	0.71
1:B:640:ASP:O	1:B:725:ILE:HG21	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:PHE:O	1:D:633:GLU:HG3	1.92	0.70
1:D:629:PHE:CZ	1:D:633:GLU:OE2	2.46	0.69
1:C:548:VAL:CG1	1:C:552:ILE:CD1	2.31	0.69
1:A:134:ASP:HB3	1:A:383:LEU:CD2	2.21	0.69
1:C:520:ASN:HB3	1:C:789:LYS:HD3	1.73	0.69
1:A:377:TRP:CD1	1:A:383:LEU:HD13	2.27	0.69
1:A:766:GLU:HG2	1:A:770:ARG:HD2	1.74	0.69
1:C:765:LYS:O	1:C:769:TRP:HB2	1.94	0.68
1:B:515:LYS:HE2	1:B:723:THR:HB	1.74	0.67
1:D:806:LEU:HD13	1:D:806:LEU:C	2.14	0.67
1:A:377:TRP:HD1	1:A:383:LEU:HD13	1.59	0.67
1:A:493:VAL:HA	1:A:496:LYS:HD3	1.76	0.67
1:C:548:VAL:HG12	1:C:552:ILE:CG1	2.23	0.67
1:A:184:ARG:HE	1:A:213:GLN:HA	1.57	0.67
1:C:267:LYS:O	1:C:271:GLU:CG	2.40	0.66
1:A:605:ARG:HH12	1:B:549:LEU:HD22	1.60	0.66
1:C:101:HIS:H	1:C:117:PHE:HB3	1.60	0.66
1:B:802:VAL:O	1:B:806:LEU:HB3	1.95	0.66
1:A:407:VAL:HG22	1:A:483:LEU:HB2	1.78	0.65
1:A:433:GLY:HA2	1:A:768:TRP:CE3	2.30	0.65
1:C:507:LEU:HB3	1:C:710:THR:HG23	1.78	0.65
1:C:525:SER:HA	1:C:528:ASN:OD1	1.97	0.65
1:A:209:GLN:HG3	1:A:213:GLN:HE21	1.63	0.64
1:D:407:VAL:HB	1:D:452:ILE:HA	1.79	0.64
1:B:143:SER:HB3	1:B:170:ARG:HH11	1.63	0.64
1:A:433:GLY:C	1:A:768:TRP:CE2	2.70	0.64
1:B:512:LEU:HB3	1:B:705:LEU:HB3	1.80	0.62
1:A:208:ALA:HB2	1:A:236:LEU:HD22	1.80	0.62
1:A:407:VAL:HB	1:A:452:ILE:HA	1.80	0.62
1:C:515:LYS:HB2	1:C:721:ASN:C	2.19	0.62
1:C:744:TYR:HA	1:C:747:LYS:HB2	1.82	0.62
1:B:803:LEU:C	1:B:807:VAL:HG12	2.18	0.62
1:C:268:TRP:CE2	1:C:272:ARG:O	2.52	0.62
1:A:714:TYR:HD1	1:A:769:TRP:HA	1.65	0.62
1:D:718:ARG:NH2	1:D:771:GLY:CA	2.63	0.61
1:B:268:TRP:HE3	1:B:288:MET:HE3	1.65	0.61
1:D:383:LEU:O	1:D:383:LEU:HG	2.01	0.61
1:D:602:LEU:HG	1:D:605:ARG:HB2	1.82	0.60
1:D:446:LEU:HD22	1:D:747:LYS:HB3	1.82	0.60
1:C:522:SER:HA	1:C:790:ILE:HD13	1.82	0.60
1:B:147:VAL:HG12	1:B:176:LEU:HD12	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:TYR:HA	1:B:201:ASP:HB3	1.84	0.60
1:C:53:GLN:HE21	1:C:66:LYS:HD2	1.66	0.60
1:A:539:LEU:O	1:A:542:TYR:HB3	2.02	0.59
1:B:473:VAL:HG13	1:B:498:ILE:HD11	1.83	0.59
1:C:514:ARG:HA	1:C:722:LEU:HA	1.84	0.59
1:B:101:HIS:O	1:B:118:TYR:HA	2.02	0.59
1:C:381:ASP:OD2	1:C:384:ASN:ND2	2.35	0.59
1:C:507:LEU:HD12	1:C:732:LYS:HB2	1.85	0.59
1:C:415:PHE:HA	1:C:434:TYR:HB3	1.84	0.59
1:C:269:SER:HB3	1:C:287:VAL:H	1.68	0.59
1:D:200:PHE:HE2	1:D:226:PHE:HB3	1.66	0.59
1:A:124:ASP:HB3	1:A:127:SER:HB3	1.84	0.59
1:C:614:PHE:HA	1:C:617:ILE:HD12	1.85	0.59
1:D:222:GLU:O	1:D:247:ASN:ND2	2.35	0.58
1:C:317:LEU:HA	1:C:323:LYS:HE3	1.84	0.58
1:B:268:TRP:CE3	1:B:288:MET:HE3	2.38	0.58
1:C:261:VAL:HG13	1:C:343:LEU:HB3	1.84	0.58
1:A:605:ARG:HH12	1:B:549:LEU:HD13	1.65	0.58
1:B:714:TYR:CB	1:B:769:TRP:CD1	2.75	0.58
1:B:159:GLU:O	1:B:166:ARG:NH2	2.36	0.58
1:B:714:TYR:CA	1:B:769:TRP:HD1	2.17	0.58
1:C:27:HIS:HB3	1:C:268:TRP:HH2	1.69	0.58
1:B:512:LEU:HD11	1:B:722:LEU:HB3	1.85	0.57
1:B:767:LYS:HA	1:B:770:ARG:HE	1.68	0.57
1:A:605:ARG:HH12	1:B:549:LEU:CD2	2.16	0.57
1:A:46:THR:OG1	1:A:311:GLN:NE2	2.38	0.57
1:D:718:ARG:HE	1:D:771:GLY:C	2.05	0.57
1:A:715:ILE:O	1:A:719:ASN:N	2.36	0.57
1:D:427:GLY:HA2	1:D:430:ARG:HH11	1.68	0.57
1:C:527:LEU:HD22	1:C:532:PRO:HB3	1.86	0.57
1:A:25:GLU:O	1:A:29:PHE:N	2.38	0.57
1:A:433:GLY:CA	1:A:768:TRP:CZ2	2.84	0.57
1:B:348:VAL:HG13	1:B:358:ASP:HB3	1.87	0.57
1:C:552:ILE:HG22	1:C:552:ILE:O	2.04	0.57
1:C:416:VAL:HG13	1:C:436:ILE:HD11	1.86	0.57
1:B:154:LEU:HA	1:B:157:LEU:HB2	1.87	0.56
1:D:377:TRP:HB2	1:D:383:LEU:HD13	1.86	0.56
1:C:512:LEU:HD23	1:C:705:LEU:HD23	1.88	0.56
1:C:513:TYR:HB3	1:C:725:ILE:HG13	1.88	0.56
1:A:121:LEU:HD12	1:A:356:ARG:HB2	1.87	0.56
1:A:315:ASN:HD22	1:A:325:TRP:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:GLU:HA	1:D:242:ARG:HE	1.71	0.56
1:D:350:ASN:N	1:D:355:LEU:O	2.37	0.56
1:B:15:ASP:HB3	1:B:18:ASN:HB2	1.87	0.56
1:A:548:VAL:HG21	1:B:801:LEU:HD22	1.87	0.56
1:D:718:ARG:NH2	1:D:771:GLY:C	2.59	0.56
1:D:806:LEU:HD13	1:D:806:LEU:O	2.06	0.56
1:B:106:TRP:HD1	1:B:122:TYR:HD2	1.54	0.56
1:B:707:MET:SD	1:B:711:THR:OG1	2.60	0.56
1:B:350:ASN:HB2	1:B:357:THR:HG22	1.88	0.55
1:C:162:MET:HB2	1:C:166:ARG:HH21	1.70	0.55
1:B:26:GLU:HG2	1:B:30:ARG:HE	1.70	0.55
1:C:301:ILE:HD11	1:C:347:ILE:HG21	1.87	0.55
1:D:509:VAL:HG12	1:D:729:ILE:HD12	1.87	0.55
1:B:532:PRO:HA	1:B:535:TRP:HD1	1.71	0.55
1:C:515:LYS:HE3	1:C:723:THR:HB	1.87	0.55
1:D:718:ARG:HH22	1:D:771:GLY:H	1.46	0.55
1:B:265:VAL:HG13	1:B:287:VAL:HA	1.88	0.55
1:A:714:TYR:CD1	1:A:769:TRP:HA	2.41	0.55
1:B:266:GLU:O	1:B:269:SER:OG	2.16	0.55
1:C:512:LEU:HB3	1:C:705:LEU:HB3	1.87	0.55
1:B:24:ALA:CA	1:B:268:TRP:HH2	2.15	0.55
1:A:377:TRP:CD1	1:A:383:LEU:CD1	2.87	0.55
1:C:3:HIS:HB3	1:C:46:THR:HG22	1.89	0.55
1:A:134:ASP:C	1:A:383:LEU:HD22	2.27	0.54
1:C:736:ILE:HD11	1:C:752:ILE:HD11	1.89	0.54
1:A:84:GLY:O	1:A:88:ASN:HB2	2.06	0.54
1:C:346:ARG:O	1:C:356:ARG:NH2	2.40	0.54
1:B:243:TYR:HA	1:B:368:GLU:HG3	1.88	0.54
1:D:346:ARG:NH2	1:D:360:ASP:OD2	2.40	0.54
1:D:489:THR:HA	1:D:734:TYR:HA	1.89	0.54
1:D:685:SER:O	1:D:697:ARG:NH2	2.40	0.54
1:B:163:ALA:O	1:B:167:TYR:N	2.39	0.54
1:A:511:ILE:HB	1:A:725:ILE:HB	1.88	0.54
1:C:117:PHE:HD1	1:C:332:MET:HG3	1.72	0.54
1:A:159:GLU:OE1	1:A:166:ARG:NH2	2.41	0.54
1:B:349:PHE:HA	1:B:356:ARG:HA	1.90	0.54
1:C:435:CYS:HA	1:C:438:LEU:HB3	1.88	0.54
1:D:809:VAL:O	1:D:809:VAL:HG23	2.08	0.54
1:A:605:ARG:HH11	1:B:549:LEU:CD1	2.01	0.54
1:B:147:VAL:HG22	1:B:174:ARG:HB2	1.89	0.54
1:A:690:ASN:HD22	1:A:693:GLU:HB2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ALA:HA	1:B:268:TRP:CH2	2.29	0.53
1:A:364:ILE:HD12	1:A:371:LEU:HD21	1.91	0.53
1:A:605:ARG:HH12	1:B:549:LEU:CD1	2.19	0.53
1:B:603:SER:O	1:B:606:ILE:HG12	2.08	0.53
1:D:406:ILE:HB	1:D:481:ALA:HA	1.89	0.53
1:A:3:HIS:HB3	1:A:46:THR:HA	1.91	0.53
1:C:308:ARG:HH12	1:C:338:ALA:HA	1.72	0.53
1:A:208:ALA:HA	1:A:211:LEU:HD12	1.90	0.53
1:A:522:SER:CB	1:A:523:VAL:HA	2.29	0.53
1:B:714:TYR:HB2	1:B:769:TRP:NE1	2.23	0.53
1:D:477:ILE:HD11	1:D:497:ALA:HB1	1.90	0.53
1:A:430:ARG:HH12	1:A:454:LEU:HD11	1.74	0.53
1:A:439:LEU:HD22	1:A:485:VAL:HG21	1.90	0.53
1:D:209:GLN:HE21	1:D:213:GLN:HE21	1.57	0.53
1:A:375:GLY:HA3	1:A:385:ILE:HA	1.91	0.53
1:B:376:VAL:HG22	1:B:384:ASN:HD22	1.73	0.53
1:B:71:LEU:HD22	1:B:317:LEU:HB2	1.90	0.53
1:C:718:ARG:CD	1:C:771:GLY:C	2.76	0.53
1:C:551:VAL:HG11	1:D:805:VAL:HG13	1.90	0.53
1:A:709:SER:HA	1:A:712:ILE:HD12	1.90	0.53
1:C:100:PRO:HG3	1:C:332:MET:HG2	1.91	0.53
1:A:111:LEU:HD11	1:A:353:SER:HB2	1.91	0.53
1:C:552:ILE:C	1:C:554:ARG:H	2.12	0.53
1:D:415:PHE:HA	1:D:434:TYR:HB3	1.91	0.53
1:A:350:ASN:H	1:A:355:LEU:H	1.57	0.52
1:D:602:LEU:HD23	1:D:606:ILE:CG2	2.34	0.52
1:D:715:ILE:O	1:D:719:ASN:N	2.42	0.52
1:D:430:ARG:HH12	1:D:453:ARG:HA	1.72	0.52
1:D:609:GLY:O	1:D:613:PHE:HB2	2.09	0.52
1:B:56:HIS:ND1	1:B:62:GLU:OE1	2.39	0.52
1:B:249:THR:HA	1:B:365:SER:HA	1.91	0.52
1:B:640:ASP:O	1:B:725:ILE:CG2	2.58	0.52
1:D:183:SER:O	1:D:187:LEU:N	2.40	0.52
1:A:434:TYR:CG	1:A:769:TRP:CH2	2.98	0.52
1:D:602:LEU:HD21	1:D:606:ILE:HG23	1.91	0.52
1:A:183:SER:O	1:A:187:LEU:N	2.39	0.52
1:D:361:LEU:HD12	1:D:377:TRP:HB3	1.91	0.52
1:B:142:ARG:H	1:B:197:ARG:HH22	1.58	0.52
1:B:174:ARG:NH1	1:B:190:MET:SD	2.83	0.52
1:C:766:GLU:OE1	1:C:770:ARG:NE	2.43	0.51
1:A:788:GLN:HG2	1:D:534:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:LYS:HA	1:B:770:ARG:NE	2.25	0.51
1:B:17:PRO:O	1:B:20:GLN:NE2	2.43	0.51
1:C:548:VAL:HG12	1:C:552:ILE:HD11	0.59	0.51
1:C:665:PHE:HB3	1:C:677:TRP:HB2	1.93	0.51
1:D:339:GLN:HG2	1:D:348:VAL:HA	1.93	0.51
1:A:195:GLU:OE1	1:A:197:ARG:NH1	2.44	0.51
1:A:765:LYS:HA	1:A:769:TRP:CE3	2.46	0.51
1:B:27:HIS:CD2	1:B:271:GLU:OE1	2.64	0.51
1:C:136:VAL:O	1:C:140:LYS:N	2.40	0.51
1:C:40:ARG:NH1	1:C:44:PRO:O	2.44	0.51
1:A:477:ILE:HD11	1:A:497:ALA:HB1	1.93	0.51
1:B:415:PHE:HE1	1:B:769:TRP:HZ2	1.58	0.51
1:D:189:GLU:HA	1:D:192:ARG:HE	1.76	0.51
1:A:196:PHE:O	1:A:225:HIS:N	2.43	0.51
1:A:318:GLN:HB2	1:A:321:ARG:HE	1.76	0.51
1:D:764:MET:HA	1:D:767:LYS:HG2	1.93	0.51
1:C:419:ARG:NH2	1:C:431:PHE:O	2.43	0.51
1:D:133:LEU:HD11	1:D:166:ARG:HD3	1.93	0.51
1:D:514:ARG:HD3	1:D:699:LEU:HA	1.91	0.51
1:A:79:PHE:HA	1:A:102:ILE:HB	1.92	0.51
1:A:204:HIS:HB2	1:A:236:LEU:HD11	1.91	0.51
1:D:24:ALA:O	1:D:28:ALA:HB2	2.10	0.51
1:D:324:ALA:HB3	1:D:326:ARG:HH21	1.75	0.51
1:A:177:PRO:HD3	1:A:186:LEU:HD22	1.92	0.50
1:B:88:ASN:HA	1:B:91:GLN:HB3	1.92	0.50
1:A:434:TYR:CD1	1:A:769:TRP:CZ3	2.99	0.50
1:B:340:TRP:HD1	1:B:347:ILE:HD12	1.77	0.50
1:B:760:LYS:HA	1:B:763:ILE:HB	1.93	0.50
1:A:82:SER:HA	1:A:107:LYS:HD2	1.94	0.50
1:C:129:SER:HA	1:C:132:ILE:HD12	1.94	0.50
1:B:125:TYR:HA	1:B:128:LEU:HD12	1.94	0.50
1:B:208:ALA:HA	1:B:211:LEU:HD12	1.93	0.50
1:A:377:TRP:HD1	1:A:383:LEU:HD12	1.73	0.50
1:B:138:SER:O	1:B:140:LYS:NZ	2.42	0.50
1:B:268:TRP:HE3	1:B:288:MET:CE	2.25	0.50
1:D:657:LYS:HB3	1:D:689:LYS:HG2	1.94	0.50
1:A:242:ARG:HE	1:A:366:LEU:HD11	1.75	0.50
1:B:184:ARG:HH21	1:B:213:GLN:HA	1.76	0.50
1:A:415:PHE:HA	1:A:434:TYR:HB3	1.92	0.50
1:A:479:HIS:HE1	1:A:740:MET:H	1.59	0.50
1:B:13:TYR:HB2	1:B:16:GLY:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:ILE:HD13	1:D:752:ILE:HD11	1.93	0.50
1:B:26:GLU:OE2	1:B:54:ARG:NH2	2.44	0.49
1:D:204:HIS:HB2	1:D:233:LEU:HB2	1.94	0.49
1:A:43:LEU:HB3	1:A:46:THR:HB	1.94	0.49
1:B:3:HIS:HB3	1:B:46:THR:HG22	1.93	0.49
1:C:157:LEU:HB3	1:C:160:LEU:HD12	1.94	0.49
1:D:33:ALA:HA	1:D:48:LEU:HD23	1.95	0.49
1:C:317:LEU:HD23	1:C:323:LYS:HG2	1.94	0.49
1:C:483:LEU:HD23	1:C:748:ILE:HD11	1.94	0.49
1:D:265:VAL:HG22	1:D:288:MET:HB3	1.94	0.49
1:B:340:TRP:HB3	1:B:347:ILE:HB	1.95	0.49
1:C:349:PHE:HA	1:C:356:ARG:HA	1.94	0.49
1:D:242:ARG:HD3	1:D:370:GLY:HA3	1.93	0.49
1:B:402:ASN:HD21	1:B:448:PHE:HA	1.78	0.49
1:C:97:LEU:HD22	1:C:317:LEU:HB3	1.95	0.49
1:C:118:TYR:H	1:C:332:MET:HE1	1.78	0.49
1:C:644:ASP:HA	1:C:647:LYS:HG2	1.95	0.49
1:C:83:GLN:O	1:C:86:THR:OG1	2.24	0.49
1:B:148:TYR:O	1:B:176:LEU:N	2.41	0.49
1:B:407:VAL:HG22	1:B:483:LEU:HB3	1.95	0.49
1:B:652:GLU:HB3	1:B:686:ALA:HB2	1.94	0.49
1:B:254:LEU:HA	1:B:344:THR:HG22	1.94	0.49
1:C:242:ARG:HB2	1:C:366:LEU:HD11	1.94	0.49
1:A:27:HIS:HB3	1:A:268:TRP:HH2	1.78	0.49
1:C:436:ILE:HG22	1:C:440:LYS:HE3	1.95	0.49
1:D:119:VAL:HG11	1:D:335:ILE:HG22	1.95	0.49
1:C:477:ILE:HG13	1:C:498:ILE:HG23	1.95	0.48
1:B:766:GLU:O	1:B:770:ARG:HG3	2.13	0.48
1:B:6:ARG:H	1:B:314:VAL:HG21	1.78	0.48
1:C:346:ARG:HH22	1:C:379:PRO:HD2	1.78	0.48
1:D:316:SER:O	1:D:321:ARG:NH1	2.47	0.48
1:B:301:ILE:HG12	1:B:340:TRP:HB2	1.94	0.48
1:B:633:GLU:O	1:B:636:GLU:HG2	2.14	0.48
1:C:142:ARG:HH22	1:C:168:ASN:HB3	1.77	0.48
1:C:233:LEU:HG	1:C:238:LEU:HD11	1.94	0.48
1:D:141:TRP:HA	1:D:197:ARG:HH11	1.78	0.48
1:B:211:LEU:HB3	1:B:241:TYR:CZ	2.49	0.48
1:D:252:ARG:HB2	1:D:364:ILE:HD13	1.95	0.48
1:D:243:TYR:HA	1:D:368:GLU:HG2	1.96	0.48
1:C:321:ARG:HH21	1:C:323:LYS:HB2	1.78	0.48
1:B:10:ILE:HG12	1:B:53:GLN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLN:HE21	1:B:474:LYS:HE3	1.78	0.48
1:A:434:TYR:CD1	1:A:769:TRP:HZ3	2.32	0.48
1:C:478:ASP:HB2	1:C:480:LYS:HG3	1.95	0.48
1:C:438:LEU:HD13	1:C:761:LEU:HD21	1.94	0.48
1:D:135:LEU:HD13	1:D:383:LEU:HD21	1.96	0.48
1:C:114:LYS:NZ	1:D:57:PHE:O	2.46	0.48
1:A:742:SER:H	1:A:745:ARG:HH12	1.60	0.48
1:B:106:TRP:O	1:B:156:ARG:NH2	2.47	0.48
1:C:515:LYS:HD3	1:C:517:ASN:HD21	1.79	0.48
1:D:24:ALA:O	1:D:28:ALA:CB	2.62	0.48
1:D:328:GLY:O	1:D:332:MET:HB2	2.14	0.48
1:A:33:ALA:HA	1:A:48:LEU:HD23	1.96	0.47
1:A:433:GLY:CA	1:A:768:TRP:CZ3	2.65	0.47
1:C:763:ILE:O	1:C:767:LYS:HB2	2.14	0.47
1:D:196:PHE:O	1:D:225:HIS:N	2.47	0.47
1:B:376:VAL:O	1:B:384:ASN:HB2	2.14	0.47
1:A:212:LYS:O	1:A:216:ALA:HB2	2.14	0.47
1:C:183:SER:OG	1:C:213:GLN:NE2	2.47	0.47
1:D:153:GLY:HA2	1:D:156:ARG:HG3	1.96	0.47
1:B:35:ILE:HA	1:B:38:ARG:HD2	1.96	0.47
1:C:183:SER:H	1:C:213:GLN:HE22	1.62	0.47
1:D:416:VAL:HG22	1:D:435:CYS:HB2	1.97	0.47
1:A:519:THR:HG22	1:A:520:ASN:H	1.79	0.47
1:B:764:MET:HA	1:B:767:LYS:HB3	1.97	0.47
1:B:507:LEU:O	1:B:732:LYS:N	2.48	0.47
1:A:93:ILE:HG12	1:B:61:PHE:HB2	1.97	0.47
1:C:13:TYR:HB2	1:C:16:GLY:H	1.78	0.47
1:B:28:ALA:HB2	1:B:268:TRP:HZ3	1.79	0.47
1:B:261:VAL:HG22	1:B:343:LEU:HD13	1.95	0.47
1:B:749:THR:O	1:B:753:LEU:HB2	2.13	0.47
1:C:261:VAL:HA	1:C:343:LEU:HD22	1.96	0.47
1:B:636:GLU:OE2	1:B:636:GLU:HA	2.15	0.47
1:B:695:ILE:HD11	1:B:715:ILE:HG12	1.97	0.47
1:B:438:LEU:HD13	1:B:761:LEU:HD21	1.97	0.47
1:D:430:ARG:NH1	1:D:452:ILE:O	2.48	0.47
1:D:491:THR:O	1:D:495:GLU:N	2.46	0.47
1:A:652:GLU:HB2	1:A:703:TYR:HA	1.96	0.47
1:B:415:PHE:CE1	1:B:769:TRP:HZ2	2.33	0.47
1:C:364:ILE:HA	1:C:373:LYS:HA	1.97	0.47
1:D:475:GLU:O	1:D:480:LYS:N	2.48	0.47
1:B:502:LYS:HE2	1:B:752:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:O	1:D:39:ASN:N	2.40	0.47
1:D:646:ALA:HB2	1:D:676:MET:HG3	1.96	0.47
1:A:514:ARG:HA	1:A:722:LEU:HA	1.96	0.46
1:C:305:THR:HA	1:C:308:ARG:HD2	1.97	0.46
1:A:512:LEU:HD12	1:A:712:ILE:HG23	1.98	0.46
1:B:658:ASP:O	1:B:689:LYS:NZ	2.48	0.46
1:A:433:GLY:H	1:A:768:TRP:HH2	1.60	0.46
1:A:683:LYS:HD2	1:A:684:PRO:HD2	1.98	0.46
1:A:694:GLY:HA3	1:A:705:LEU:HD13	1.98	0.46
1:C:466:LYS:HD2	1:C:470:ASN:HD22	1.79	0.46
1:D:209:GLN:HA	1:D:212:LYS:HD2	1.97	0.46
1:B:507:LEU:HB2	1:B:709:SER:H	1.80	0.46
1:C:504:PHE:HE1	1:C:736:ILE:HG23	1.80	0.46
1:D:514:ARG:HD3	1:D:699:LEU:HD23	1.96	0.46
1:C:152:THR:HA	1:C:155:ILE:HD12	1.98	0.46
1:A:261:VAL:HG13	1:A:343:LEU:HD22	1.97	0.46
1:A:765:LYS:HD2	1:A:769:TRP:HE3	1.72	0.46
1:B:765:LYS:HA	1:B:769:TRP:CZ3	2.51	0.46
1:C:191:LYS:NZ	1:C:224:TYR:OH	2.45	0.46
1:C:366:LEU:HA	1:C:371:LEU:HA	1.98	0.46
1:C:680:MET:HB3	1:C:687:LEU:HG	1.98	0.46
1:D:8:GLY:HA2	1:D:51:ASP:HB3	1.97	0.46
1:A:508:GLY:HA3	1:A:728:LEU:HB3	1.98	0.46
1:B:27:HIS:HD2	1:B:271:GLU:OE1	1.98	0.46
1:B:76:VAL:HG13	1:B:314:VAL:HG13	1.98	0.46
1:B:135:LEU:HG	1:B:383:LEU:HD22	1.97	0.46
1:C:134:ASP:OD2	1:C:377:TRP:NE1	2.41	0.45
1:C:652:GLU:HB3	1:C:703:TYR:HD1	1.81	0.45
1:C:515:LYS:HE3	1:C:723:THR:CB	2.46	0.45
1:A:142:ARG:HG3	1:A:169:ILE:HA	1.98	0.45
1:A:730:ASP:OD1	1:A:730:ASP:N	2.49	0.45
1:C:170:ARG:HH22	1:C:172:LYS:HB2	1.81	0.45
1:A:472:MET:HA	1:A:475:GLU:HB2	1.97	0.45
1:C:476:LEU:HD22	1:C:739:PRO:HD3	1.98	0.45
1:B:142:ARG:HH22	1:B:168:ASN:HB3	1.80	0.45
1:D:750:ILE:HA	1:D:753:LEU:HD12	1.98	0.45
1:C:194:ARG:HH12	1:C:224:TYR:HE1	1.64	0.45
1:A:474:LYS:HA	1:A:477:ILE:HB	1.99	0.45
1:A:655:ALA:HB3	1:A:687:LEU:HD23	1.99	0.45
1:C:120:ASN:HB3	1:C:355:LEU:HB3	1.99	0.45
1:A:145:THR:HB	1:A:198:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:O	1:A:216:ALA:CB	2.65	0.45
1:C:805:VAL:C	1:C:807:VAL:H	2.20	0.45
1:C:636:GLU:HB3	1:C:638:PRO:HB3	2.00	0.44
1:D:463:GLN:HA	1:D:469:TRP:HA	1.99	0.44
1:A:652:GLU:O	1:A:704:ALA:N	2.50	0.44
1:A:714:TYR:CD1	1:A:769:TRP:HD1	2.36	0.44
1:B:406:ILE:HB	1:B:482:ASP:H	1.82	0.44
1:C:54:ARG:O	1:C:66:LYS:NZ	2.48	0.44
1:D:146:VAL:HG12	1:D:171:LEU:HD13	1.99	0.44
1:B:802:VAL:HG13	1:B:806:LEU:HB3	1.98	0.44
1:B:9:GLY:O	1:B:53:GLN:N	2.45	0.44
1:D:510:SER:HA	1:D:729:ILE:HG13	1.99	0.44
1:A:714:TYR:CD1	1:A:769:TRP:CD1	3.06	0.44
1:B:27:HIS:CD2	1:B:271:GLU:CD	2.90	0.44
1:C:512:LEU:HD13	1:C:712:ILE:HG23	1.99	0.44
1:C:551:VAL:HG11	1:D:805:VAL:CG1	2.48	0.44
1:D:765:LYS:O	1:D:769:TRP:HB2	2.17	0.44
1:A:119:VAL:HG11	1:A:335:ILE:HG22	1.99	0.44
1:B:317:LEU:HD23	1:B:323:LYS:HE2	1.98	0.44
1:B:250:GLY:N	1:B:364:ILE:O	2.50	0.44
1:C:268:TRP:HD1	1:C:288:MET:HA	1.83	0.44
1:C:329:GLY:O	1:C:332:MET:HB2	2.17	0.44
1:C:439:LEU:HD22	1:C:485:VAL:HG11	2.00	0.44
1:C:514:ARG:HD3	1:C:699:LEU:HA	2.00	0.44
1:C:520:ASN:C	1:C:522:SER:H	2.21	0.44
1:D:439:LEU:HD22	1:D:485:VAL:HG11	1.99	0.44
1:C:92:SER:OG	1:D:59:ASP:OD1	2.36	0.44
1:C:5:ILE:O	1:C:49:THR:OG1	2.31	0.44
1:D:184:ARG:HA	1:D:187:LEU:HB2	1.98	0.44
1:A:381:ASP:OD1	1:A:381:ASP:N	2.50	0.44
1:A:764:MET:O	1:A:768:TRP:HD1	1.99	0.44
1:B:330:ARG:O	1:B:333:ASN:HB2	2.18	0.44
1:C:551:VAL:CG1	1:D:805:VAL:HG13	2.48	0.44
1:D:532:PRO:HA	1:D:535:TRP:HD1	1.83	0.44
1:D:53:GLN:HE21	1:D:70:GLN:HG3	1.83	0.44
1:D:502:LYS:HZ2	1:D:753:LEU:HD11	1.83	0.44
1:C:120:ASN:O	1:C:356:ARG:N	2.43	0.43
1:C:10:ILE:HG12	1:C:53:GLN:HB2	1.99	0.43
1:D:694:GLY:HA3	1:D:705:LEU:HD13	2.00	0.43
1:A:124:ASP:HA	1:A:355:LEU:HD21	2.00	0.43
1:D:512:LEU:HB3	1:D:705:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TYR:CG	1:A:769:TRP:HH2	2.35	0.43
1:C:321:ARG:HE	1:C:323:LYS:HB2	1.84	0.43
1:B:718:ARG:HH12	1:B:769:TRP:HA	1.83	0.43
1:C:87:THR:HG21	1:C:107:LYS:HE2	2.01	0.43
1:A:258:ASN:HD22	1:A:261:VAL:HG23	1.83	0.43
1:B:174:ARG:HD3	1:B:186:LEU:HD11	2.00	0.43
1:C:126:ALA:O	1:C:130:HIS:ND1	2.52	0.43
1:C:194:ARG:HA	1:C:194:ARG:HD2	1.71	0.43
1:C:645:LEU:HA	1:C:648:GLN:HE21	1.83	0.43
1:D:718:ARG:CZ	1:D:771:GLY:N	2.71	0.43
1:D:406:ILE:HG23	1:D:453:ARG:HH11	1.83	0.43
1:A:114:LYS:NZ	1:B:14:ALA:O	2.51	0.43
1:C:40:ARG:HD2	1:C:44:PRO:HA	2.00	0.43
1:B:27:HIS:NE2	1:B:271:GLU:HB3	2.33	0.43
1:B:806:LEU:C	1:B:806:LEU:HD13	2.39	0.43
1:A:313:THR:OG1	1:A:325:TRP:NE1	2.47	0.43
1:B:629:PHE:O	1:B:633:GLU:HG3	2.19	0.43
1:D:184:ARG:HA	1:D:187:LEU:HD12	2.01	0.43
1:D:305:THR:HA	1:D:308:ARG:HG2	2.00	0.43
1:B:142:ARG:H	1:B:197:ARG:NH2	2.17	0.43
1:B:240:PRO:HA	1:B:243:TYR:HD2	1.83	0.43
1:B:680:MET:HG2	1:B:687:LEU:HD21	2.01	0.43
1:C:708:GLU:OE2	1:C:734:TYR:OH	2.36	0.43
1:A:403:ARG:NH2	1:A:744:TYR:OH	2.52	0.42
1:C:473:VAL:HG13	1:C:498:ILE:HG12	2.02	0.42
1:C:525:SER:C	1:C:527:LEU:H	2.23	0.42
1:D:657:LYS:HA	1:D:662:MET:HG3	2.00	0.42
1:A:254:LEU:HB3	1:A:256:VAL:HG23	2.02	0.42
1:C:330:ARG:O	1:C:333:ASN:HB2	2.19	0.42
1:A:617:ILE:O	1:A:621:SER:OG	2.27	0.42
1:A:414:PRO:HG3	1:A:769:TRP:CG	2.46	0.42
1:C:439:LEU:HB2	1:C:485:VAL:HG21	2.00	0.42
1:C:470:ASN:HA	1:C:474:LYS:HE3	2.00	0.42
1:C:26:GLU:HG2	1:C:52:ILE:HD13	2.01	0.42
1:A:764:MET:HG2	1:A:768:TRP:CD1	2.55	0.42
1:B:331:PHE:O	1:B:335:ILE:N	2.50	0.42
1:C:765:LYS:HD2	1:C:769:TRP:CG	2.55	0.42
1:C:155:ILE:HG12	1:D:151:SER:HB3	2.02	0.42
1:D:185:PRO:HA	1:D:188:LYS:HD2	2.01	0.42
1:B:326:ARG:HH11	1:B:327:PHE:HA	1.84	0.42
1:D:150:ASP:N	1:D:150:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:THR:HG21	1:A:745:ARG:HB2	2.02	0.42
1:A:760:LYS:HA	1:A:763:ILE:HD12	2.01	0.42
1:C:183:SER:O	1:C:187:LEU:N	2.51	0.42
1:D:42:LEU:HD21	1:D:303:SER:HB3	2.02	0.42
1:A:514:ARG:HD3	1:A:699:LEU:HA	2.01	0.42
1:C:685:SER:O	1:C:697:ARG:NH1	2.47	0.42
1:D:512:LEU:HD22	1:D:705:LEU:HD23	2.00	0.42
1:A:657:LYS:HB2	1:A:687:LEU:HB3	2.02	0.42
1:A:670:ILE:HB	1:A:673:PHE:HD2	1.85	0.42
1:B:106:TRP:HB3	1:B:156:ARG:HE	1.84	0.42
1:C:185:PRO:HA	1:C:188:LYS:HD2	2.00	0.42
1:C:184:ARG:HG2	1:C:187:LEU:HD12	2.02	0.42
1:C:332:MET:HE3	1:C:336:LYS:HE3	2.01	0.42
1:A:413:GLU:HA	1:A:414:PRO:HA	1.90	0.41
1:B:58:HIS:H	1:B:83:GLN:HG3	1.85	0.41
1:B:662:MET:HG2	1:B:677:TRP:HZ3	1.85	0.41
1:C:405:LEU:HD12	1:C:448:PHE:HB2	2.01	0.41
1:C:514:ARG:NH1	1:C:699:LEU:O	2.53	0.41
1:C:738:THR:HG21	1:C:745:ARG:HA	2.00	0.41
1:D:695:ILE:HG23	1:D:722:LEU:HD21	2.02	0.41
1:A:765:LYS:HA	1:A:769:TRP:HE3	1.83	0.41
1:C:414:PRO:HG2	1:C:769:TRP:CD1	2.55	0.41
1:B:13:TYR:CE2	1:B:54:ARG:HD3	2.55	0.41
1:A:337:GLU:HA	1:A:351:LYS:HE3	2.03	0.41
1:A:434:TYR:HA	1:A:768:TRP:CD1	2.55	0.41
1:C:665:PHE:HA	1:C:668:SER:HB3	2.01	0.41
1:A:434:TYR:N	1:A:768:TRP:CE2	2.88	0.41
1:A:184:ARG:HB2	1:A:213:GLN:HG2	2.03	0.41
1:A:462:ALA:N	1:A:470:ASN:OD1	2.54	0.41
1:A:641:SER:HB2	1:D:650:LYS:HG3	2.03	0.41
1:A:790:ILE:HG22	1:A:793:ILE:HB	2.02	0.41
1:B:198:ILE:H	1:B:226:PHE:HD1	1.69	0.41
1:C:234:TYR:HD2	1:C:287:VAL:HG22	1.86	0.41
1:C:697:ARG:HG2	1:C:703:TYR:CG	2.55	0.41
1:D:406:ILE:O	1:D:482:ASP:N	2.54	0.41
1:B:297:ASP:OD2	1:B:343:LEU:N	2.45	0.41
1:B:58:HIS:NE2	1:B:83:GLN:OE1	2.53	0.41
1:C:446:LEU:HD12	1:C:448:PHE:HE1	1.85	0.41
1:B:613:PHE:O	1:B:617:ILE:HG12	2.21	0.41
1:D:514:ARG:HA	1:D:722:LEU:HA	2.03	0.41
1:B:670:ILE:HG13	1:B:670:ILE:H	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:HIS:HB3	1:D:268:TRP:HH2	1.85	0.41
1:D:638:PRO:O	1:D:640:ASP:N	2.54	0.41
1:A:148:TYR:O	1:A:176:LEU:N	2.48	0.41
1:A:226:PHE:HB2	1:A:248:LEU:HD12	2.02	0.41
1:A:145:THR:HG23	1:A:172:LYS:HB2	2.04	0.40
1:A:36:ILE:O	1:A:40:ARG:NH2	2.38	0.40
1:C:265:VAL:HG22	1:C:288:MET:HB3	2.02	0.40
1:D:519:THR:OG1	1:D:520:ASN:N	2.54	0.40
1:D:65:LYS:HA	1:D:65:LYS:HD2	1.88	0.40
1:D:511:ILE:HG13	1:D:729:ILE:HD11	2.02	0.40
1:D:755:LEU:O	1:D:759:ASP:N	2.55	0.40
1:A:305:THR:HA	1:A:308:ARG:HG2	2.04	0.40
1:B:35:ILE:HD11	1:B:296:TYR:HE1	1.85	0.40
1:B:13:TYR:HE2	1:B:54:ARG:HD3	1.87	0.40
1:D:603:SER:O	1:D:606:ILE:HG13	2.21	0.40
1:A:15:ASP:HB2	1:A:19:ALA:HB2	2.04	0.40
1:A:417:MET:N	1:A:432:GLU:O	2.53	0.40
1:A:434:TYR:HA	1:A:768:TRP:CE2	2.56	0.40
1:B:253:ILE:HG12	1:B:344:THR:HB	2.02	0.40
1:C:181:ASP:HB3	1:C:209:GLN:HG2	2.03	0.40
1:C:455:VAL:HG13	1:C:458:GLY:H	1.86	0.40
1:D:643:ASP:HA	1:D:672:THR:HG21	2.03	0.40
1:B:27:HIS:HD2	1:B:271:GLU:CD	2.24	0.40
1:D:602:LEU:HB3	1:D:603:SER:H	1.72	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	705/832 (85%)	650 (92%)	54 (8%)	1 (0%)	53 88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	705/832 (85%)	652 (92%)	47 (7%)	6 (1%)	19	61
1	C	705/832 (85%)	652 (92%)	46 (6%)	7 (1%)	17	60
1	D	705/832 (85%)	656 (93%)	47 (7%)	2 (0%)	43	81
All	All	2820/3328 (85%)	2610 (93%)	194 (7%)	16 (1%)	31	70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	SER
1	B	638	PRO
1	D	807	VAL
1	B	351	LYS
1	B	517	ASN
1	B	603	SER
1	C	521	PRO
1	C	793	ILE
1	D	603	SER
1	A	43	LEU
1	C	553	ALA
1	C	526	PHE
1	B	43	LEU
1	C	806	LEU
1	C	485	VAL
1	C	638	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	619/715 (87%)	608 (98%)	11 (2%)	62	82
1	B	619/715 (87%)	613 (99%)	6 (1%)	78	89
1	C	618/715 (86%)	609 (98%)	9 (2%)	67	85
1	D	619/715 (87%)	609 (98%)	10 (2%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2475/2860 (86%)	2439 (98%)	36 (2%)	70 85

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	118	TYR
1	A	119	VAL
1	A	136	VAL
1	A	161	ILE
1	A	171	LEU
1	A	221	THR
1	A	234	TYR
1	A	381	ASP
1	A	409	THR
1	A	448	PHE
1	B	221	THR
1	B	326	ARG
1	B	502	LYS
1	B	532	PRO
1	B	602	LEU
1	B	807	VAL
1	C	119	VAL
1	C	173	ILE
1	C	317	LEU
1	C	326	ARG
1	C	522	SER
1	C	523	VAL
1	C	552	ILE
1	C	619	ILE
1	C	634	ARG
1	D	78	ILE
1	D	87	THR
1	D	152	THR
1	D	348	VAL
1	D	507	LEU
1	D	527	LEU
1	D	602	LEU
1	D	603	SER
1	D	806	LEU
1	D	807	VAL

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

Mol	Chain	Res	Type
1	A	45	ASN
1	A	109	HIS
1	A	120	ASN
1	A	175	GLN
1	A	213	GLN
1	A	258	ASN
1	A	300	HIS
1	A	311	GLN
1	A	315	ASN
1	A	479	HIS
1	A	528	ASN
1	A	690	ASN
1	A	754	GLN
1	B	27	HIS
1	B	45	ASN
1	B	113	ASN
1	B	209	GLN
1	B	225	HIS
1	B	247	ASN
1	B	255	ASN
1	B	402	ASN
1	B	468	GLN
1	C	53	GLN
1	C	175	GLN
1	C	213	GLN
1	C	247	ASN
1	C	260	HIS
1	C	318	GLN
1	C	339	GLN
1	D	204	HIS
1	D	209	GLN
1	D	225	HIS
1	D	517	ASN
1	D	696	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.