Full wwPDB EM Validation Report (i)

Dec 13, 2022 – 05:00 PM JST

PDB ID	:	6KSP
EMDB ID	:	EMD-0773
Title	:	Rat GluD1 receptor(splayed conformation) in complex with 7-CKA and Calcium ions
Authors	:	Burada, A.P.; Kumar, J.
Deposited on	:	2019-08-24
Resolution	:	8.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

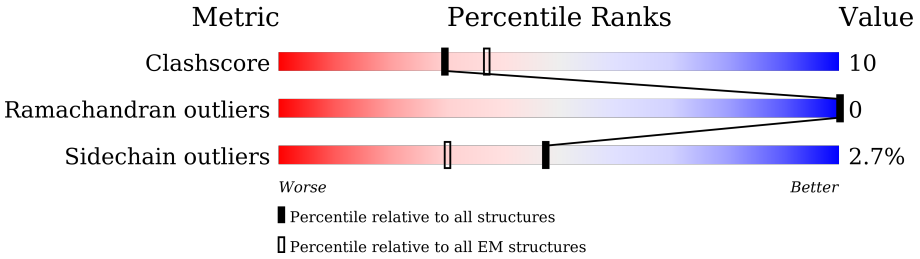
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	856	64% 23% • 12%
1	B	856	63% 24% • 12%
1	C	856	65% 22% • 12%
1	D	856	67% 21% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23744 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, delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	753	5936	3785	1010	1109	32	0	0
1	B	753	5936	3785	1010	1109	32	0	0
1	C	753	5936	3785	1010	1109	32	0	0
1	D	753	5936	3785	1010	1109	32	0	0

There are 20 discrepancies between the modelled and reference sequences:

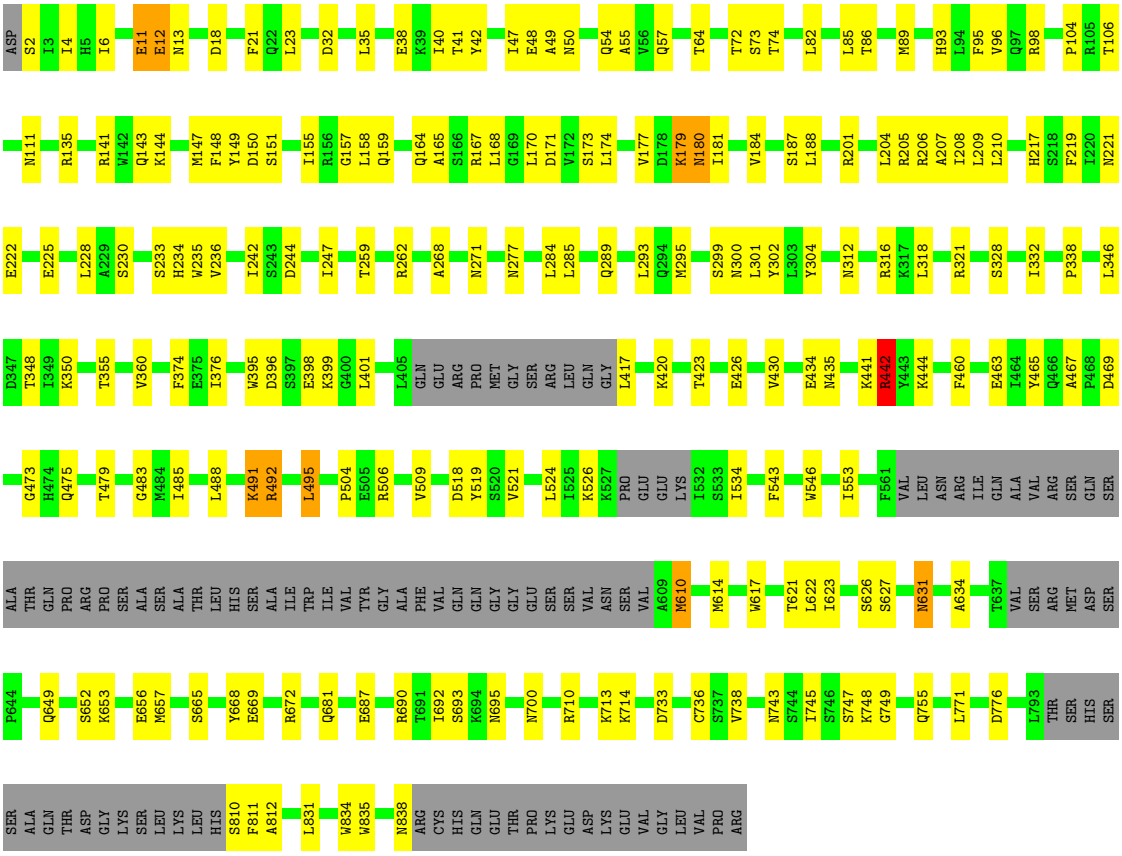
Chain	Residue	Modelled	Actual	Comment	Reference
A	852	GLY	-	See sequence details	UNP Q62640
A	853	LEU	-	See sequence details	UNP Q62640
A	854	VAL	-	See sequence details	UNP Q62640
A	855	PRO	-	See sequence details	UNP Q62640
A	856	ARG	-	See sequence details	UNP Q62640
B	852	GLY	-	See sequence details	UNP Q62640
B	853	LEU	-	See sequence details	UNP Q62640
B	854	VAL	-	See sequence details	UNP Q62640
B	855	PRO	-	See sequence details	UNP Q62640
B	856	ARG	-	See sequence details	UNP Q62640
C	852	GLY	-	See sequence details	UNP Q62640
C	853	LEU	-	See sequence details	UNP Q62640
C	854	VAL	-	See sequence details	UNP Q62640
C	855	PRO	-	See sequence details	UNP Q62640
C	856	ARG	-	See sequence details	UNP Q62640
D	852	GLY	-	See sequence details	UNP Q62640
D	853	LEU	-	See sequence details	UNP Q62640
D	854	VAL	-	See sequence details	UNP Q62640
D	855	PRO	-	See sequence details	UNP Q62640
D	856	ARG	-	See sequence details	UNP Q62640

3 Residue-property plots (i)

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

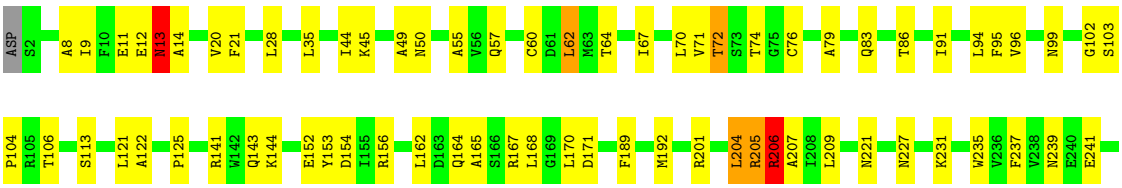
- Molecule 1: Glutamate receptor ionotropic, delta-1

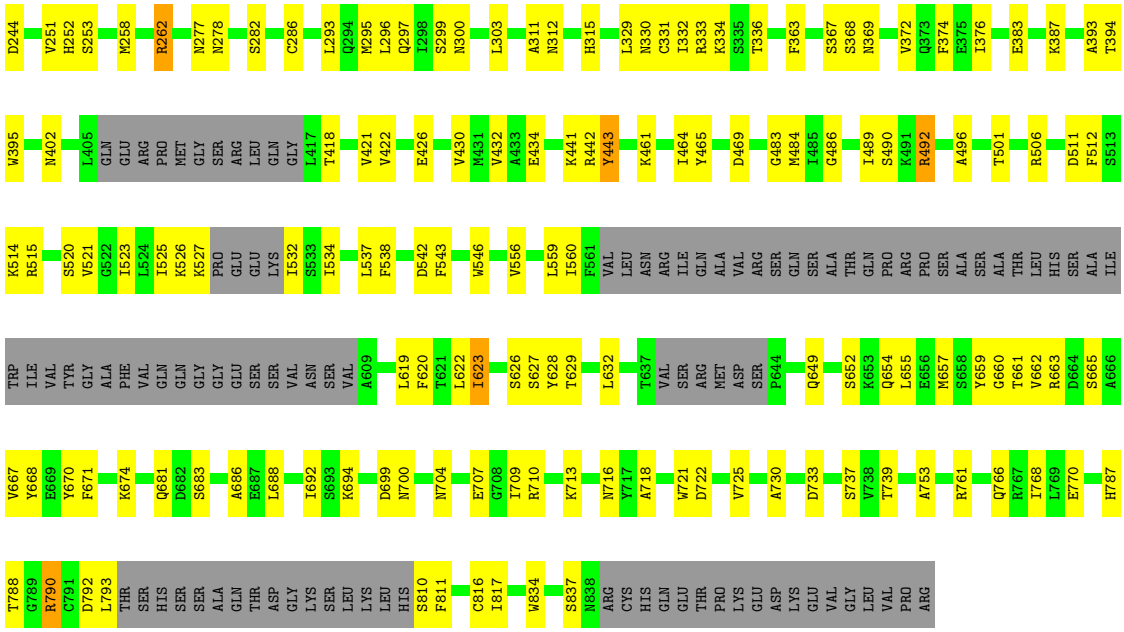
Chain A: 64% 23% • 12%



- Molecule 1: Glutamate receptor ionotropic, delta-1

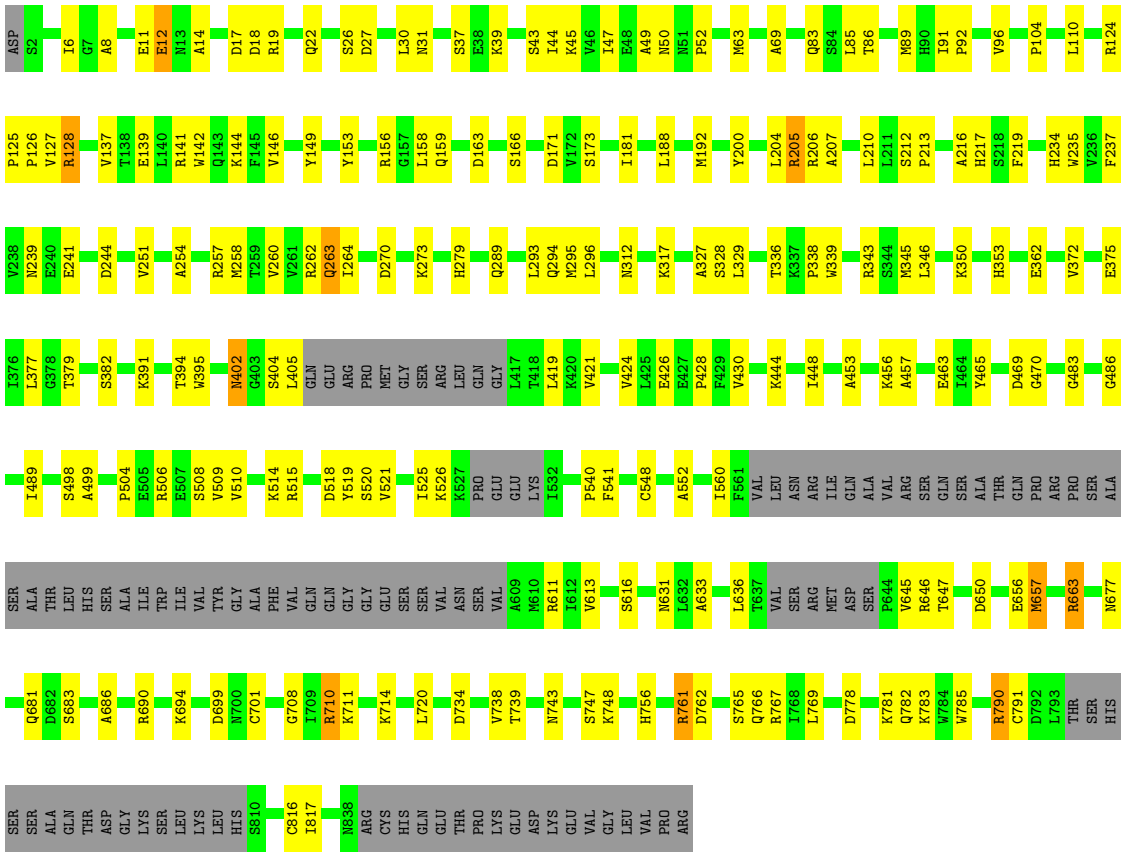
Chain B: 63% 24% • 12%





• Molecule 1: Glutamate receptor ionotropic, delta-1

Chain C: 65% 22% • 12%



• Molecule 1: Glutamate receptor ionotropic, delta-1

Chain D: 67% 21% 12%

ASP S2 E11 E12 N13 D18 R19 V20 F21 Q22 N31 I44 E48 N51 L62 G66 V71 T72 S73 T74 A81 H90 I91 P92 H93 V96 Q97 R98 N99 P104 R105 T106 P112 S113 P114 E117 L121 A122 S123 R124 V137 T138

M147 F148 Y149 Y153 D154 I155 L158 L162 D163 Q164 L168 L174 E196 R199 D202 T203 L204 R205 I208 L209 H217 I220 L228 W235 V236 F237 V238 N239 E240 E241 I242 V251 R257 W258 T259 V260 V261 R262 K269 C274 N277

I281 S282 S283 C286 D287 P288 N300 L310 W339 K350 H353 I354 T355 V360 M361 S367 S368 N369 I376 L377 G378 T379 D388 D396 L405 GLN GLU ARG PRO MET GLY SER ARG LEU GLN GLY L417 T418 L419 K420 V421 V422 E426 V430 E434

N435 P440 K441 R442 D449 A457 E463 I464 Y465 D469 G470 R471 Y472 G473 H474 Q475 L476 H477 N478 T479 S480 W481 N482 I485 L488 K491 A496 T501 I502 R506 V510 K514 D518 L524 K527 PRO GLU GLU LYS I532 S533 D542 F543

W546 A547 C548 A551 F561 VAL LEU ASN ARG ILE GLN ALA VAL ARG SER GLN SER ALA THR GLN PRO ARG PRO SER ALA SER ALA THR LEU HIS SER ALA ILE TRP ILE VAL TYR GLY ALA PHE VAL GLN GLN GLY GLY GLU SER SER VAL ASN SER VAL A609 S626 T629

A633 T637 VAL SER ARG MET ASP SER P644 D650 K653 Q654 L655 E656 T661 F671 R672 A673 K674 N677 D682 F685 L688 W689 S693 K694 N695 D699 S706 E707 G708 I709 R710 K711 L720 V726 L731 V738 S747 K748 G749 Y750

G751 I752 A753 L754 Q755 Y760 R761 F764 S765 Q766 R767 I768 L769 Q772 D773 D778 V779 L780 K781 Q782 W785 P786 H787 D792 L793 THR SER HIS SER SER ALA GLN THR ASP GLY LYS SER LEU LYS LEU HIS S810 F811 F815 L818 L824 L833 N836 S837

N838 ARG CYS HIS GLN GLU THR PRO LYS GLU ASP LYS GLU VAL GLY LEU VAL PRO ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14939	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 ($e^-/Å^2$)	40.38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.32	0/6059	0.56	0/8208
1	B	0.32	0/6059	0.59	2/8208 (0.0%)
1	C	0.32	0/6059	0.57	0/8208
1	D	0.30	0/6059	0.56	0/8208
All	All	0.31	0/24236	0.57	2/32832 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	1
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	ASN	N-CA-C	-6.70	92.91	111.00
1	B	13	ASN	CB-CA-C	5.17	120.74	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	ARG	Sidechain
1	A	492	ARG	Sidechain
1	B	205	ARG	Sidechain
1	B	206	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	333	ARG	Sidechain
1	B	492	ARG	Sidechain
1	C	128	ARG	Sidechain

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	5936	0	5898	129	0
1	B	5936	0	5900	132	0
1	C	5936	0	5898	137	0
1	D	5936	0	5900	111	0
All	All	23744	0	23596	477	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 10.

All (477) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLU:HG2	1:B:49:ALA:HB2	1.44	0.99
1:B:442:ARG:HA	1:B:442:ARG:NH2	1.90	0.86
1:A:434:GLU:HB2	1:A:442:ARG:HB3	1.61	0.82
1:B:62:LEU:HD12	1:B:62:LEU:O	1.91	0.71
1:A:653:LYS:HD2	1:A:656:GLU:HG3	1.73	0.71
1:B:206:ARG:HB2	1:B:206:ARG:HH21	1.58	0.68
1:C:137:VAL:HG12	1:C:142:TRP:HB2	1.75	0.68
1:C:426:GLU:HG2	1:C:428:PRO:HD2	1.76	0.67
1:D:532:ILE:HG13	1:D:811:PHE:HB2	1.76	0.67
1:D:695:ASN:HD22	1:D:699:ASP:HB2	1.60	0.67
1:D:104:PRO:HB3	1:D:240:GLU:H	1.60	0.66
1:C:444:LYS:HB3	1:C:783:LYS:HZ1	1.61	0.66
1:B:559:LEU:O	1:B:559:LEU:HG	1.96	0.65
1:B:9:ILE:HG12	1:B:45:LYS:HD3	1.76	0.65
1:C:681:GLN:HG3	1:C:683:SER:H	1.61	0.65
1:A:236:VAL:HA	1:A:259:THR:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLU:CG	1:B:49:ALA:HB2	2.24	0.64
1:D:672:ARG:HG2	1:D:689:TRP:HE1	1.62	0.64
1:D:209:LEU:HB2	1:D:237:PHE:HA	1.78	0.64
1:C:19:ARG:NH2	1:C:289:GLN:OE1	2.31	0.63
1:A:11:GLU:HB2	1:A:47:ILE:HG13	1.79	0.63
1:B:206:ARG:HB2	1:B:206:ARG:NH2	2.14	0.63
1:B:209:LEU:HB2	1:B:237:PHE:HA	1.81	0.63
1:B:671:PHE:HA	1:B:674:LYS:HB2	1.81	0.63
1:C:293:LEU:O	1:C:293:LEU:HD22	1.99	0.63
1:A:518:ASP:HA	1:A:749:GLY:HA2	1.79	0.62
1:A:420:LYS:HA	1:A:463:GLU:HB2	1.81	0.62
1:A:614:MET:SD	1:A:614:MET:N	2.72	0.62
1:B:556:VAL:HA	1:B:559:LEU:HB3	1.82	0.62
1:C:317:LYS:NZ	1:C:345:MET:SD	2.74	0.61
1:A:149:TYR:HA	1:A:210:LEU:HB2	1.83	0.61
1:B:426:GLU:H	1:B:430:VAL:HB	1.66	0.61
1:B:374:PHE:HB2	1:B:395:TRP:HB3	1.83	0.61
1:A:181:ILE:HG21	1:A:219:PHE:HA	1.82	0.61
1:B:221:ASN:HD21	1:B:253:SER:HB2	1.66	0.60
1:A:150:ASP:HA	1:A:177:VAL:HB	1.82	0.60
1:A:111:ASN:HD22	1:B:50:ASN:HB3	1.67	0.60
1:A:155:ILE:O	1:A:159:GLN:NE2	2.32	0.60
1:B:442:ARG:HA	1:B:442:ARG:CZ	2.31	0.60
1:A:217:HIS:O	1:A:221:ASN:ND2	2.33	0.60
1:C:264:ILE:HD12	1:C:375:GLU:HB2	1.84	0.60
1:D:420:LYS:HA	1:D:463:GLU:HB2	1.83	0.60
1:B:62:LEU:HD11	1:B:67:ILE:HG23	1.84	0.59
1:A:188:LEU:HD11	1:B:167:ARG:HH21	1.67	0.59
1:C:8:ALA:HB3	1:C:44:ILE:HA	1.84	0.59
1:D:259:THR:HA	1:D:378:GLY:HA2	1.84	0.59
1:B:102:GLY:O	1:B:239:ASN:ND2	2.35	0.59
1:A:230:SER:HB3	1:A:233:SER:HB3	1.85	0.59
1:C:504:PRO:O	1:D:766:GLN:NE2	2.36	0.59
1:B:730:ALA:O	1:B:790:ARG:NH1	2.36	0.59
1:A:4:ILE:HB	1:A:40:ILE:HA	1.84	0.59
1:C:251:VAL:HA	1:C:254:ALA:HB3	1.83	0.59
1:A:295:MET:O	1:A:300:ASN:ND2	2.36	0.59
1:A:426:GLU:O	1:A:430:VAL:N	2.36	0.59
1:B:9:ILE:H	1:B:72:THR:HB	1.68	0.59
1:C:234:HIS:HA	1:C:257:ARG:HB2	1.85	0.59
1:C:128:ARG:HB3	1:C:395:TRP:HH2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:ASP:HA	1:D:749:GLY:HA2	1.85	0.58
1:D:242:ILE:O	1:D:262:ARG:NH1	2.35	0.58
1:C:181:ILE:HG12	1:C:219:PHE:HB2	1.86	0.58
1:A:374:PHE:HB2	1:A:395:TRP:HB3	1.85	0.58
1:B:106:THR:HG22	1:B:156:ARG:HH21	1.68	0.58
1:C:457:ALA:O	1:C:767:ARG:NH1	2.36	0.58
1:D:833:LEU:HD23	1:D:836:ASN:HD22	1.69	0.58
1:B:201:ARG:HA	1:B:204:LEU:HB3	1.85	0.57
1:B:704:ASN:H	1:B:707:GLU:HB2	1.69	0.57
1:B:660:GLY:HA2	1:B:692:ILE:HG22	1.85	0.57
1:C:762:ASP:O	1:C:766:GLN:HB2	2.04	0.57
1:B:60:CYS:O	1:B:330:ASN:ND2	2.37	0.57
1:D:422:VAL:HA	1:D:465:TYR:HB2	1.85	0.57
1:B:442:ARG:HA	1:B:442:ARG:HH21	1.66	0.57
1:D:426:GLU:O	1:D:430:VAL:N	2.35	0.57
1:B:11:GLU:HB2	1:B:74:THR:HG22	1.87	0.57
1:B:788:THR:OG1	1:B:790:ARG:NH2	2.36	0.57
1:B:104:PRO:HG2	1:B:153:TYR:HB2	1.87	0.57
1:D:496:ALA:HB3	1:D:753:ALA:HB3	1.87	0.57
1:C:645:VAL:HG22	1:C:647:THR:H	1.69	0.56
1:B:521:VAL:HG11	1:B:667:VAL:HG21	1.86	0.56
1:B:282:SER:HA	1:B:286:CYS:HB2	1.87	0.56
1:D:533:SER:O	1:D:810:SER:N	2.38	0.56
1:A:141:ARG:O	1:A:206:ARG:NH2	2.39	0.56
1:B:713:LYS:NZ	1:B:718:ALA:O	2.37	0.56
1:D:501:THR:O	1:D:506:ARG:NH2	2.39	0.56
1:C:37:SER:O	1:C:39:LYS:NZ	2.38	0.56
1:A:346:LEU:HG	1:A:350:LYS:HE2	1.88	0.56
1:D:31:ASN:ND2	1:D:282:SER:O	2.38	0.56
1:D:350:LYS:O	1:D:353:HIS:NE2	2.39	0.56
1:D:469:ASP:OD1	1:D:471:ARG:NH1	2.39	0.56
1:A:23:LEU:HD11	1:A:289:GLN:HE21	1.71	0.55
1:C:213:PRO:O	1:C:217:HIS:ND1	2.39	0.55
1:C:469:ASP:HB3	1:C:483:GLY:HA2	1.88	0.55
1:C:636:LEU:O	1:C:646:ARG:NH1	2.40	0.55
1:B:704:ASN:HB2	1:B:707:GLU:H	1.71	0.55
1:C:11:GLU:HG3	1:C:47:ILE:HD11	1.89	0.55
1:B:11:GLU:HB3	1:B:74:THR:HA	1.88	0.55
1:C:734:ASP:OD1	1:C:790:ARG:NH1	2.40	0.55
1:B:79:ALA:O	1:B:83:GLN:N	2.40	0.54
1:A:485:ILE:HG21	1:A:506:ARG:HE	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:VAL:HG11	1:D:310:LEU:HD11	1.89	0.54
1:A:6:ILE:HB	1:A:42:TYR:HB3	1.89	0.54
1:B:99:ASN:ND2	1:B:241:GLU:OE1	2.41	0.54
1:C:85:LEU:O	1:C:89:MET:N	2.40	0.54
1:D:473:GLY:HA3	1:D:485:ILE:HG12	1.89	0.54
1:A:151:SER:OG	1:A:179:LYS:NZ	2.39	0.54
1:D:761:ARG:O	1:D:764:PHE:HB2	2.08	0.54
1:B:79:ALA:HB3	1:B:95:PHE:HE1	1.72	0.54
1:B:144:LYS:HG2	1:B:171:ASP:HB2	1.90	0.54
1:C:353:HIS:ND1	1:C:362:GLU:OE2	2.41	0.54
1:C:790:ARG:NH2	1:C:791:CYS:SG	2.78	0.54
1:C:89:MET:HA	1:C:338:PRO:HG3	1.90	0.54
1:C:258:MET:H	1:C:379:THR:HB	1.73	0.54
1:C:525:ILE:O	1:C:739:THR:N	2.36	0.54
1:D:121:LEU:HA	1:D:367:SER:HB3	1.90	0.54
1:D:769:LEU:O	1:D:773:ASP:N	2.39	0.54
1:A:82:LEU:O	1:A:85:LEU:HB3	2.08	0.54
1:A:519:TYR:HB3	1:A:748:LYS:HB2	1.90	0.54
1:B:311:ALA:O	1:B:315:HIS:ND1	2.36	0.54
1:B:538:PHE:HB3	1:B:542:ASP:HB3	1.90	0.54
1:D:654:GLN:HE22	1:D:688:LEU:HD12	1.73	0.54
1:A:48:GLU:H	1:A:54:GLN:HE21	1.56	0.53
1:A:473:GLY:O	1:A:506:ARG:NH2	2.39	0.53
1:C:14:ALA:O	1:C:18:ASP:N	2.39	0.53
1:C:128:ARG:HH11	1:C:372:VAL:HG23	1.74	0.53
1:C:156:ARG:HA	1:D:155:ILE:HD11	1.90	0.53
1:D:73:SER:HA	1:D:96:VAL:HB	1.91	0.53
1:B:99:ASN:O	1:B:297:GLN:NE2	2.41	0.53
1:D:158:LEU:O	1:D:162:LEU:N	2.38	0.53
1:D:524:LEU:HD11	1:D:738:VAL:HB	1.90	0.53
1:B:164:GLN:O	1:B:168:LEU:N	2.36	0.53
1:C:11:GLU:HG2	1:C:49:ALA:HA	1.91	0.53
1:C:548:CYS:O	1:C:552:ALA:N	2.41	0.53
1:B:665:SER:H	1:B:668:TYR:HB3	1.73	0.53
1:B:733:ASP:O	1:B:790:ARG:NH1	2.41	0.53
1:D:488:LEU:O	1:D:755:GLN:NE2	2.42	0.53
1:D:671:PHE:HA	1:D:674:LYS:HB3	1.90	0.53
1:C:816:CYS:SG	1:C:817:ILE:N	2.82	0.53
1:D:543:PHE:HA	1:D:546:TRP:HB2	1.89	0.53
1:B:523:ILE:N	1:B:659:TYR:OH	2.39	0.53
1:A:164:GLN:OE1	1:A:167:ARG:NH1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:CYS:HA	1:B:95:PHE:HZ	1.74	0.52
1:A:12:GLU:HG2	1:A:49:ALA:HB2	1.91	0.52
1:B:376:ILE:HB	1:B:393:ALA:HB3	1.92	0.52
1:B:739:THR:HG23	1:B:793:LEU:HG	1.90	0.52
1:C:52:PRO:HB2	1:D:81:ALA:HB2	1.92	0.52
1:C:125:PRO:HG2	1:C:263:GLN:HG3	1.92	0.52
1:B:9:ILE:HA	1:B:45:LYS:HB2	1.91	0.52
1:B:363:PHE:HB3	1:B:367:SER:HA	1.92	0.52
1:C:778:ASP:OD2	1:C:782:GLN:NE2	2.42	0.52
1:A:106:THR:HA	1:A:157:GLY:HA3	1.92	0.52
1:A:209:LEU:HD11	1:A:235:TRP:HB3	1.90	0.52
1:C:163:ASP:OD2	1:D:149:TYR:OH	2.27	0.52
1:D:90:HIS:HB2	1:D:339:TRP:HB3	1.91	0.52
1:C:104:PRO:HG3	1:C:239:ASN:HA	1.91	0.52
1:C:92:PRO:HA	1:C:350:LYS:HE3	1.91	0.52
1:C:663:ARG:HB3	1:C:701:CYS:HB3	1.91	0.52
1:B:512:PHE:HA	1:B:753:ALA:HA	1.92	0.51
1:C:237:PHE:HD2	1:C:260:VAL:HG13	1.75	0.51
1:C:521:VAL:HG13	1:C:720:LEU:HD11	1.91	0.51
1:A:526:LYS:HA	1:A:738:VAL:HA	1.92	0.51
1:D:48:GLU:HB2	1:D:51:ASN:HD22	1.76	0.51
1:B:694:LYS:NZ	1:B:699:ASP:O	2.41	0.51
1:A:623:ILE:O	1:A:627:SER:OG	2.25	0.51
1:A:73:SER:HA	1:A:96:VAL:HB	1.92	0.51
1:B:231:LYS:HB3	1:B:383:GLU:HG3	1.93	0.51
1:D:251:VAL:HG11	1:D:379:THR:HG21	1.93	0.51
1:A:104:PRO:HG2	1:A:158:LEU:HD11	1.92	0.51
1:A:649:GLN:H	1:A:652:SER:HB2	1.75	0.51
1:B:20:VAL:HG11	1:B:300:ASN:HB3	1.91	0.51
1:B:206:ARG:HB2	1:B:206:ARG:CZ	2.39	0.51
1:B:434:GLU:HB3	1:B:442:ARG:CG	2.40	0.51
1:C:6:ILE:HG22	1:C:69:ALA:H	1.76	0.51
1:D:196:GLU:HA	1:D:199:ARG:HE	1.76	0.51
1:B:125:PRO:HG3	1:B:372:VAL:HB	1.93	0.50
1:B:501:THR:O	1:B:506:ARG:NH2	2.44	0.50
1:B:654:GLN:HE22	1:B:688:LEU:HD13	1.76	0.50
1:B:418:THR:HG22	1:B:461:LYS:HB2	1.94	0.50
1:D:261:VAL:HG13	1:D:376:ILE:HG13	1.93	0.50
1:A:50:ASN:O	1:B:113:SER:OG	2.28	0.50
1:A:623:ILE:O	1:A:626:SER:OG	2.23	0.50
1:A:681:GLN:NE2	1:C:690:ARG:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:HIS:HA	1:B:387:LYS:HE3	1.94	0.50
1:C:244:ASP:OD1	1:C:262:ARG:NH2	2.44	0.50
1:A:355:THR:HG22	1:A:360:VAL:HG22	1.92	0.50
1:A:810:SER:OG	1:A:811:PHE:N	2.45	0.50
1:C:139:GLU:O	1:C:141:ARG:NH1	2.44	0.50
1:A:148:PHE:N	1:A:208:ILE:O	2.44	0.50
1:A:174:LEU:HD21	1:B:162:LEU:HB3	1.94	0.50
1:D:476:LEU:HD13	1:D:478:ASN:HD22	1.76	0.50
1:A:12:GLU:N	1:A:12:GLU:OE2	2.44	0.49
1:A:710:ARG:O	1:A:714:LYS:N	2.45	0.49
1:B:164:GLN:HE21	1:B:168:LEU:HG	1.75	0.49
1:C:205:ARG:HD3	1:C:206:ARG:HG3	1.94	0.49
1:A:147:MET:N	1:A:173:SER:O	2.41	0.49
1:D:650:ASP:N	1:D:650:ASP:OD1	2.44	0.49
1:B:94:LEU:HA	1:B:121:LEU:HB2	1.94	0.49
1:C:657:MET:SD	1:C:657:MET:N	2.75	0.49
1:A:144:LYS:HA	1:A:171:ASP:HB3	1.93	0.49
1:A:534:ILE:HG23	1:A:812:ALA:HB3	1.94	0.49
1:C:159:GLN:HE21	1:D:155:ILE:HD13	1.77	0.49
1:C:631:ASN:ND2	1:D:629:THR:OG1	2.45	0.49
1:D:449:ASP:HB3	1:D:780:LEU:HD22	1.94	0.49
1:C:747:SER:O	1:D:772:GLN:NE2	2.45	0.49
1:D:22:GLN:HE21	1:D:44:ILE:HD12	1.78	0.49
1:B:165:ALA:O	1:B:170:LEU:N	2.46	0.49
1:B:421:VAL:O	1:B:465:TYR:N	2.46	0.49
1:C:156:ARG:HG2	1:D:155:ILE:HG13	1.95	0.49
1:C:43:SER:HB3	1:C:45:LYS:HE3	1.95	0.48
1:C:510:VAL:HA	1:C:756:HIS:HB2	1.95	0.48
1:C:12:GLU:HA	1:C:49:ALA:HB2	1.95	0.48
1:D:457:ALA:O	1:D:767:ARG:NH1	2.45	0.48
1:A:89:MET:HA	1:A:338:PRO:HA	1.94	0.48
1:B:534:ILE:O	1:B:537:LEU:HB3	2.13	0.48
1:C:11:GLU:HG3	1:C:47:ILE:HG13	1.95	0.48
1:C:149:TYR:HD2	1:C:153:TYR:HB3	1.78	0.48
1:C:560:ILE:HG13	1:C:611:ARG:HH11	1.77	0.48
1:A:519:TYR:O	1:A:747:SER:OG	2.32	0.48
1:B:681:GLN:HE22	1:B:686:ALA:H	1.62	0.48
1:C:11:GLU:HG3	1:C:47:ILE:CD1	2.44	0.48
1:C:63:MET:O	1:C:328:SER:OG	2.32	0.48
1:A:47:ILE:HD13	1:A:55:ALA:HB2	1.94	0.48
1:C:144:LYS:HG2	1:C:171:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:689:TRP:O	1:D:693:SER:N	2.47	0.48
1:A:72:THR:OG1	1:A:93:HIS:NE2	2.41	0.48
1:A:316:ARG:HH21	1:A:348:THR:HG22	1.78	0.48
1:D:396:ASP:OD1	1:D:396:ASP:N	2.45	0.48
1:C:31:ASN:O	1:C:279:HIS:ND1	2.43	0.48
1:A:442:ARG:HG2	1:A:444:LYS:NZ	2.29	0.48
1:C:506:ARG:HA	1:C:509:VAL:HG22	1.96	0.48
1:C:514:LYS:HZ2	1:D:514:LYS:HD3	1.79	0.48
1:D:164:GLN:O	1:D:168:LEU:HB2	2.14	0.48
1:B:74:THR:HG21	1:B:79:ALA:HB2	1.96	0.47
1:A:150:ASP:N	1:A:150:ASP:OD1	2.46	0.47
1:C:710:ARG:HH21	1:C:714:LYS:HE2	1.78	0.47
1:A:12:GLU:CG	1:A:49:ALA:HB2	2.44	0.47
1:B:623:ILE:O	1:B:627:SER:N	2.46	0.47
1:C:207:ALA:HB3	1:C:235:TRP:HA	1.97	0.47
1:C:769:LEU:HD11	1:D:748:LYS:HG2	1.95	0.47
1:A:135:ARG:HE	1:A:401:LEU:HD23	1.78	0.47
1:B:8:ALA:HB3	1:B:44:ILE:HA	1.96	0.47
1:D:283:SER:H	1:D:286:CYS:HB2	1.78	0.47
1:D:355:THR:HG22	1:D:360:VAL:HG22	1.96	0.47
1:A:244:ASP:HA	1:A:247:ILE:HD12	1.97	0.47
1:A:398:GLU:HG3	1:A:399:LYS:HG2	1.96	0.47
1:A:488:LEU:HA	1:A:755:GLN:HE21	1.80	0.47
1:C:525:ILE:HG13	1:C:739:THR:HG23	1.97	0.47
1:A:86:THR:HG21	1:A:93:HIS:HB2	1.96	0.47
1:A:771:LEU:O	1:A:776:ASP:N	2.44	0.47
1:B:122:ALA:HB3	1:B:368:SER:HA	1.95	0.47
1:C:86:THR:HG23	1:C:91:ILE:H	1.79	0.47
1:C:212:SER:O	1:C:216:ALA:N	2.46	0.47
1:C:508:SER:OG	1:D:766:GLN:NE2	2.47	0.47
1:C:521:VAL:HA	1:C:720:LEU:HD21	1.96	0.47
1:D:474:HIS:N	1:D:482:ASN:OD1	2.36	0.47
1:D:760:TYR:O	1:D:764:PHE:N	2.45	0.47
1:C:270:ASP:HA	1:C:273:LYS:HD3	1.95	0.47
1:D:114:PRO:HB2	1:D:117:GLU:HB2	1.96	0.47
1:D:502:ILE:HD11	1:D:751:GLY:H	1.79	0.47
1:B:511:ASP:OD1	1:B:761:ARG:NH1	2.47	0.47
1:C:200:TYR:O	1:C:204:LEU:HB2	2.14	0.46
1:C:631:ASN:HD21	1:D:626:SER:HA	1.81	0.46
1:D:12:GLU:HG2	1:D:99:ASN:HD21	1.79	0.46
1:A:207:ALA:O	1:A:236:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:NH2	1:B:143:GLN:OE1	2.48	0.46
1:B:526:LYS:H	1:B:713:LYS:HG3	1.79	0.46
1:C:128:ARG:HG3	1:C:372:VAL:CG2	2.45	0.46
1:C:694:LYS:HG3	1:C:699:ASP:HB3	1.97	0.46
1:D:269:LYS:HE2	1:D:288:PRO:HB3	1.97	0.46
1:B:681:GLN:HG3	1:B:683:SER:H	1.79	0.46
1:B:421:VAL:HG13	1:B:496:ALA:HA	1.98	0.46
1:C:241:GLU:HA	1:C:296:LEU:HD23	1.96	0.46
1:A:614:MET:HG3	1:D:824:LEU:HG	1.97	0.46
1:B:9:ILE:HD13	1:B:55:ALA:HB1	1.98	0.46
1:B:422:VAL:HG13	1:B:484:MET:HG3	1.97	0.46
1:B:811:PHE:HB3	1:C:541:PHE:HZ	1.79	0.46
1:B:623:ILE:N	1:B:623:ILE:CD1	2.78	0.46
1:D:434:GLU:HB2	1:D:442:ARG:HB3	1.97	0.46
1:A:665:SER:H	1:A:668:TYR:HB3	1.80	0.46
1:C:128:ARG:HG3	1:C:372:VAL:HG21	1.97	0.46
1:B:619:LEU:HA	1:B:622:LEU:HB3	1.96	0.45
1:A:332:ILE:HG21	1:B:60:CYS:HB3	1.98	0.45
1:B:12:GLU:O	1:B:14:ALA:N	2.49	0.45
1:B:207:ALA:HB3	1:B:235:TRP:HD1	1.82	0.45
1:B:293:LEU:HD12	1:B:296:LEU:HD12	1.98	0.45
1:B:543:PHE:H	1:B:546:TRP:HD1	1.65	0.45
1:D:661:THR:HB	1:D:720:LEU:HB3	1.97	0.45
1:D:202:ASP:OD1	1:D:205:ARG:NH2	2.48	0.45
1:D:542:ASP:OD1	1:D:542:ASP:N	2.50	0.45
1:D:731:LEU:HB2	1:D:785:TRP:HD1	1.81	0.45
1:B:244:ASP:OD1	1:B:262:ARG:NH1	2.49	0.45
1:B:649:GLN:HB2	1:B:652:SER:H	1.80	0.45
1:A:164:GLN:O	1:A:168:LEU:N	2.41	0.45
1:A:504:PRO:O	1:B:766:GLN:NE2	2.48	0.45
1:A:733:ASP:OD2	1:A:736:CYS:N	2.50	0.45
1:B:96:VAL:HG11	1:B:299:SER:HA	1.98	0.45
1:B:670:TYR:O	1:B:674:LYS:N	2.42	0.45
1:C:514:LYS:HA	1:D:514:LYS:HZ2	1.80	0.45
1:D:62:LEU:O	1:D:66:GLY:N	2.45	0.45
1:D:653:LYS:HD2	1:D:656:GLU:HB2	1.98	0.45
1:C:394:THR:O	1:C:402:ASN:N	2.50	0.45
1:A:268:ALA:HA	1:A:285:LEU:HD22	1.97	0.45
1:A:417:LEU:HB2	1:A:460:PHE:HB3	1.99	0.45
1:A:423:THR:O	1:A:467:ALA:N	2.49	0.45
1:A:521:VAL:H	1:A:745:ILE:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:VAL:HG13	1:B:559:LEU:HD23	1.99	0.45
1:C:27:ASP:HA	1:C:30:LEU:HB3	1.98	0.45
1:B:12:GLU:O	1:B:13:ASN:C	2.55	0.45
1:B:60:CYS:SG	1:B:330:ASN:ND2	2.90	0.45
1:C:11:GLU:HG3	1:C:47:ILE:CG1	2.46	0.45
1:C:166:SER:OG	1:D:174:LEU:O	2.34	0.45
1:C:486:GLY:HA2	1:C:489:ILE:HB	1.97	0.45
1:D:274:CYS:HB3	1:D:281:ILE:HB	1.99	0.45
1:A:653:LYS:HD2	1:A:656:GLU:CG	2.45	0.45
1:A:396:ASP:OD1	1:A:396:ASP:N	2.50	0.44
1:B:251:VAL:HG12	1:B:258:MET:HG2	1.99	0.44
1:C:83:GLN:HE22	1:C:110:LEU:HB3	1.82	0.44
1:C:293:LEU:C	1:C:293:LEU:HD13	2.38	0.44
1:A:687:GLU:OE1	1:A:690:ARG:NH1	2.50	0.44
1:C:520:SER:OG	1:C:743:ASN:O	2.28	0.44
1:D:93:HIS:O	1:D:121:LEU:N	2.48	0.44
1:A:710:ARG:HD2	1:A:713:LYS:HD3	1.99	0.44
1:C:128:ARG:HB3	1:C:395:TRP:CH2	2.49	0.44
1:C:329:LEU:HB2	1:C:336:THR:HB	1.97	0.44
1:A:147:MET:HA	1:A:208:ILE:HB	1.98	0.44
1:A:621:THR:OG1	1:A:622:LEU:N	2.50	0.44
1:A:831:LEU:HA	1:A:834:TRP:HB3	1.99	0.44
1:A:18:ASP:HA	1:A:21:PHE:HB3	2.00	0.44
1:A:318:LEU:O	1:A:321:ARG:NH2	2.38	0.44
1:B:443:TYR:HE2	1:B:464:ILE:HG21	1.83	0.44
1:A:332:ILE:HG22	1:B:57:GLN:HA	1.99	0.44
1:C:22:GLN:O	1:C:26:SER:HB3	2.17	0.44
1:B:189:PHE:HA	1:B:192:MET:HG2	1.99	0.44
1:D:792:ASP:OD1	1:D:792:ASP:N	2.51	0.44
1:C:312:ASN:ND2	1:C:353:HIS:O	2.51	0.44
1:C:453:ALA:HA	1:C:456:LYS:HE3	2.00	0.44
1:C:681:GLN:HE22	1:C:686:ALA:H	1.65	0.44
1:D:20:VAL:HG21	1:D:300:ASN:HB3	2.00	0.44
1:A:64:THR:HA	1:A:328:SER:HB3	1.98	0.44
1:C:188:LEU:O	1:C:192:MET:N	2.51	0.44
1:D:361:MET:HA	1:D:369:ASN:HD21	1.82	0.44
1:D:682:ASP:HB3	1:D:685:PHE:HB2	2.00	0.44
1:B:810:SER:OG	1:B:811:PHE:N	2.47	0.43
1:C:402:ASN:ND2	1:C:402:ASN:H	2.16	0.43
1:C:426:GLU:H	1:C:430:VAL:HB	1.83	0.43
1:C:761:ARG:NH1	1:C:765:SER:OG	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LEU:HD23	1:D:228:LEU:HD11	2.00	0.43
1:D:239:ASN:HB3	1:D:242:ILE:HB	2.00	0.43
1:B:165:ALA:HB1	1:B:170:LEU:HB2	2.00	0.43
1:B:661:THR:OG1	1:B:662:VAL:N	2.43	0.43
1:C:377:LEU:HG	1:C:391:LYS:HA	1.99	0.43
1:C:419:LEU:O	1:C:463:GLU:N	2.41	0.43
1:C:424:VAL:HG22	1:C:470:GLY:HA2	2.00	0.43
1:D:510:VAL:HG11	1:D:753:ALA:HB1	2.00	0.43
1:A:435:ASN:HA	1:A:441:LYS:H	1.83	0.43
1:C:137:VAL:HA	1:C:142:TRP:H	1.82	0.43
1:C:237:PHE:HB3	1:C:260:VAL:HG22	1.99	0.43
1:A:32:ASP:HB2	1:A:35:LEU:HB2	2.00	0.43
1:A:143:GLN:H	1:A:206:ARG:HH12	1.67	0.43
1:A:284:LEU:HD22	1:A:293:LEU:HD11	2.01	0.43
1:D:518:ASP:OD2	1:D:747:SER:N	2.51	0.43
1:A:524:LEU:HD11	1:A:738:VAL:HB	1.99	0.43
1:B:432:VAL:HG22	1:B:443:TYR:HE1	1.83	0.43
1:D:97:GLN:HB3	1:D:124:ARG:HD3	2.01	0.43
1:B:525:ILE:HG12	1:B:709:ILE:HA	1.99	0.43
1:C:402:ASN:H	1:C:402:ASN:HD22	1.66	0.43
1:A:201:ARG:HH11	1:A:228:LEU:HD23	1.84	0.43
1:D:708:GLY:HA2	1:D:711:LYS:HB2	2.00	0.43
1:A:2:SER:N	1:A:38:GLU:OE1	2.52	0.43
1:A:553:ILE:H	1:A:553:ILE:HG13	1.66	0.43
1:B:394:THR:HG23	1:B:402:ASN:HB2	2.00	0.43
1:B:721:TRP:CD1	1:B:725:VAL:HB	2.54	0.43
1:C:526:LYS:HA	1:C:738:VAL:HG12	2.00	0.43
1:D:106:THR:HG1	1:D:153:TYR:HH	1.58	0.43
1:C:444:LYS:HA	1:C:448:ILE:HG13	2.00	0.43
1:D:476:LEU:N	1:D:480:SER:O	2.44	0.43
1:D:524:LEU:HD22	1:D:726:VAL:HA	2.01	0.43
1:B:28:LEU:HB3	1:B:35:LEU:HD13	2.01	0.42
1:B:331:CYS:HA	1:B:336:THR:HG21	1.99	0.42
1:D:12:GLU:HB3	1:D:13:ASN:H	1.70	0.42
1:A:692:ILE:O	1:A:700:ASN:ND2	2.52	0.42
1:B:792:ASP:OD1	1:B:792:ASP:N	2.52	0.42
1:C:540:PRO:HD3	1:C:633:ALA:HB2	2.01	0.42
1:C:708:GLY:HA2	1:C:711:LYS:HB2	2.02	0.42
1:A:374:PHE:HB3	1:A:376:ILE:HD11	2.01	0.42
1:B:486:GLY:HA2	1:B:489:ILE:HD12	2.01	0.42
1:C:128:ARG:HG3	1:C:372:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:HH11	1:C:206:ARG:HG3	1.84	0.42
1:C:650:ASP:OD1	1:C:650:ASP:N	2.52	0.42
1:D:147:MET:HA	1:D:208:ILE:HB	2.02	0.42
1:D:476:LEU:HB3	1:D:478:ASN:H	1.84	0.42
1:D:18:ASP:HA	1:D:21:PHE:HB3	2.01	0.42
1:D:419:LEU:O	1:D:463:GLU:N	2.52	0.42
1:D:435:ASN:HA	1:D:440:PRO:HA	2.01	0.42
1:A:205:ARG:O	1:A:234:HIS:N	2.52	0.42
1:A:423:THR:N	1:A:465:TYR:O	2.49	0.42
1:A:518:ASP:OD2	1:B:515:ARG:NH2	2.51	0.42
1:B:816:CYS:SG	1:B:817:ILE:HG13	2.59	0.42
1:C:96:VAL:HG13	1:C:124:ARG:HD2	2.01	0.42
1:C:498:SER:OG	1:C:499:ALA:N	2.52	0.42
1:D:91:ILE:HD13	1:D:91:ILE:HA	1.93	0.42
1:B:86:THR:HB	1:B:91:ILE:HB	2.00	0.42
1:A:506:ARG:HA	1:A:509:VAL:HG22	2.00	0.42
1:B:103:SER:OG	1:B:152:GLU:OE1	2.30	0.42
1:C:515:ARG:HD3	1:C:518:ASP:HB3	2.02	0.42
1:D:11:GLU:OE1	1:D:74:THR:HA	2.19	0.42
1:A:74:THR:HG1	1:A:95:PHE:HE1	1.67	0.42
1:A:201:ARG:HA	1:A:204:LEU:HB2	2.01	0.42
1:A:491:LYS:HA	1:A:755:GLN:HE22	1.85	0.42
1:B:434:GLU:HB3	1:B:442:ARG:HG2	2.02	0.42
1:A:180:ASN:HD22	1:A:181:ILE:H	1.67	0.42
1:D:137:VAL:HG23	1:D:138:THR:HG23	2.02	0.42
1:B:527:LYS:HG3	1:B:737:SER:HB2	2.02	0.41
1:A:634:ALA:HB1	1:B:632:LEU:HD13	2.02	0.41
1:C:404:SER:OG	1:C:405:LEU:N	2.53	0.41
1:A:4:ILE:O	1:A:41:THR:N	2.39	0.41
1:B:532:ILE:HG13	1:C:541:PHE:HB2	2.02	0.41
1:D:228:LEU:HG	1:D:235:TRP:HH2	1.86	0.41
1:A:143:GLN:HA	1:A:170:LEU:HD22	2.03	0.41
1:A:242:ILE:O	1:A:262:ARG:NE	2.48	0.41
1:A:835:TRP:HA	1:A:838:ASN:HB2	2.03	0.41
1:C:128:ARG:NH1	1:C:372:VAL:HG23	2.34	0.41
1:C:781:LYS:O	1:C:785:TRP:N	2.39	0.41
1:D:96:VAL:HG22	1:D:123:SER:HB3	2.01	0.41
1:A:222:GLU:HA	1:A:225:GLU:HB2	2.02	0.41
1:A:669:GLU:HB3	1:A:672:ARG:HH11	1.86	0.41
1:C:453:ALA:HA	1:C:456:LYS:HG2	2.02	0.41
1:D:379:THR:HA	1:D:388:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PRO:HA	1:C:126:PRO:HD3	1.88	0.41
1:C:146:VAL:HB	1:C:173:SER:HB2	2.02	0.41
1:D:548:CYS:HA	1:D:551:ALA:HB3	2.02	0.41
1:B:8:ALA:O	1:B:45:LYS:N	2.52	0.41
1:B:469:ASP:HB2	1:B:483:GLY:HA3	2.03	0.41
1:C:327:ALA:HB3	1:C:339:TRP:CD1	2.56	0.41
1:A:631:ASN:HD21	1:D:633:ALA:HA	1.86	0.41
1:C:343:ARG:HA	1:C:346:LEU:HD12	2.03	0.41
1:C:421:VAL:N	1:C:463:GLU:O	2.40	0.41
1:D:815:PHE:HA	1:D:818:LEU:HB3	2.02	0.41
1:A:165:ALA:HB1	1:A:170:LEU:HB2	2.03	0.41
1:A:184:VAL:O	1:A:187:SER:OG	2.32	0.41
1:A:610:MET:SD	1:A:610:MET:N	2.89	0.41
1:B:64:THR:HA	1:B:329:LEU:H	1.85	0.41
1:C:50:ASN:HD22	1:D:112:PRO:HD2	1.85	0.41
1:C:519:TYR:N	1:C:748:LYS:O	2.53	0.41
1:A:164:GLN:HE21	1:A:168:LEU:HG	1.86	0.41
1:A:469:ASP:HB3	1:A:483:GLY:HA2	2.03	0.41
1:C:14:ALA:HA	1:C:17:ASP:HB2	2.02	0.41
1:D:706:SER:HA	1:D:709:ILE:HD12	2.01	0.41
1:D:782:GLN:HE22	1:D:787:HIS:HB3	1.86	0.41
1:A:57:GLN:HE22	1:B:332:ILE:HA	1.85	0.40
1:A:299:SER:HA	1:A:302:TYR:HD2	1.86	0.40
1:A:301:LEU:HA	1:A:304:TYR:HB3	2.03	0.40
1:B:514:LYS:HB2	1:B:768:ILE:HG21	2.03	0.40
1:C:104:PRO:HD2	1:C:210:LEU:HD23	2.01	0.40
1:C:421:VAL:O	1:C:465:TYR:N	2.35	0.40
1:C:521:VAL:HB	1:C:743:ASN:HB3	2.02	0.40
1:D:217:HIS:HA	1:D:220:ILE:HG22	2.03	0.40
1:D:471:ARG:O	1:D:474:HIS:NE2	2.54	0.40
1:D:778:ASP:O	1:D:782:GLN:HG2	2.21	0.40
1:B:11:GLU:CB	1:B:74:THR:HA	2.49	0.40
1:C:139:GLU:OE1	1:C:404:SER:OG	2.33	0.40
1:A:475:GLN:HE22	1:A:479:THR:HA	1.87	0.40
1:A:492:ARG:HE	1:A:492:ARG:HB2	1.66	0.40
1:A:504:PRO:HB3	1:B:770:GLU:HG2	2.04	0.40
1:A:543:PHE:HA	1:A:546:TRP:HB2	2.04	0.40
1:B:520:SER:H	1:B:722:ASP:HB2	1.86	0.40
1:C:158:LEU:HA	1:C:158:LEU:HD23	1.89	0.40
1:C:708:GLY:HA2	1:C:711:LYS:HD3	2.02	0.40
1:A:181:ILE:HD12	1:A:219:PHE:HD1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LEU:HD22	1:A:495:LEU:HA	1.95	0.40
1:A:622:LEU:HD21	1:B:620:PHE:HE2	1.87	0.40
1:B:834:TRP:O	1:B:837:SER:OG	2.30	0.40
1:D:731:LEU:HB2	1:D:785:TRP:CD1	2.57	0.40
1:A:11:GLU:O	1:A:98:ARG:NH2	2.55	0.40
1:A:690:ARG:HA	1:A:693:SER:HB2	2.03	0.40
1:B:21:PHE:HB2	1:B:303:LEU:HD21	2.04	0.40
1:B:490:SER:OG	1:B:492:ARG:HG3	2.22	0.40
1:C:613:VAL:O	1:C:616:SER:OG	2.38	0.40
1:D:491:LYS:HG2	1:D:755:GLN:HE22	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	741/856 (87%)	682 (92%)	59 (8%)	0	100	100
1	B	741/856 (87%)	671 (91%)	70 (9%)	0	100	100
1	C	741/856 (87%)	682 (92%)	59 (8%)	0	100	100
1	D	741/856 (87%)	686 (93%)	55 (7%)	0	100	100
All	All	2964/3424 (87%)	2721 (92%)	243 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	650/739 (88%)	633 (97%)	17 (3%)	46	66
1	B	650/739 (88%)	618 (95%)	32 (5%)	25	50
1	C	650/739 (88%)	635 (98%)	15 (2%)	50	70
1	D	650/739 (88%)	645 (99%)	5 (1%)	81	89
All	All	2600/2956 (88%)	2531 (97%)	69 (3%)	48	65

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	12	GLU
1	A	13	ASN
1	A	179	LYS
1	A	180	ASN
1	A	271	ASN
1	A	277	ASN
1	A	312	ASN
1	A	442	ARG
1	A	491	LYS
1	A	495	LEU
1	A	610	MET
1	A	617	TRP
1	A	631	ASN
1	A	657	MET
1	A	695	ASN
1	A	743	ASN
1	B	13	ASN
1	B	62	LEU
1	B	70	LEU
1	B	71	VAL
1	B	72	THR
1	B	154	ASP
1	B	204	LEU
1	B	205	ARG
1	B	206	ARG
1	B	227	ASN
1	B	262	ARG
1	B	277	ASN
1	B	278	ASN

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Mol	Chain	Res	Type
1	B	295	MET
1	B	312	ASN
1	B	334	LYS
1	B	369	ASN
1	B	441	LYS
1	B	443	TYR
1	B	560	ILE
1	B	623	ILE
1	B	626	SER
1	B	628	TYR
1	B	629	THR
1	B	655	LEU
1	B	657	MET
1	B	663	ARG
1	B	700	ASN
1	B	710	ARG
1	B	716	ASN
1	B	787	HIS
1	B	790	ARG
1	C	12	GLU
1	C	127	VAL
1	C	205	ARG
1	C	263	GLN
1	C	294	GLN
1	C	295	MET
1	C	382	SER
1	C	402	ASN
1	C	656	GLU
1	C	657	MET
1	C	663	ARG
1	C	677	ASN
1	C	710	ARG
1	C	761	ARG
1	C	790	ARG
1	D	12	GLU
1	D	257	ARG
1	D	277	ASN
1	D	677	ASN
1	D	761	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	54	GLN
1	A	57	GLN
1	A	180	ASN
1	A	214	GLN
1	A	221	ASN
1	A	271	ASN
1	A	277	ASN
1	A	289	GLN
1	A	312	ASN
1	A	324	HIS
1	A	475	GLN
1	A	631	ASN
1	A	695	ASN
1	A	700	ASN
1	A	743	ASN
1	A	755	GLN
1	B	13	ASN
1	B	164	GLN
1	B	221	ASN
1	B	227	ASN
1	B	277	ASN
1	B	278	ASN
1	B	312	ASN
1	B	330	ASN
1	B	369	ASN
1	B	654	GLN
1	B	681	GLN
1	B	700	ASN
1	B	716	ASN
1	B	772	GLN
1	C	31	ASN
1	C	50	ASN
1	C	111	ASN
1	C	263	GLN
1	C	402	ASN
1	C	631	ASN
1	C	681	GLN
1	D	22	GLN
1	D	31	ASN
1	D	50	ASN
1	D	51	ASN
1	D	130	ASN

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Mol	Chain	Res	Type
1	D	217	HIS
1	D	277	ASN
1	D	478	ASN
1	D	677	ASN
1	D	695	ASN
1	D	755	GLN
1	D	766	GLN
1	D	836	ASN

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 monosaccharides 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.