Full wwPDB EM Validation Report

Oct 28, 2024 – 01:28 PM JST

PDB ID	:	8JF7
EMDB ID	:	EMD-36209
Title	:	Triheteromeric NMDA receptor GluN1-GluN2A-GluN3A in complex with glycine, glutamate, a GluN1-specific Fab,and a GluN2A-specific Fab
Authors	:	Kou, Z.; Zhu, S.
Deposited on	:	2023-05-17
Resolution	:	7.73 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 ⓘ symbol.

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

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

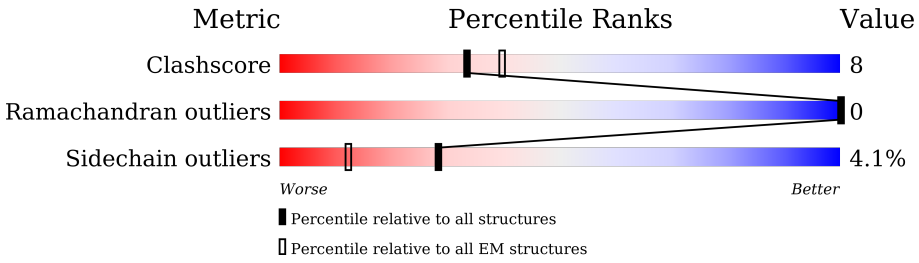
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 7.73 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	847	57% 19% • 23%
1	C	847	59% 18% • 22%
2	B	1116	43% 13% • 43%
3	D	1228	45% 12% • 42%
4	E	237	74% 26%
4	G	237	75% 24% •
5	F	217	81% 18% •
5	H	217	78% 21%
6	K	212	80% 20%

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Mol	Chain	Length	Quality of chain
7	J	227	79% 21%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31416 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, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	651	Total	C	N	O	S	0	0
			5169	3266	908	967	28		
1	C	657	Total	C	N	O	S	0	0
			5224	3300	919	977	28		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A,Enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	640	Total	C	N	O	S	0	0
			5063	3235	843	957	28		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	LYS	-	linker	UNP Q00959
B	844	SER	-	linker	UNP Q00959
B	845	ARG	-	linker	UNP Q00959
B	846	ALA	-	linker	UNP Q00959
B	847	GLU	-	linker	UNP Q00959
B	848	ALA	-	linker	UNP Q00959
B	849	LYS	-	linker	UNP Q00959
B	850	ARG	-	linker	UNP Q00959
B	851	MET	-	linker	UNP Q00959
B	852	LYS	-	linker	UNP Q00959
B	853	GLY	-	linker	UNP Q00959
B	854	LEU	-	linker	UNP Q00959
B	855	GLU	-	linker	UNP Q00959
B	856	VAL	-	linker	UNP Q00959
B	857	LEU	-	linker	UNP Q00959
B	858	PHE	-	linker	UNP Q00959
B	859	GLN	-	linker	UNP Q00959
B	860	GLY	-	linker	UNP Q00959

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Chain	Residue	Modelled	Actual	Comment	Reference
B	861	PRO	-	linker	UNP Q00959
B	862	ALA	-	linker	UNP Q00959
B	863	ALA	-	linker	UNP Q00959
B	864	ALA	-	linker	UNP Q00959
B	865	ALA	-	linker	UNP Q00959
B	866	VAL	-	linker	UNP Q00959
B	1071	LYS	ALA	conflict	UNP A0A7G8ZY66
B	1109	HIS	-	expression tag	UNP A0A7G8ZY66
B	1110	HIS	-	expression tag	UNP A0A7G8ZY66
B	1111	HIS	-	expression tag	UNP A0A7G8ZY66
B	1112	HIS	-	expression tag	UNP A0A7G8ZY66
B	1113	HIS	-	expression tag	UNP A0A7G8ZY66
B	1114	HIS	-	expression tag	UNP A0A7G8ZY66
B	1115	HIS	-	expression tag	UNP A0A7G8ZY66
B	1116	HIS	-	expression tag	UNP A0A7G8ZY66

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 3A,Enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	714	Total	C	N	O	S	0	0
			5643	3591	947	1068	37		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	927	GLU	GLY	conflict	UNP Q9R1M7
D	966	LEU	-	linker	UNP Q9R1M7
D	967	GLU	-	linker	UNP Q9R1M7
D	968	VAL	-	linker	UNP Q9R1M7
D	969	LEU	-	linker	UNP Q9R1M7
D	970	PHE	-	linker	UNP Q9R1M7
D	971	GLN	-	linker	UNP Q9R1M7
D	972	GLY	-	linker	UNP Q9R1M7
D	973	PRO	-	linker	UNP Q9R1M7
D	974	ALA	-	linker	UNP Q9R1M7
D	975	ALA	-	linker	UNP Q9R1M7
D	976	ALA	-	linker	UNP Q9R1M7
D	977	ALA	-	linker	UNP Q9R1M7
D	978	VAL	-	linker	UNP Q9R1M7
D	1183	LYS	ALA	conflict	UNP A0A7G8ZY66
D	1221	TRP	-	expression tag	UNP A0A7G8ZY66

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1222	SER	-	expression tag	UNP A0A7G8ZY66
D	1223	HIS	-	expression tag	UNP A0A7G8ZY66
D	1224	PRO	-	expression tag	UNP A0A7G8ZY66
D	1225	GLN	-	expression tag	UNP A0A7G8ZY66
D	1226	PHE	-	expression tag	UNP A0A7G8ZY66
D	1227	GLU	-	expression tag	UNP A0A7G8ZY66
D	1228	LYS	-	expression tag	UNP A0A7G8ZY66

- Molecule 4 is a protein called GluN1-specific antibody fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	237	Total	C	N	O	S	0	0
			1811	1132	303	370	6		
4	G	237	Total	C	N	O	S	0	0
			1811	1132	303	370	6		

- Molecule 5 is a protein called GluN1-specific antibody fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	217	Total	C	N	O	S	0	0
			1651	1047	267	331	6		
5	H	217	Total	C	N	O	S	0	0
			1651	1047	267	331	6		

- Molecule 6 is a protein called GluN2A-specific antibody fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	212	Total	C	N	O	S	0	0
			1636	1025	274	332	5		

- Molecule 7 is a protein called GluN2A-specific antibody fragment heavy chain.

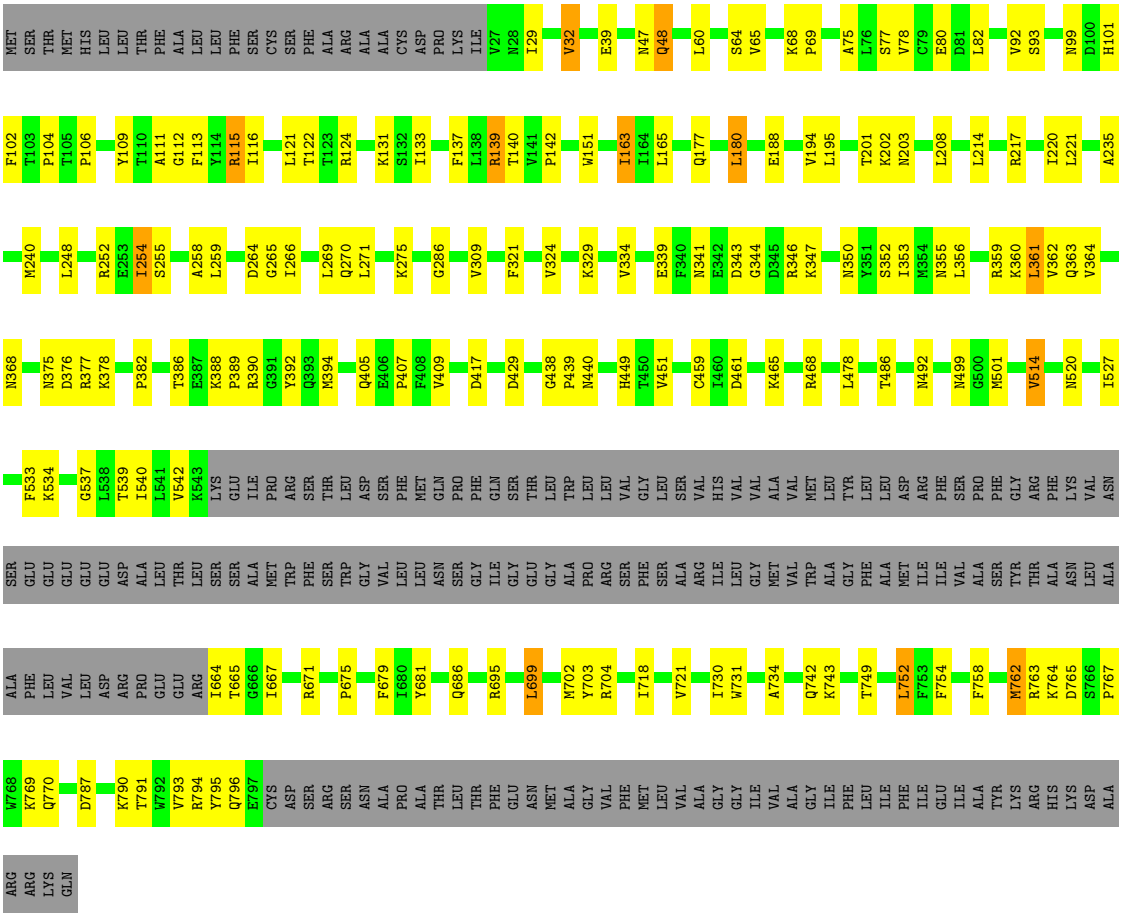
Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	227	Total	C	N	O	S	0	0
			1757	1110	297	345	5		

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.

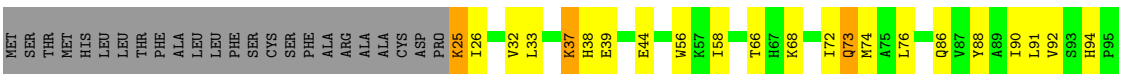
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

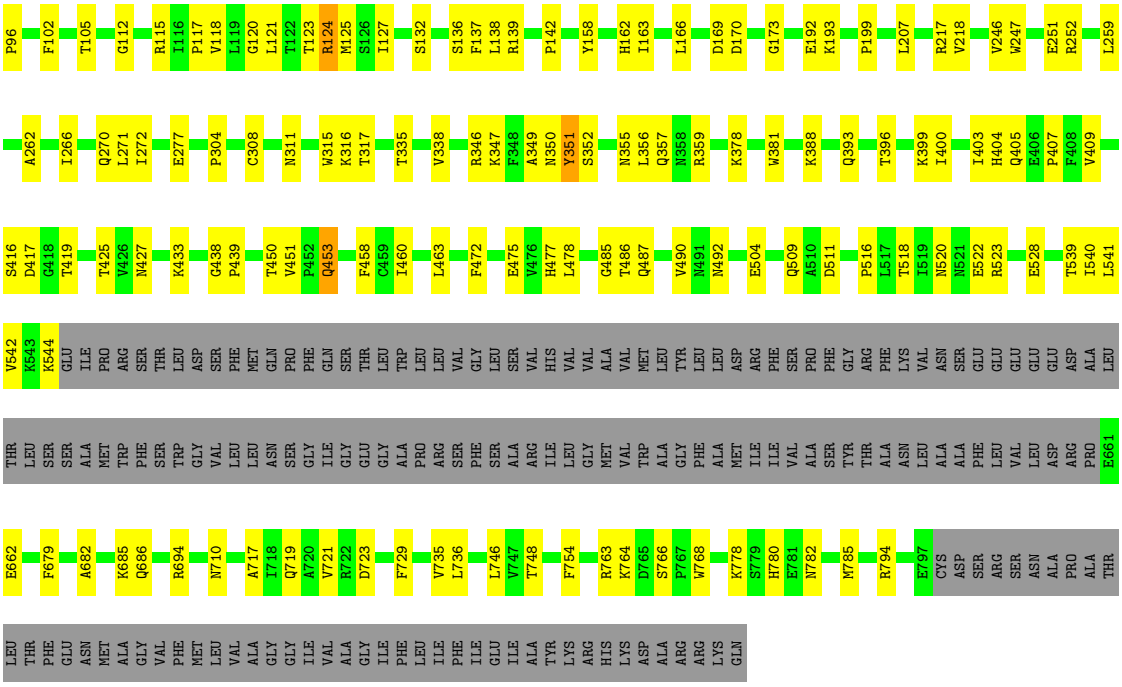
Chain A:



- Molecule 1: Glutamate receptor ionotropic, NMDA 1

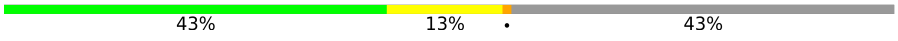
Chain C:

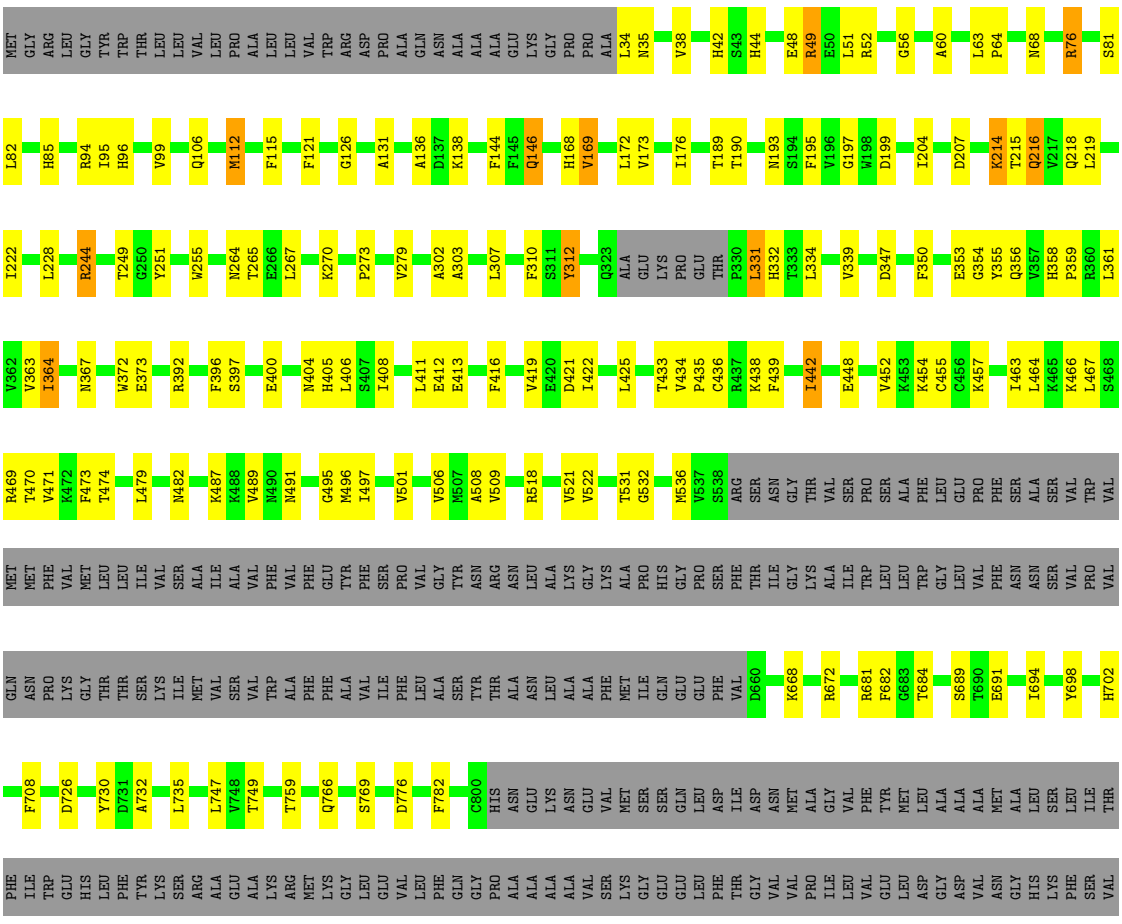


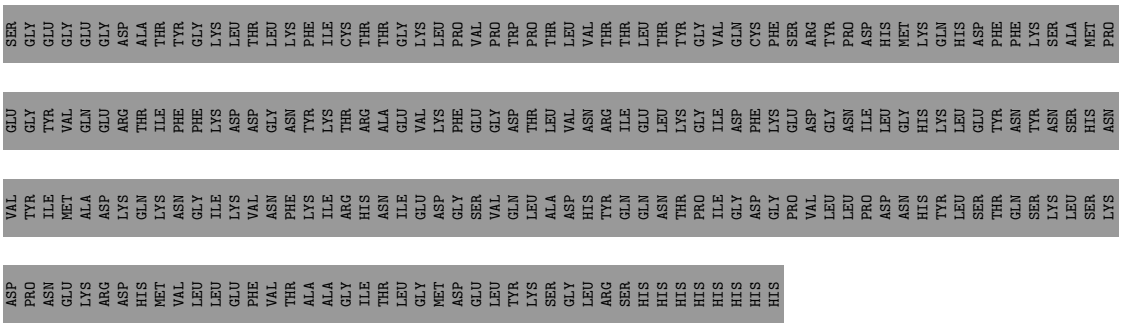


• Molecule 2: Glutamate receptor ionotropic, NMDA 2A,Enhanced green fluorescent protein

Chain B:

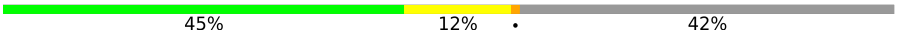


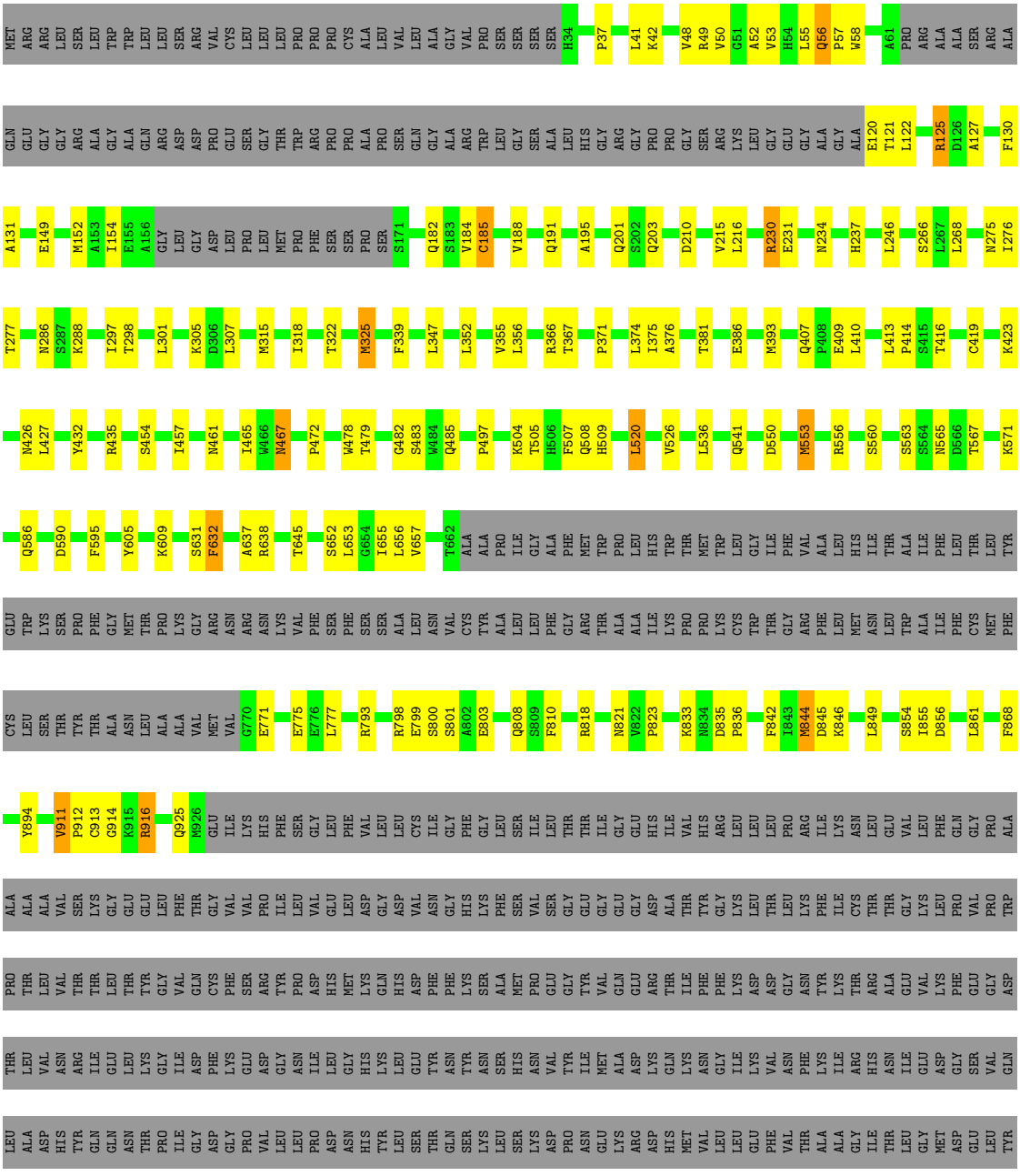




• Molecule 3: Glutamate receptor ionotropic, NMDA 3A,Enhanced green fluorescent protein

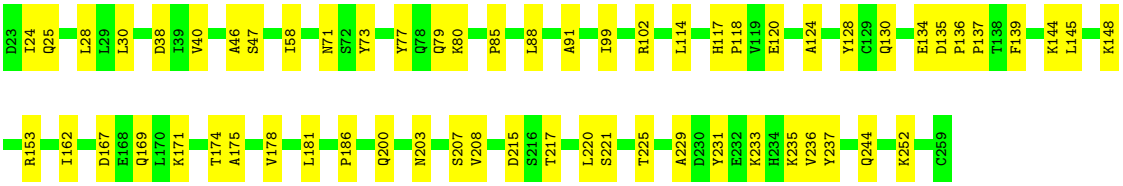
Chain D:





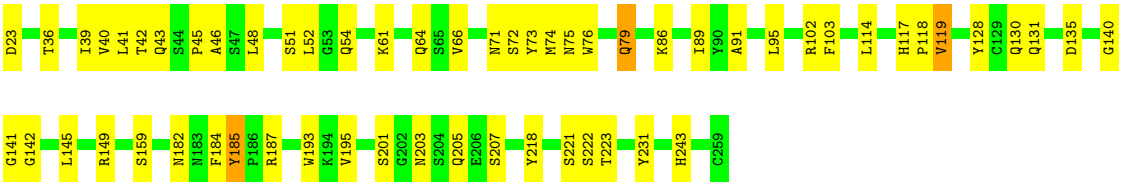
• Molecule 4: GluN1-specific antibody fragment light chain

Chain E:



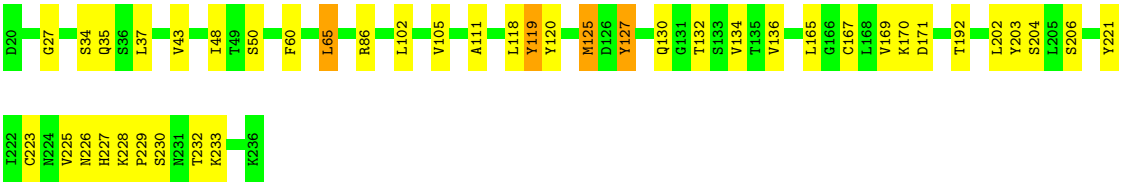
• Molecule 4: GluN1-specific antibody fragment light chain

Chain G:



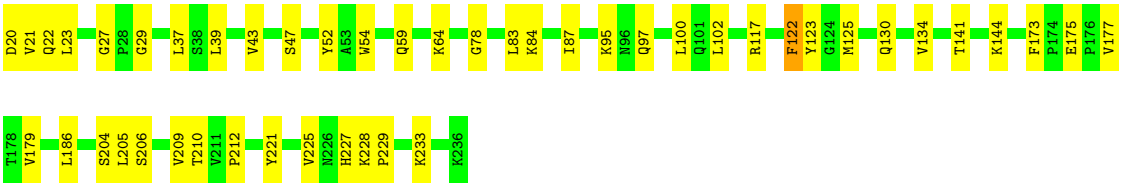
• Molecule 5: GluN1-specific antibody fragment heavy chain

Chain F:



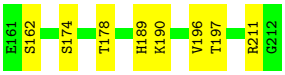
• Molecule 5: GluN1-specific antibody fragment heavy chain

Chain H:



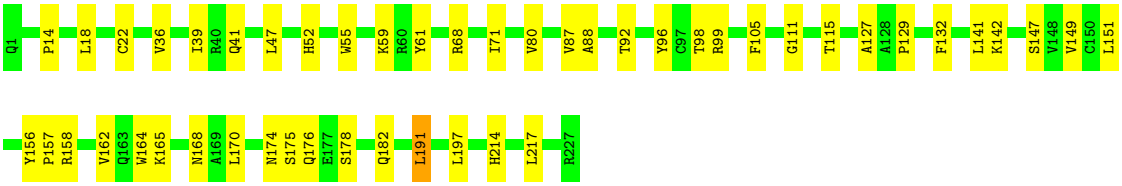
• Molecule 6: GluN2A-specific antibody fragment light chain

Chain K:



• Molecule 7: GluN2A-specific antibody fragment heavy chain

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162395	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (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	0.24	0/5282	0.40	0/7152
1	C	0.24	0/5337	0.39	0/7223
2	B	0.24	0/5176	0.40	0/7021
3	D	0.24	0/5779	0.40	0/7853
4	E	0.24	0/1852	0.44	0/2520
4	G	0.24	0/1852	0.43	0/2520
5	F	0.24	0/1695	0.45	0/2314
5	H	0.24	0/1695	0.45	0/2314
6	K	0.24	0/1673	0.42	0/2271
7	J	0.24	0/1799	0.45	0/2446
All	All	0.24	0/32140	0.41	0/43634

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

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	5169	0	5124	89	0
1	C	5224	0	5186	90	0
2	B	5063	0	4995	91	0
3	D	5643	0	5515	85	0
4	E	1811	0	1739	38	0
4	G	1811	0	1737	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1651	0	1596	25	0
5	H	1651	0	1596	29	0
6	K	1636	0	1576	24	0
7	J	1757	0	1725	27	0
All	All	31416	0	30789	502	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 8.

All (502) 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:490:VAL:HG13	1:C:492:ASN:H	1.59	0.67
2:B:172:LEU:HA	2:B:228:LEU:HB2	1.76	0.66
2:B:364:ILE:HG13	2:B:372:TRP:HB3	1.76	0.66
1:A:459:CYS:HB2	1:A:514:VAL:HB	1.77	0.65
1:A:355:ASN:H	1:A:363:GLN:HA	1.62	0.64
4:G:102:ARG:HB3	4:G:118:PRO:HG2	1.78	0.64
4:E:88:LEU:HA	4:E:99:ILE:HG13	1.80	0.64
1:C:72:ILE:HD11	3:D:419:CYS:HB3	1.80	0.63
1:C:338:VAL:HB	1:C:347:LYS:HE3	1.79	0.63
1:A:762:MET:SD	1:A:763:ARG:N	2.72	0.62
2:B:81:SER:O	2:B:85:HIS:ND1	2.33	0.62
1:C:405:GLN:HE22	1:C:516:PRO:HD2	1.64	0.61
2:B:411:LEU:HD23	2:B:496:MET:HB3	1.81	0.61
4:G:75:ASN:HB2	4:G:130:GLN:HB3	1.81	0.61
1:A:355:ASN:HB3	1:A:362:VAL:HG23	1.81	0.61
5:H:141:THR:O	5:H:144:LYS:NZ	2.34	0.61
3:D:520:LEU:HD21	3:D:631:SER:HB3	1.82	0.61
1:A:266:ILE:HD11	1:A:356:LEU:HD12	1.83	0.60
1:A:78:VAL:HG13	1:A:82:LEU:HD12	1.83	0.60
1:A:790:LYS:HA	1:A:794:ARG:HG3	1.82	0.60
3:D:325:MET:SD	3:D:325:MET:N	2.74	0.60
3:D:472:PRO:HG3	3:D:508:GLN:HG2	1.83	0.60
3:D:55:LEU:HD22	3:D:125:ARG:HH12	1.65	0.60
5:H:47:SER:O	5:H:117:ARG:NH2	2.32	0.60
1:A:378:LYS:NZ	1:A:386:THR:O	2.35	0.59
1:A:742:GLN:HG3	1:A:743:LYS:HG2	1.84	0.59
2:B:138:LYS:HD2	2:B:353:GLU:HB2	1.84	0.59
1:C:251:GLU:HB3	1:C:271:LEU:HG	1.84	0.59
3:D:297:ILE:HG23	3:D:298:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ASN:HD21	1:C:523:ARG:HH11	1.51	0.59
2:B:35:ASN:HD21	2:B:96:HIS:H	1.50	0.59
1:C:778:LYS:O	1:C:782:ASN:ND2	2.35	0.59
1:C:66:THR:OG1	1:C:68:LYS:NZ	2.35	0.59
3:D:541:GLN:NE2	3:D:595:PHE:O	2.35	0.58
1:A:375:ASN:ND2	1:A:377:ARG:O	2.36	0.58
4:E:71:ASN:ND2	4:E:91:ALA:O	2.36	0.58
5:H:175:GLU:HG3	5:H:205:LEU:HD13	1.84	0.58
1:C:56:TRP:HD1	1:C:58:ILE:HG23	1.67	0.58
1:C:541:LEU:HD21	1:C:746:LEU:HD13	1.84	0.58
1:A:142:PRO:HG3	1:A:346:ARG:HG2	1.86	0.58
4:E:25:GLN:NE2	4:E:139:PHE:O	2.37	0.58
2:B:408:ILE:HG21	2:B:509:VAL:HG13	1.86	0.57
3:D:56:GLN:NE2	3:D:57:PRO:O	2.37	0.57
5:F:37:LEU:HB3	5:F:102:LEU:HB3	1.86	0.57
3:D:556:ARG:NH1	3:D:560:SER:OG	2.37	0.57
4:E:200:GLN:HG2	5:F:119:TYR:H	1.70	0.57
1:A:92:VAL:HG11	1:A:104:PRO:HB3	1.85	0.57
2:B:214:LYS:HD3	2:B:215:THR:HG23	1.86	0.57
1:C:112:GLY:HA2	1:C:136:SER:HB3	1.85	0.57
1:A:438:GLY:HA3	1:A:478:LEU:HB3	1.84	0.57
1:A:208:LEU:HD13	1:A:240:MET:HG3	1.85	0.57
1:A:177:GLN:NE2	1:A:194:VAL:O	2.38	0.57
1:A:112:GLY:O	1:A:115:ARG:NH2	2.38	0.57
2:B:434:VAL:HG21	2:B:464:LEU:HD11	1.86	0.57
1:C:218:VAL:HA	1:C:246:VAL:HB	1.86	0.57
7:J:165:LYS:HB3	7:J:168:ASN:HB2	1.87	0.57
6:K:86:TYR:HB2	6:K:102:THR:HB	1.87	0.57
1:A:394:MET:SD	1:A:394:MET:N	2.77	0.56
5:H:29:GLY:HA2	5:H:134:VAL:HG22	1.87	0.56
2:B:487:LYS:HG3	2:B:489:VAL:HG22	1.87	0.56
3:D:381:THR:OG1	3:D:461:ASN:ND2	2.38	0.56
4:G:45:PRO:O	4:G:187:ARG:NH1	2.38	0.56
4:E:134:GLU:HG3	4:E:136:PRO:HD2	1.86	0.56
2:B:189:THR:O	2:B:193:ASN:ND2	2.39	0.56
1:A:264:ASP:OD1	1:A:359:ARG:NH2	2.39	0.56
4:G:203:ASN:N	5:H:125:MET:SD	2.79	0.56
5:H:39:LEU:HB3	5:H:100:LEU:HD13	1.87	0.56
6:K:160:GLN:HB3	7:J:182:GLN:HG2	1.88	0.56
2:B:303:ALA:O	2:B:307:LEU:HB2	2.06	0.56
5:F:167:CYS:HB3	5:F:223:CYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:ARG:NH1	2:B:470:THR:OG1	2.38	0.56
1:A:270:GLN:OE1	1:A:352:SER:OG	2.23	0.55
3:D:798:ARG:HH12	3:D:823:PRO:HA	1.71	0.55
5:H:78:GLY:HA3	5:H:84:LYS:HD2	1.88	0.55
1:A:796:GLN:NE2	3:D:771:GLU:OE1	2.39	0.55
1:C:166:LEU:HD11	1:C:207:LEU:HB3	1.88	0.55
1:C:539:THR:HG23	1:C:736:LEU:HD12	1.88	0.55
7:J:22:CYS:HB3	7:J:80:VAL:HB	1.88	0.55
1:A:201:THR:OG1	1:A:203:ASN:ND2	2.39	0.55
2:B:279:VAL:HG13	2:B:363:VAL:HG22	1.88	0.55
2:B:766:GLN:HB3	2:B:769:SER:HB2	1.87	0.55
1:C:487:GLN:H	1:C:694:ARG:HH12	1.54	0.55
4:G:71:ASN:ND2	4:G:91:ALA:O	2.39	0.55
7:J:132:PHE:HB2	7:J:151:LEU:HB3	1.88	0.55
7:J:157:PRO:HB2	7:J:214:HIS:HE2	1.72	0.55
1:A:527:ILE:HA	1:A:764:LYS:HB2	1.88	0.55
1:A:439:PRO:HA	1:A:449:HIS:HB2	1.87	0.55
1:C:472:PHE:HB3	1:C:768:TRP:HZ3	1.72	0.55
1:C:217:ARG:HE	1:C:393:GLN:HE21	1.53	0.55
1:C:541:LEU:HD11	1:C:746:LEU:HB3	1.89	0.55
1:A:131:LYS:NZ	1:A:343:ASP:O	2.39	0.55
2:B:350:PHE:HB3	2:B:354:GLY:HA2	1.88	0.55
1:C:405:GLN:O	1:C:409:VAL:N	2.33	0.55
3:D:230:ARG:NH2	3:D:237:HIS:O	2.39	0.55
1:A:539:THR:HB	1:A:752:LEU:HB3	1.87	0.55
1:A:361:LEU:O	1:A:377:ARG:NH2	2.39	0.54
1:C:132:SER:HB3	3:D:231:GLU:HB2	1.90	0.54
1:C:685:LYS:HB2	1:C:710:ASN:HB3	1.89	0.54
2:B:501:VAL:HG13	2:B:521:VAL:HG11	1.88	0.54
3:D:266:SER:HB2	3:D:325:MET:HA	1.87	0.54
3:D:854:SER:HB2	3:D:911:VAL:HG12	1.90	0.54
4:E:174:THR:HA	4:E:225:THR:HG23	1.89	0.54
4:E:178:VAL:HG13	4:E:221:SER:HA	1.89	0.54
5:F:227:HIS:HB2	5:F:232:THR:H	1.72	0.54
1:C:92:VAL:H	1:C:120:GLY:HA3	1.72	0.54
1:A:265:GLY:HA3	1:A:382:PRO:HG3	1.90	0.54
2:B:146:GLN:NE2	2:B:354:GLY:O	2.40	0.54
2:B:747:LEU:HD23	2:B:747:LEU:H	1.71	0.54
3:D:347:LEU:HD13	3:D:352:LEU:HD22	1.89	0.54
4:E:24:ILE:HD12	5:F:170:LYS:HD3	1.90	0.54
4:E:38:ASP:O	5:F:204:SER:OG	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:235:LYS:HG2	4:E:236:VAL:HG13	1.90	0.54
2:B:536:MET:HB2	2:B:735:LEU:HD13	1.90	0.54
1:C:123:THR:O	1:C:139:ARG:NH2	2.41	0.54
1:C:125:MET:HG2	1:C:127:ILE:HG22	1.90	0.54
1:C:169:ASP:HB3	1:C:173:GLY:H	1.71	0.53
3:D:185:CYS:HA	3:D:188:VAL:HG12	1.90	0.53
1:A:29:ILE:HG21	1:A:60:LEU:HD12	1.90	0.53
1:A:355:ASN:HB2	1:A:364:VAL:HG13	1.90	0.53
4:G:201:SER:HB3	5:H:130:GLN:HE21	1.74	0.53
1:A:235:ALA:HB1	1:A:240:MET:HB2	1.90	0.53
1:A:388:LYS:HD2	1:A:389:PRO:HD2	1.90	0.53
1:C:685:LYS:HG2	1:C:686:GLN:HG3	1.89	0.53
4:G:42:THR:O	4:G:61:LYS:NZ	2.41	0.53
2:B:491:ASN:HB2	6:K:52:THR:HG21	1.91	0.53
3:D:426:ASN:HD22	3:D:427:LEU:HD23	1.74	0.53
5:F:171:ASP:HA	5:F:202:LEU:HD12	1.91	0.53
1:C:721:VAL:HG11	1:C:729:PHE:HB2	1.91	0.53
3:D:49:ARG:NH1	3:D:191:GLN:OE1	2.41	0.53
2:B:219:LEU:HD13	2:B:222:ILE:HD12	1.89	0.53
1:A:140:THR:O	1:A:346:ARG:NH2	2.42	0.53
2:B:244:ARG:NH1	2:B:397:SER:OG	2.41	0.53
2:B:273:PRO:HB2	2:B:396:PHE:HB3	1.91	0.53
5:H:175:GLU:HA	5:H:205:LEU:HD22	1.90	0.53
3:D:371:PRO:HD2	3:D:374:LEU:HD13	1.91	0.53
6:K:160:GLN:HB2	6:K:178:THR:HB	1.90	0.53
1:C:763:ARG:HB2	1:C:766:SER:HB3	1.91	0.52
4:G:39:ILE:HD12	4:G:141:GLY:HA2	1.91	0.52
3:D:52:ALA:HB3	3:D:152:MET:HA	1.90	0.52
4:E:169:GLN:HB3	4:E:175:ALA:HA	1.91	0.52
2:B:94:ARG:NH1	2:B:312:TYR:OH	2.40	0.52
1:C:346:ARG:HD3	1:C:349:ALA:HB2	1.91	0.52
1:A:47:ASN:ND2	1:A:48:GLN:OE1	2.43	0.52
4:G:40:VAL:HG13	5:H:204:SER:HB2	1.92	0.52
7:J:170:LEU:O	7:J:174:ASN:ND2	2.36	0.52
1:C:117:PRO:HB3	1:C:138:LEU:HB2	1.92	0.52
7:J:127:ALA:HA	7:J:156:TYR:H	1.74	0.52
6:K:46:LEU:HD21	6:K:49:TYR:HB3	1.91	0.52
3:D:246:LEU:HD13	3:D:275:ASN:HB2	1.92	0.52
1:C:407:PRO:HG3	1:C:735:VAL:HG13	1.90	0.52
3:D:407:GLN:HB3	3:D:410:LEU:HB2	1.91	0.52
2:B:413:GLU:HB2	2:B:416:PHE:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:52:LEU:HG	4:G:119:VAL:HB	1.92	0.52
3:D:127:ALA:HA	3:D:386:GLU:HG3	1.91	0.52
1:A:665:THR:HG23	1:A:749:THR:HG21	1.92	0.51
3:D:632:PHE:HE1	3:D:638:ARG:HH11	1.57	0.51
5:H:177:VAL:HA	5:H:228:LYS:HE2	1.92	0.51
1:C:416:SER:HB2	1:C:419:THR:HB	1.91	0.51
3:D:56:GLN:O	3:D:201:GLN:NE2	2.43	0.51
1:A:429:ASP:HB3	1:A:791:THR:HG21	1.93	0.51
1:A:537:GLY:H	1:A:758:PHE:HE1	1.58	0.51
1:C:33:LEU:HD13	1:C:39:GLU:HA	1.92	0.51
1:C:451:VAL:O	1:C:453:GLN:NE2	2.44	0.51
1:C:68:LYS:HB2	1:C:74:MET:HB2	1.93	0.51
3:D:37:PRO:HB3	3:D:409:GLU:HG3	1.92	0.51
4:G:203:ASN:HD21	5:H:122:PHE:HE1	1.58	0.51
1:C:262:ALA:O	1:C:359:ARG:NH2	2.44	0.51
1:C:335:THR:OG1	1:C:350:ASN:ND2	2.39	0.51
4:E:73:TYR:HA	4:E:91:ALA:HA	1.92	0.51
6:K:21:ILE:HD12	6:K:73:LEU:HD23	1.93	0.51
1:A:407:PRO:HD3	1:A:731:TRP:HE1	1.74	0.51
1:A:533:PHE:HD1	1:A:534:LYS:HG2	1.76	0.51
2:B:482:ASN:HB3	2:B:495:GLY:HA2	1.92	0.51
1:A:93:SER:HA	1:A:122:THR:HB	1.93	0.51
1:C:308:CYS:SG	1:C:311:ASN:ND2	2.84	0.51
4:E:30:LEU:HD21	4:E:208:VAL:HG21	1.93	0.51
1:A:346:ARG:HE	1:A:347:LYS:H	1.56	0.51
1:C:90:ILE:HB	1:C:118:VAL:HA	1.93	0.51
4:G:185:TYR:H	4:G:243:HIS:HD2	1.59	0.51
7:J:61:TYR:HE1	7:J:71:ILE:HG22	1.76	0.51
1:A:360:LYS:HZ2	4:E:235:LYS:HD2	1.75	0.50
3:D:356:LEU:HB2	3:D:376:ALA:HA	1.93	0.50
4:G:76:TRP:HB2	4:G:89:ILE:HB	1.93	0.50
2:B:422:ILE:HB	2:B:454:LYS:HA	1.93	0.50
1:A:121:LEU:HD23	1:A:121:LEU:H	1.77	0.50
4:E:102:ARG:NH2	4:E:120:GLU:OE2	2.45	0.50
1:A:39:GLU:OE2	1:A:64:SER:OG	2.29	0.50
1:A:68:LYS:HZ3	1:A:69:PRO:HD2	1.77	0.50
1:A:113:PHE:HE1	2:B:106:GLN:HE21	1.59	0.50
3:D:844:MET:SD	3:D:845:ASP:N	2.71	0.50
4:E:47:SER:OG	4:E:144:LYS:O	2.29	0.50
5:H:87:ILE:HG21	5:H:102:LEU:HD23	1.93	0.50
1:C:403:ILE:HG12	1:C:404:HIS:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:79:GLN:HG2	4:E:85:PRO:HB3	1.93	0.50
4:G:195:VAL:HG11	5:H:123:TYR:HB3	1.92	0.50
4:E:28:LEU:HD23	4:E:28:LEU:H	1.75	0.50
2:B:691:GLU:HB3	2:B:702:HIS:HE1	1.77	0.50
2:B:190:THR:HA	2:B:193:ASN:HD21	1.76	0.49
1:C:38:HIS:NE2	1:C:277:GLU:OE1	2.44	0.49
3:D:497:PRO:HB3	3:D:507:PHE:HB2	1.93	0.49
4:E:40:VAL:HG12	5:F:206:SER:HB2	1.94	0.49
7:J:14:PRO:HB3	7:J:88:ALA:HA	1.94	0.49
5:F:102:LEU:HD22	5:F:105:VAL:HG22	1.94	0.49
6:K:145:LYS:HB3	6:K:197:THR:HB	1.94	0.49
1:C:112:GLY:O	1:C:115:ARG:NH1	2.44	0.49
3:D:653:LEU:O	3:D:846:LYS:NZ	2.45	0.49
2:B:694:ILE:O	2:B:698:TYR:N	2.42	0.49
1:C:25:LYS:HD3	1:C:26:ILE:HG23	1.94	0.49
6:K:30:TYR:HE2	6:K:33:LEU:HB2	1.77	0.49
6:K:162:SER:HB2	7:J:182:GLN:HB2	1.94	0.49
1:C:486:THR:HG23	1:C:686:GLN:HG2	1.94	0.49
6:K:189:HIS:O	6:K:211:ARG:NH1	2.46	0.49
1:A:254:ILE:HA	1:A:258:ALA:HB3	1.95	0.49
3:D:55:LEU:HD12	3:D:154:ILE:HB	1.94	0.49
1:C:528:GLU:OE2	1:C:764:LYS:NZ	2.42	0.49
1:C:541:LEU:HB2	1:C:736:LEU:HD22	1.95	0.49
2:B:347:ASP:HB2	2:B:358:HIS:HB2	1.94	0.49
3:D:563:SER:OG	3:D:565:ASN:OD1	2.25	0.49
3:D:656:LEU:HD11	3:D:861:LEU:HB3	1.94	0.48
1:C:169:ASP:HA	1:C:199:PRO:HG3	1.95	0.48
1:C:438:GLY:HA3	1:C:478:LEU:HB3	1.95	0.48
6:K:61:ARG:HB2	6:K:76:ASN:HB2	1.94	0.48
1:A:376:ASP:OD1	1:A:376:ASP:N	2.46	0.48
2:B:42:HIS:HD2	2:B:44:HIS:HB3	1.79	0.48
3:D:210:ASP:OD1	3:D:234:ASN:ND2	2.46	0.48
4:E:124:ALA:HA	4:E:145:LEU:HB2	1.96	0.48
2:B:463:ILE:HA	2:B:466:LYS:HE3	1.95	0.48
6:K:1:ASP:OD1	6:K:3:GLN:NE2	2.46	0.48
1:A:363:GLN:HG2	1:A:377:ARG:HE	1.79	0.48
4:E:167:ASP:OD2	4:E:171:LYS:NZ	2.40	0.48
5:H:186:LEU:O	5:H:221:TYR:OH	2.31	0.48
3:D:550:ASP:HB3	3:D:553:MET:HB2	1.94	0.48
3:D:560:SER:HB3	3:D:565:ASN:HD21	1.77	0.48
4:G:205:GLN:HB3	4:G:222:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HB	2:B:76:ARG:HG2	1.96	0.48
3:D:301:LEU:HD13	3:D:307:LEU:HA	1.96	0.48
3:D:413:LEU:HD12	3:D:414:PRO:HD2	1.94	0.48
4:G:73:TYR:HA	4:G:91:ALA:HA	1.95	0.48
7:J:18:LEU:HD23	7:J:87:VAL:HG11	1.95	0.48
2:B:396:PHE:N	2:B:400:GLU:OE1	2.44	0.48
3:D:315:MET:HA	3:D:318:ILE:HG12	1.96	0.48
3:D:586:GLN:NE2	3:D:590:ASP:OD2	2.47	0.48
4:G:23:ASP:N	4:G:135:ASP:OD2	2.46	0.48
4:G:46:ALA:HA	4:G:187:ARG:HG3	1.96	0.48
2:B:168:HIS:ND1	2:B:197:GLY:O	2.47	0.48
2:B:48:GLU:O	2:B:52:ARG:NH1	2.45	0.47
4:E:46:ALA:HB3	4:E:148:LYS:HE3	1.96	0.47
4:E:58:ILE:HB	4:E:114:LEU:HD23	1.96	0.47
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.96	0.47
5:H:23:LEU:HG	5:H:117:ARG:HG3	1.95	0.47
4:G:159:SER:HB3	4:G:182:ASN:HB2	1.96	0.47
1:C:542:VAL:H	1:C:748:THR:HA	1.80	0.47
3:D:652:SER:OG	3:D:868:PHE:O	2.31	0.47
5:F:65:LEU:HD23	5:F:65:LEU:H	1.79	0.47
1:A:165:LEU:HD21	1:A:180:LEU:HG	1.96	0.47
1:A:329:LYS:HE3	1:A:339:GLU:H	1.79	0.47
1:A:341:ASN:OD1	1:A:344:GLY:N	2.47	0.47
2:B:169:VAL:HA	2:B:199:ASP:HB3	1.96	0.47
3:D:215:VAL:HG13	3:D:216:LEU:HG	1.96	0.47
4:E:229:ALA:O	4:E:233:LYS:HG2	2.14	0.47
7:J:41:GLN:HB2	7:J:47:LEU:HG	1.96	0.47
1:C:439:PRO:HD3	1:C:450:THR:HG22	1.95	0.47
4:E:181:LEU:HD22	4:E:220:LEU:HD13	1.96	0.47
5:F:34:SER:O	5:F:35:GLN:NE2	2.48	0.47
2:B:392:ARG:NH1	7:J:59:LYS:O	2.48	0.47
5:F:27:GLY:O	5:F:228:LYS:NZ	2.44	0.47
5:F:130:GLN:HE21	5:F:192:THR:HB	1.80	0.47
7:J:36:VAL:HG21	7:J:80:VAL:HG21	1.97	0.47
2:B:421:ASP:HA	2:B:454:LYS:HD3	1.96	0.47
3:D:505:THR:HB	3:D:509:HIS:HB3	1.97	0.47
1:A:133:ILE:HG23	2:B:136:ALA:HB3	1.96	0.47
2:B:176:ILE:HB	2:B:207:ASP:HA	1.95	0.47
4:E:117:HIS:HB2	4:E:118:PRO:HD3	1.97	0.47
4:G:89:ILE:HG12	4:G:95:LEU:HG	1.96	0.47
4:G:205:GLN:HE22	5:H:59:GLN:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:173:PHE:HB2	5:H:227:HIS:HD2	1.80	0.47
6:K:39:LYS:HD2	6:K:42:LYS:HD2	1.97	0.47
2:B:302:ALA:HB1	2:B:334:LEU:HD11	1.97	0.47
2:B:38:VAL:HA	2:B:99:VAL:HG13	1.97	0.46
1:C:399:LYS:H	1:C:511:ASP:HB2	1.80	0.46
4:E:200:GLN:NE2	4:E:203:ASN:HD21	2.13	0.46
4:G:117:HIS:HB2	4:G:118:PRO:HD3	1.96	0.46
6:K:94:THR:HB	6:K:95:PRO:HD3	1.97	0.46
2:B:367:ASN:HB2	2:B:373:GLU:HB2	1.97	0.46
2:B:467:LEU:HD12	2:B:782:PHE:HE2	1.79	0.46
1:A:286:GLY:HA3	1:A:334:VAL:HG23	1.96	0.46
4:G:223:THR:HG21	5:H:64:LYS:HD2	1.97	0.46
5:H:179:VAL:HA	5:H:225:VAL:HG13	1.97	0.46
1:C:433:LYS:HA	1:C:460:ILE:HG21	1.96	0.46
3:D:657:VAL:HG21	3:D:775:GLU:HB2	1.97	0.46
3:D:655:ILE:HG21	3:D:777:LEU:HD12	1.97	0.46
1:A:350:ASN:HA	1:A:368:ASN:HA	1.98	0.46
2:B:681:ARG:HA	2:B:708:PHE:HB3	1.98	0.46
1:C:485:GLY:H	1:C:686:GLN:HB3	1.80	0.46
4:G:103:PHE:HB3	4:G:114:LEU:HD11	1.97	0.46
1:A:540:ILE:HG22	1:A:730:ILE:HG12	1.98	0.46
3:D:454:SER:HA	3:D:457:ILE:HD11	1.97	0.46
6:K:120:PRO:HD3	6:K:132:VAL:HG22	1.98	0.46
6:K:146:VAL:HA	6:K:196:VAL:HA	1.97	0.46
1:A:109:TYR:HD2	2:B:115:PHE:HB2	1.81	0.46
2:B:521:VAL:HG12	2:B:522:VAL:HG13	1.98	0.46
3:D:605:TYR:HB2	3:D:800:SER:HA	1.98	0.46
5:F:60:PHE:HD1	5:F:111:ALA:HB2	1.80	0.46
1:A:671:ARG:HE	1:A:679:PHE:HZ	1.64	0.46
2:B:204:ILE:HD12	2:B:218:GLN:HB3	1.98	0.46
2:B:452:VAL:HG21	2:B:454:LYS:HE3	1.98	0.46
3:D:276:ILE:H	3:D:276:ILE:HG13	1.56	0.45
4:G:43:GLN:HE22	4:G:142:GLY:H	1.65	0.45
3:D:50:VAL:HG22	3:D:195:ALA:HB3	1.99	0.45
5:H:52:TYR:HB2	5:H:54:TRP:CE2	2.52	0.45
2:B:406:LEU:HB3	2:B:506:VAL:HG11	1.98	0.45
1:C:259:LEU:HD23	1:C:259:LEU:H	1.81	0.45
4:G:131:GLN:HE22	4:G:135:ASP:H	1.65	0.45
5:H:209:VAL:HG21	5:H:212:PRO:HG2	1.97	0.45
6:K:55:ALA:HB1	7:J:105:PHE:HB3	1.98	0.45
1:C:719:GLN:NE2	1:C:723:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:36:THR:HB	5:H:205:LEU:HD11	1.98	0.45
1:A:137:PHE:HE2	1:A:139:ARG:HH21	1.64	0.45
2:B:404:ASN:O	2:B:474:THR:OG1	2.35	0.45
1:C:76:LEU:HD22	3:D:182:GLN:HG3	1.99	0.45
2:B:436:CYS:N	2:B:454:LYS:O	2.45	0.45
3:D:818:ARG:O	3:D:821:ASN:ND2	2.50	0.45
4:G:149:ARG:NH1	4:G:218:TYR:OH	2.42	0.45
1:A:75:ALA:HB2	1:A:106:PRO:HB2	1.99	0.45
2:B:339:VAL:HA	2:B:350:PHE:HD2	1.82	0.45
1:C:400:ILE:HG21	1:C:463:LEU:HD21	1.99	0.45
1:C:487:GLN:HE22	1:C:522:GLU:HB3	1.81	0.45
5:F:169:VAL:HG11	5:F:225:VAL:HG21	1.99	0.45
2:B:531:THR:HB	2:B:732:ALA:HB3	1.98	0.45
1:C:163:ILE:HA	1:C:218:VAL:HB	1.99	0.45
3:D:833:LYS:NZ	3:D:856:ASP:OD1	2.39	0.45
5:F:227:HIS:HB3	5:F:230:SER:HB3	1.98	0.45
3:D:656:LEU:HB2	3:D:849:LEU:HD13	1.98	0.45
2:B:408:ILE:HG23	2:B:508:ALA:HA	1.98	0.45
2:B:411:LEU:HD11	2:B:482:ASN:HB2	2.00	0.45
3:D:297:ILE:HD12	3:D:307:LEU:HD11	1.98	0.45
4:E:207:SER:HB2	4:E:221:SER:H	1.82	0.45
7:J:175:SER:HB2	7:J:178:SER:HB2	1.99	0.45
7:J:176:GLN:HE22	7:J:191:LEU:HD13	1.82	0.45
2:B:433:THR:HG22	2:B:457:LYS:HB3	1.98	0.44
1:C:162:HIS:HB3	1:C:192:GLU:HB2	1.99	0.44
1:C:315:TRP:NE1	1:C:317:THR:OG1	2.50	0.44
1:A:486:THR:H	1:A:686:GLN:HB3	1.82	0.44
1:A:255:SER:OG	5:F:50:SER:O	2.29	0.44
1:A:542:VAL:HG23	1:A:664:ILE:HG13	1.99	0.44
2:B:82:LEU:HD23	2:B:112:MET:HG2	1.99	0.44
1:C:399:LYS:HB3	1:C:477:HIS:CE1	2.52	0.44
2:B:359:PRO:HG2	2:B:361:LEU:HD23	1.99	0.44
1:A:124:ARG:NH1	1:A:252:ARG:H	2.15	0.44
5:F:226:ASN:HD22	5:F:233:LYS:HD2	1.81	0.44
5:H:27:GLY:HA3	5:H:39:LEU:HD12	1.98	0.44
3:D:432:TYR:HA	3:D:435:ARG:HG2	1.99	0.44
1:A:259:LEU:HB2	1:A:359:ARG:HD2	1.98	0.44
1:A:269:LEU:HA	1:A:353:ILE:HG12	1.99	0.44
3:D:48:VAL:O	3:D:149:GLU:N	2.49	0.44
3:D:130:PHE:HD2	3:D:386:GLU:HG2	1.82	0.44
6:K:137:ASN:OD1	6:K:174:SER:OG	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:39:ILE:O	7:J:96:TYR:N	2.40	0.44
6:K:2:ILE:HG12	6:K:28:ASN:HB3	1.99	0.44
2:B:356:GLN:HE21	2:B:359:PRO:HB3	1.83	0.44
1:C:266:ILE:HB	1:C:356:LEU:HD12	2.00	0.44
3:D:465:ILE:HD12	3:D:482:GLY:HA3	1.97	0.44
3:D:656:LEU:HB3	3:D:842:PHE:HB3	1.99	0.44
5:H:37:LEU:HD21	5:H:134:VAL:HG21	1.99	0.44
7:J:156:TYR:HB3	7:J:157:PRO:HD3	1.99	0.44
4:G:40:VAL:HG12	5:H:206:SER:HB2	2.00	0.43
1:A:440:ASN:HD21	1:A:451:VAL:HB	1.82	0.43
2:B:249:THR:HA	2:B:255:TRP:HH2	1.83	0.43
2:B:331:LEU:HD12	2:B:332:HIS:H	1.83	0.43
3:D:131:ALA:HB1	3:D:393:MET:HG3	2.00	0.43
6:K:140:TYR:HB3	6:K:141:PRO:HD3	2.01	0.43
1:C:158:TYR:HD1	1:C:388:LYS:HE2	1.84	0.43
7:J:14:PRO:HA	7:J:87:VAL:HG23	2.00	0.43
2:B:42:HIS:CD2	2:B:44:HIS:HB3	2.53	0.43
2:B:48:GLU:HA	2:B:51:LEU:HD13	2.00	0.43
3:D:638:ARG:NH1	3:D:801:SER:OG	2.51	0.43
5:F:228:LYS:HB3	5:F:229:PRO:HD3	2.00	0.43
4:G:64:GLN:HG3	4:G:66:VAL:HG13	1.99	0.43
2:B:204:ILE:HG13	2:B:222:ILE:HD11	2.00	0.43
3:D:483:SER:HB2	3:D:485:GLN:HE22	1.82	0.43
4:G:128:TYR:HB3	4:G:140:GLY:H	1.83	0.43
1:C:68:LYS:HG3	1:C:73:GLN:HE22	1.83	0.43
3:D:799:GLU:N	3:D:803:GLU:OE1	2.49	0.43
4:E:200:GLN:HB2	5:F:125:MET:HA	1.99	0.43
2:B:56:GLY:HA2	2:B:60:ALA:HB2	2.00	0.43
1:C:251:GLU:HB2	1:C:270:GLN:HA	2.01	0.43
3:D:798:ARG:HG2	3:D:799:GLU:HG2	2.00	0.43
1:A:32:VAL:HG12	1:A:65:VAL:HB	2.00	0.43
2:B:251:TYR:HB2	2:B:405:HIS:HE1	1.84	0.43
2:B:442:ILE:HD11	2:B:448:GLU:HB3	2.00	0.43
1:C:37:LYS:HE3	1:C:37:LYS:HB3	1.92	0.43
1:C:169:ASP:HB3	1:C:173:GLY:N	2.34	0.43
3:D:339:PHE:HZ	3:D:356:LEU:HD11	1.84	0.43
4:G:207:SER:HB2	4:G:221:SER:H	1.84	0.43
2:B:216:GLN:HE21	2:B:216:GLN:HB2	1.66	0.43
3:D:216:LEU:HB3	3:D:416:THR:HG21	2.00	0.43
3:D:637:ALA:HB3	3:D:808:GLN:HE22	1.83	0.42
6:K:6:GLN:HA	6:K:23:CYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ILE:HA	1:A:721:VAL:HG12	2.01	0.42
2:B:264:ASN:HD22	2:B:267:LEU:H	1.67	0.42
1:C:142:PRO:HD3	1:C:346:ARG:HD2	2.01	0.42
1:C:272:ILE:HG13	1:C:352:SER:H	1.85	0.42
1:C:475:GLU:OE1	1:C:477:HIS:ND1	2.52	0.42
4:E:77:TYR:O	4:E:128:TYR:N	2.46	0.42
5:H:20:ASP:HB2	5:H:22:GLN:HE22	1.83	0.42
1:A:77:SER:HA	1:A:80:GLU:HG2	2.02	0.42
1:A:405:GLN:H	1:A:409:VAL:HB	1.84	0.42
2:B:438:LYS:HE2	2:B:479:LEU:HD13	2.00	0.42
1:C:425:THR:HG23	1:C:427:ASN:H	1.84	0.42
1:C:458:PHE:HZ	1:C:785:MET:HE3	1.85	0.42
4:E:38:ASP:HB3	5:F:203:TYR:CZ	2.54	0.42
5:F:127:TYR:HD1	5:F:127:TYR:HA	1.75	0.42
4:G:71:ASN:ND2	4:G:72:SER:O	2.52	0.42
1:A:429:ASP:HB2	1:A:787:ASP:HB3	2.01	0.42
1:A:675:PRO:HB3	1:A:681:TYR:HE1	1.84	0.42
3:D:53:VAL:HG23	3:D:184:VAL:HG21	2.02	0.42
4:E:200:GLN:HA	5:F:118:LEU:HA	2.01	0.42
1:A:151:TRP:CE2	1:A:248:LEU:HB3	2.54	0.42
1:A:214:LEU:O	1:A:217:ARG:NH1	2.51	0.42
1:A:667:ILE:HG22	3:D:916:ARG:HH22	1.84	0.42
2:B:518:ARG:NH2	2:B:689:SER:OG	2.53	0.42
2:B:536:MET:HG3	2:B:749:THR:HA	2.01	0.42
1:C:169:ASP:OD1	1:C:170:ASP:N	2.53	0.42
1:C:396:THR:HA	1:C:472:PHE:HB2	2.02	0.42
1:C:518:THR:O	1:C:520:ASN:ND2	2.53	0.42
3:D:367:THR:HG22	3:D:478:TRP:HZ2	1.84	0.42
1:A:99:ASN:HD21	1:A:106:PRO:HD3	1.83	0.42
1:A:165:LEU:HA	1:A:220:ILE:HB	2.02	0.42
2:B:411:LEU:HD11	2:B:482:ASN:H	1.84	0.42
3:D:835:ASP:HB2	3:D:836:PRO:HD3	2.02	0.42
1:C:124:ARG:HD2	1:C:252:ARG:HH11	1.85	0.42
1:C:504:GLU:HB3	1:C:509:GLN:HB3	2.00	0.42
3:D:268:LEU:HD11	3:D:325:MET:HB3	2.01	0.42
3:D:855:ILE:HA	3:D:912:PRO:HD2	2.02	0.42
1:C:351:TYR:HD1	1:C:351:TYR:HA	1.74	0.42
1:C:520:ASN:ND2	1:C:523:ARG:HH11	2.17	0.42
4:E:135:ASP:HB3	4:E:136:PRO:HD3	2.00	0.42
4:E:215:ASP:OD1	4:E:217:THR:OG1	2.32	0.42
5:F:43:VAL:HG11	5:F:48:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:96:TYR:HE1	7:J:111:GLY:HA3	1.85	0.42
1:A:699:LEU:HB2	1:A:702:MET:HB3	2.02	0.42
2:B:68:ASN:HD22	2:B:95:ILE:HD11	1.85	0.42
3:D:467:ASN:O	3:D:479:THR:OG1	2.38	0.42
7:J:162:VAL:HB	7:J:176:GLN:HG2	2.01	0.42
1:A:492:ASN:HD21	1:A:499:ASN:HB3	1.83	0.41
6:K:190:LYS:HA	6:K:211:ARG:HH12	1.85	0.41
2:B:63:LEU:HB3	2:B:64:PRO:HD3	2.02	0.41
2:B:173:VAL:HG22	2:B:204:ILE:HB	2.01	0.41
1:A:321:PHE:HA	1:A:324:VAL:HG22	2.03	0.41
1:C:544:LYS:HG2	1:C:662:GLU:HG2	2.02	0.41
2:B:684:THR:OG1	2:B:691:GLU:OE2	2.35	0.41
3:D:854:SER:HA	3:D:914:GLY:HA2	2.01	0.41
7:J:98:THR:OG1	7:J:99:ARG:N	2.54	0.41
7:J:129:PRO:HD3	7:J:217:LEU:HD21	2.03	0.41
5:F:165:LEU:HD12	5:F:221:TYR:H	1.84	0.41
4:G:79:GLN:O	4:G:79:GLN:NE2	2.54	0.41
7:J:149:VAL:HA	7:J:164:TRP:HH2	1.85	0.41
1:A:695:ARG:HA	1:A:695:ARG:HD3	1.92	0.41
2:B:412:GLU:HG3	2:B:419:VAL:HG21	2.03	0.41
2:B:471:VAL:HB	2:B:473:PHE:HD1	1.85	0.41
2:B:682:PHE:HE1	2:B:726:ASP:HB3	1.86	0.41
6:K:24:ARG:HG2	6:K:25:ALA:H	1.86	0.41
2:B:406:LEU:HD13	2:B:506:VAL:HG11	2.03	0.41
1:C:88:TYR:HE2	1:C:304:PRO:HD2	1.86	0.41
1:A:667:ILE:HG22	3:D:916:ARG:HH12	1.85	0.41
2:B:532:GLY:HA2	2:B:759:THR:HG22	2.01	0.41
3:D:565:ASN:HD22	3:D:567:THR:HG23	1.86	0.41
5:H:54:TRP:HE1	5:H:117:ARG:HE	1.68	0.41
1:C:247:TRP:H	1:C:381:TRP:HZ3	1.67	0.41
1:C:355:ASN:HD22	1:C:357:GLN:HB2	1.86	0.41
1:C:378:LYS:HE2	1:C:378:LYS:HB2	1.94	0.41
3:D:504:LYS:HG2	3:D:505:THR:H	1.85	0.41
4:E:77:TYR:HE1	4:E:130:GLN:HB2	1.86	0.41
1:A:99:ASN:O	1:A:101:HIS:ND1	2.38	0.41
1:A:392:TYR:HE2	1:A:767:PRO:HB3	1.86	0.41
1:C:32:VAL:HG12	1:C:94:HIS:HE1	1.85	0.41
1:C:539:THR:OG1	1:C:540:ILE:N	2.53	0.41
4:G:41:LEU:HD22	4:G:140:GLY:HA2	2.04	0.41
5:H:228:LYS:HB2	5:H:229:PRO:HD3	2.03	0.41
7:J:92:THR:HG23	7:J:115:THR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:HD13	1:A:163:ILE:H	1.86	0.40
1:A:465:LYS:HA	1:A:468:ARG:HG2	2.03	0.40
2:B:126:GLY:HA2	2:B:131:ALA:HB1	2.03	0.40
1:C:396:THR:HG22	1:C:472:PHE:HA	2.03	0.40
2:B:497:ILE:HG21	2:B:518:ARG:HH11	1.86	0.40
1:C:682:ALA:HB1	1:C:717:ALA:HB1	2.04	0.40
3:D:286:ASN:HD21	3:D:288:LYS:HB2	1.86	0.40
3:D:355:VAL:HG13	3:D:375:ILE:HB	2.02	0.40
3:D:590:ASP:OD2	3:D:894:TYR:OH	2.28	0.40
4:G:48:LEU:HD23	4:G:145:LEU:HD11	2.03	0.40
4:G:51:SER:H	4:G:54:GLN:NE2	2.19	0.40
1:A:734:ALA:HB2	1:A:793:VAL:HG13	2.03	0.40
2:B:48:GLU:HB2	2:B:49:ARG:NH2	2.37	0.40
1:C:96:PRO:HA	1:C:102:PHE:HE1	1.87	0.40
4:E:136:PRO:HA	4:E:137:PRO:HD3	1.95	0.40
4:E:162:ILE:HD12	4:E:252:LYS:HB2	2.03	0.40
4:G:193:TRP:HB3	4:G:195:VAL:HG23	2.02	0.40
6:K:118:PHE:HZ	7:J:147:SER:HB3	1.86	0.40
3:D:58:TRP:CD1	3:D:122:LEU:HB2	2.56	0.40
4:E:186:PRO:HB3	4:E:208:VAL:HG11	2.02	0.40
2:B:435:PRO:HA	2:B:455:CYS:HA	2.03	0.40
3:D:120:GLU:HG3	3:D:121:THR:HG23	2.02	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	647/847 (76%)	618 (96%)	29 (4%)	0	100	100
1	C	653/847 (77%)	637 (98%)	16 (2%)	0	100	100
2	B	634/1116 (57%)	613 (97%)	21 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	706/1228 (58%)	695 (98%)	11 (2%)	0	100	100
4	E	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
4	G	235/237 (99%)	229 (97%)	6 (3%)	0	100	100
5	F	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
5	H	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
6	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
7	J	225/227 (99%)	209 (93%)	16 (7%)	0	100	100
All	All	3975/5385 (74%)	3847 (97%)	128 (3%)	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	568/730 (78%)	537 (94%)	31 (6%)	18	39
1	C	574/730 (79%)	555 (97%)	19 (3%)	33	52
2	B	565/967 (58%)	539 (95%)	26 (5%)	23	44
3	D	639/1068 (60%)	610 (96%)	29 (4%)	23	45
4	E	202/202 (100%)	197 (98%)	5 (2%)	42	61
4	G	202/202 (100%)	195 (96%)	7 (4%)	31	51
5	F	189/189 (100%)	180 (95%)	9 (5%)	21	43
5	H	189/189 (100%)	181 (96%)	8 (4%)	25	46
6	K	185/185 (100%)	182 (98%)	3 (2%)	58	73
7	J	197/197 (100%)	189 (96%)	8 (4%)	26	47
All	All	3510/4659 (75%)	3365 (96%)	145 (4%)	28	47

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	48	GLN
1	A	102	PHE
1	A	115	ARG
1	A	139	ARG
1	A	163	ILE
1	A	180	LEU
1	A	188	GLU
1	A	195	LEU
1	A	202	LYS
1	A	221	LEU
1	A	254	ILE
1	A	271	LEU
1	A	275	LYS
1	A	361	LEU
1	A	390	ARG
1	A	417	ASP
1	A	461	ASP
1	A	501	MET
1	A	514	VAL
1	A	520	ASN
1	A	699	LEU
1	A	703	TYR
1	A	704	ARG
1	A	752	LEU
1	A	754	PHE
1	A	762	MET
1	A	765	ASP
1	A	769	LYS
1	A	770	GLN
1	A	795	TYR
2	B	34	LEU
2	B	49	ARG
2	B	76	ARG
2	B	112	MET
2	B	121	PHE
2	B	144	PHE
2	B	146	GLN
2	B	169	VAL
2	B	195	PHE
2	B	214	LYS
2	B	216	GLN
2	B	244	ARG

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Mol	Chain	Res	Type
2	B	265	THR
2	B	270	LYS
2	B	310	PHE
2	B	312	TYR
2	B	331	LEU
2	B	355	TYR
2	B	364	ILE
2	B	425	LEU
2	B	439	PHE
2	B	442	ILE
2	B	668	LYS
2	B	672	ARG
2	B	730	TYR
2	B	776	ASP
1	C	25	LYS
1	C	37	LYS
1	C	44	GLU
1	C	73	GLN
1	C	86	GLN
1	C	91	LEU
1	C	105	THR
1	C	121	LEU
1	C	124	ARG
1	C	137	PHE
1	C	193	LYS
1	C	316	LYS
1	C	351	TYR
1	C	417	ASP
1	C	453	GLN
1	C	679	PHE
1	C	754	PHE
1	C	780	HIS
1	C	794	ARG
3	D	41	LEU
3	D	42	LYS
3	D	56	GLN
3	D	125	ARG
3	D	185	CYS
3	D	203	GLN
3	D	230	ARG
3	D	277	THR
3	D	305	LYS

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Mol	Chain	Res	Type
3	D	322	THR
3	D	325	MET
3	D	366	ARG
3	D	423	LYS
3	D	467	ASN
3	D	520	LEU
3	D	526	VAL
3	D	536	LEU
3	D	553	MET
3	D	571	LYS
3	D	609	LYS
3	D	632	PHE
3	D	645	THR
3	D	793	ARG
3	D	810	PHE
3	D	844	MET
3	D	911	VAL
3	D	913	CYS
3	D	916	ARG
3	D	925	GLN
4	E	80	LYS
4	E	153	ARG
4	E	231	TYR
4	E	237	TYR
4	E	244	GLN
5	F	65	LEU
5	F	86	ARG
5	F	119	TYR
5	F	120	TYR
5	F	125	MET
5	F	127	TYR
5	F	132	THR
5	F	134	VAL
5	F	136	VAL
4	G	74	MET
4	G	79	GLN
4	G	86	LYS
4	G	119	VAL
4	G	184	PHE
4	G	185	TYR
4	G	231	TYR
5	H	21	VAL

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Mol	Chain	Res	Type
5	H	43	VAL
5	H	83	LEU
5	H	95	LYS
5	H	97	GLN
5	H	122	PHE
5	H	210	THR
5	H	233	LYS
6	K	51	THR
6	K	61	ARG
6	K	142	ARG
7	J	52	HIS
7	J	55	TRP
7	J	68	ARG
7	J	141	LEU
7	J	142	LYS
7	J	158	ARG
7	J	191	LEU
7	J	197	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	48	GLN
1	A	86	GLN
1	A	99	ASN
1	A	177	GLN
1	A	203	ASN
1	A	257	ASN
1	A	290	GLN
1	A	358	ASN
1	A	440	ASN
1	A	492	ASN
1	A	521	ASN
1	A	742	GLN
1	A	770	GLN
2	B	35	ASN
2	B	53	ASN
2	B	68	ASN
2	B	119	GLN
2	B	146	GLN
2	B	193	ASN

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Mol	Chain	Res	Type
2	B	201	GLN
2	B	216	GLN
2	B	356	GLN
2	B	405	HIS
2	B	503	GLN
2	B	703	GLN
2	B	709	ASN
2	B	774	GLN
1	C	73	GLN
1	C	94	HIS
1	C	162	HIS
1	C	196	GLN
1	C	311	ASN
1	C	350	ASN
1	C	355	ASN
1	C	375	ASN
1	C	405	GLN
1	C	487	GLN
1	C	709	HIS
1	C	742	GLN
1	C	782	ASN
3	D	56	GLN
3	D	186	HIS
3	D	201	GLN
3	D	203	GLN
3	D	275	ASN
3	D	296	ASN
3	D	314	GLN
3	D	317	ASN
3	D	337	GLN
3	D	390	GLN
3	D	407	GLN
3	D	426	ASN
3	D	461	ASN
3	D	635	ASN
3	D	808	GLN
3	D	893	GLN
3	D	897	HIS
3	D	925	GLN
4	E	25	GLN
4	E	71	ASN
4	E	182	ASN

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Mol	Chain	Res	Type
4	E	203	ASN
4	E	244	GLN
5	F	97	GLN
5	F	226	ASN
4	G	64	GLN
4	G	71	ASN
4	G	79	GLN
4	G	130	GLN
4	G	205	GLN
4	G	243	HIS
5	H	97	GLN
5	H	101	GLN
5	H	130	GLN
6	K	40	GLN
6	K	89	GLN
6	K	147	GLN
6	K	160	GLN
7	J	13	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.