Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Dec 13, 2016 – 02:19 PM EST

PDB ID	:	5FN5
EMDB ID:	:	EMD-3240
Title	:	Cryo-EM structure of gamma secretase in class 3 of the apo- state ensemble
Authors	:	Bai, X.C.; Rajendra, E.; Yang, G.H.; Shi, Y.G.; Scheres, S.H.W.
Deposited on	:	2015-11-10
Resolution	:	4.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

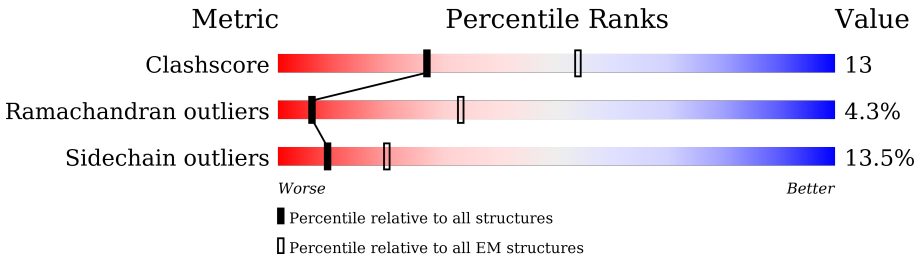
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	709	63% 26% • • 6%
2	B	467	24% 19% 5% 52%
3	C	265	56% 31% 5% 8%
4	D	101	71% 21% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9645 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 NICASTRIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	665	5222	3312	888	1001	21	0	0

- Molecule 2 is a protein called PRESENILIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	223	1735	1189	256	280	10	0	0

- Molecule 3 is a protein called GAMMA-SECRETASE SUBUNIT APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	243	1868	1252	299	313	4	0	0

- Molecule 4 is a protein called GAMMA-SECRETASE SUBUNIT PEN-2.

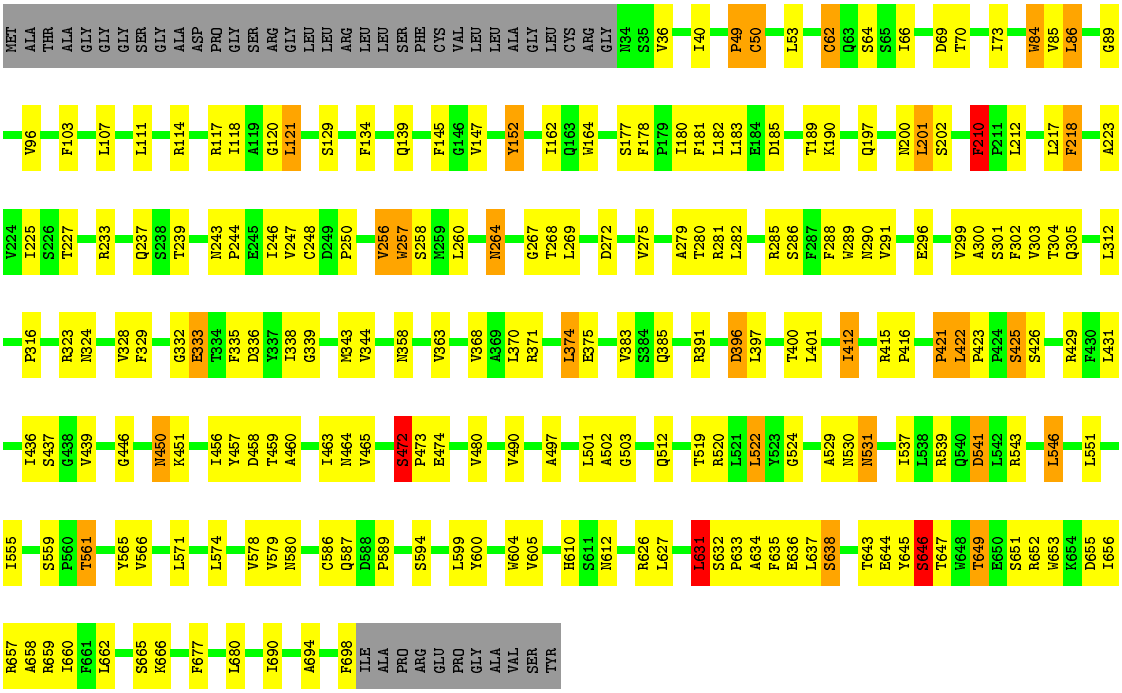
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	96	820	560	129	130	1	0	0

3 Residue-property plots (i)

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

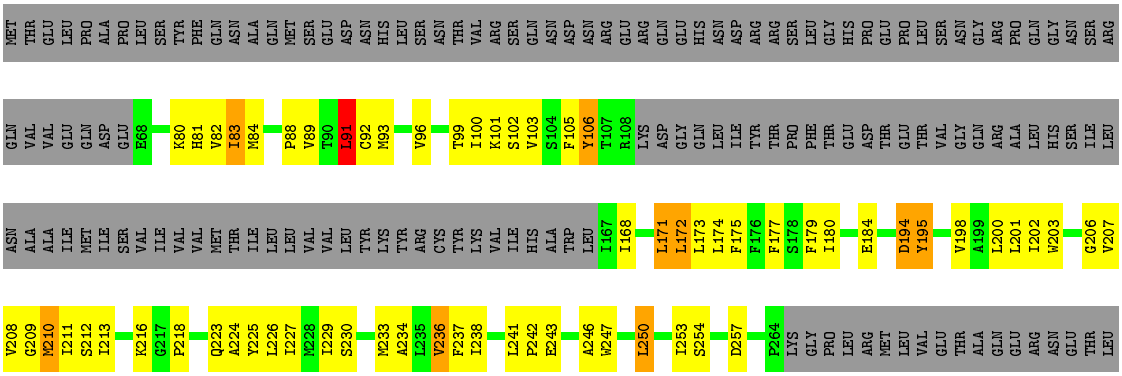
- Molecule 1: NICASTRIN

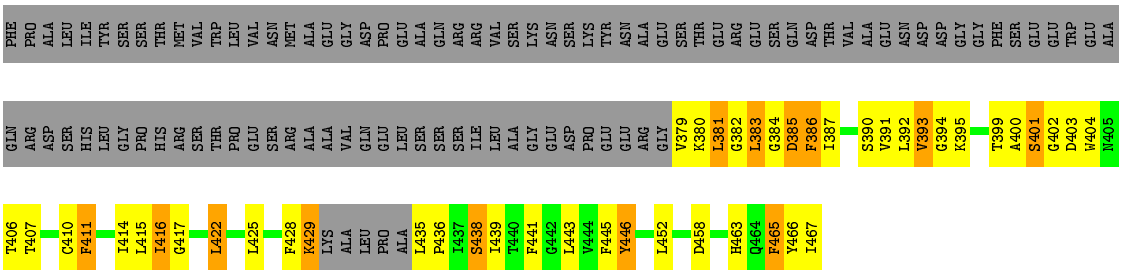
Chain A:



- Molecule 2: PRESENILIN-1

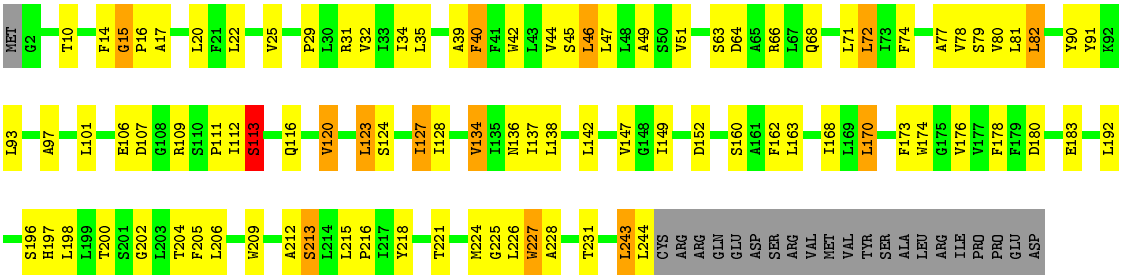
Chain B:





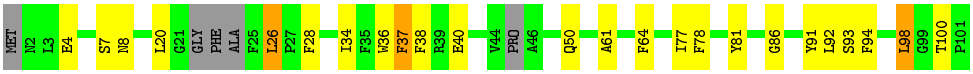
• Molecule 3: GAMMA-SECRETASE SUBUNIT APH-1A

Chain C:



• Molecule 4: GAMMA-SECRETASE SUBUNIT PEN-2

Chain D:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	66720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.54	1/5345 (0.0%)	0.82	1/7284 (0.0%)
2	B	0.75	0/1780	1.03	3/2430 (0.1%)
3	C	0.67	0/1920	0.95	1/2619 (0.0%)
4	D	0.76	0/849	0.89	0/1155
All	All	0.63	1/9894 (0.0%)	0.90	5/13488 (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	8
2	B	0	5
3	C	0	2
4	D	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	TRP	CB-CG	-5.26	1.40	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	250	LEU	CA-CB-CG	5.99	129.08	115.30
2	B	91	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	218	PHE	N-CA-CB	5.26	120.07	110.60
3	C	244	LEU	CA-CB-CG	5.18	127.21	115.30
2	B	381	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	VAL	Peptide
1	A	290	ASN	Peptide
1	A	472	SER	Peptide
1	A	49	PRO	Peptide
1	A	546	LEU	Peptide
1	A	612	ASN	Peptide
1	A	62	CYS	Peptide
1	A	646	SER	Peptide
2	B	106	TYR	Peptide
2	B	400	ALA	Peptide
2	B	401	SER	Peptide
2	B	402	GLY	Peptide
2	B	465	PHE	Peptide
3	C	113	SER	Peptide
3	C	213	SER	Peptide
4	D	4	GLU	Peptide

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	5222	0	5120	101	0
2	B	1735	0	1790	97	0
3	C	1868	0	1907	67	0
4	D	820	0	810	15	0
All	All	9645	0	9627	253	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 13.

All (253) 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)
2:B:452:LEU:HD13	3:C:51:VAL:HG22	1.43	0.97
2:B:441:PHE:O	2:B:445:PHE:HB3	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:LEU:HD23	2:B:246:ALA:HB3	1.51	0.89
1:A:529:ALA:HB1	1:A:546:LEU:HD22	1.54	0.87
1:A:73:ILE:HG21	1:A:660:ILE:HD11	1.60	0.80
3:C:170:LEU:HD22	3:C:221:THR:HG23	1.67	0.76
2:B:100:ILE:HD13	2:B:394:GLY:HA2	1.67	0.75
2:B:417:GLY:HA3	2:B:438:SER:HA	1.68	0.74
4:D:34:ILE:O	4:D:38:PHE:HB3	1.87	0.73
2:B:237:PHE:CD2	2:B:246:ALA:HB1	2.23	0.73
2:B:207:VAL:HG21	4:D:26:LEU:HD11	1.71	0.73
2:B:247:TRP:O	2:B:250:LEU:HG	1.89	0.73
2:B:416:ILE:HG12	3:C:40:PHE:HB2	1.70	0.71
3:C:34:ILE:O	3:C:90:TYR:OH	2.07	0.71
2:B:250:LEU:O	2:B:253:ILE:HG22	1.91	0.70
3:C:20:LEU:HD12	3:C:123:LEU:HD23	1.74	0.70
1:A:303:VAL:HG21	1:A:522:LEU:HD12	1.74	0.69
2:B:175:PHE:CE1	2:B:206:GLY:HA3	2.28	0.68
1:A:303:VAL:HG21	1:A:522:LEU:CD1	2.22	0.68
2:B:417:GLY:HA3	2:B:438:SER:CA	2.25	0.67
2:B:234:ALA:HA	2:B:391:VAL:HG22	1.77	0.67
2:B:168:ILE:HG23	2:B:171:LEU:HD13	1.78	0.66
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.77	0.65
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.79	0.65
2:B:233:MET:O	2:B:236:VAL:HG12	1.97	0.65
2:B:466:TYR:HB2	3:C:204:THR:HG21	1.77	0.64
3:C:47:LEU:O	3:C:51:VAL:HG23	1.97	0.64
1:A:303:VAL:HG11	1:A:522:LEU:HD13	1.80	0.64
1:A:182:LEU:HB2	1:A:288:PHE:CD2	2.33	0.64
2:B:411:PHE:HA	2:B:414:ILE:HD12	1.81	0.63
4:D:34:ILE:HD11	4:D:61:ALA:HA	1.80	0.63
3:C:20:LEU:HD12	3:C:123:LEU:CD2	2.28	0.63
1:A:121:LEU:HD21	1:A:178:PHE:CE1	2.34	0.63
2:B:387:ILE:O	2:B:391:VAL:HG23	1.99	0.63
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.80	0.62
2:B:210:MET:N	2:B:210:MET:SD	2.72	0.62
2:B:198:VAL:HG21	4:D:94:PHE:CD2	2.35	0.62
2:B:425:LEU:O	2:B:429:LYS:N	2.33	0.62
1:A:401:LEU:HD13	1:A:439:VAL:HG11	1.81	0.62
2:B:89:VAL:HA	2:B:386:PHE:CE1	2.35	0.61
3:C:116:GLN:O	3:C:120:VAL:HG13	2.00	0.61
1:A:299:VAL:O	1:A:303:VAL:HG23	2.00	0.61
2:B:226:LEU:HD13	2:B:380:LYS:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG21	3:C:137:ILE:HG22	1.83	0.61
2:B:91:LEU:HD12	2:B:92:CYS:N	2.16	0.60
1:A:223:ALA:HB2	1:A:247:VAL:HG22	1.82	0.60
2:B:237:PHE:O	2:B:241:LEU:HG	2.01	0.60
2:B:383:LEU:O	2:B:387:ILE:HG13	2.01	0.60
1:A:96:VAL:HG13	1:A:118:ILE:HD11	1.84	0.60
3:C:40:PHE:O	3:C:44:VAL:HG23	2.01	0.60
2:B:208:VAL:HG11	4:D:28:PHE:CD1	2.37	0.59
1:A:299:VAL:HA	1:A:302:PHE:CE2	2.36	0.59
1:A:260:LEU:HD13	1:A:312:LEU:CD1	2.33	0.59
1:A:368:VAL:HG11	1:A:490:VAL:HG11	1.84	0.59
2:B:436:PRO:HA	2:B:439:ILE:HD12	1.83	0.59
1:A:162:ILE:HD11	1:A:164:TRP:CD2	2.38	0.59
1:A:145:PHE:O	1:A:429:ARG:NH2	2.35	0.58
3:C:16:PRO:O	3:C:20:LEU:HG	2.04	0.58
1:A:375:GLU:HA	1:A:412:ILE:HG23	1.86	0.58
1:A:680:LEU:HD13	3:C:15:GLY:HA2	1.86	0.58
2:B:257:ASP:HB3	2:B:435:LEU:HD23	1.85	0.58
2:B:404:TRP:O	2:B:407:THR:HG22	2.04	0.58
2:B:84:MET:O	2:B:88:PRO:HD2	2.05	0.57
2:B:466:TYR:CE2	3:C:163:LEU:HB3	2.40	0.57
2:B:416:ILE:CG1	3:C:40:PHE:HB2	2.34	0.56
4:D:92:LEU:HD12	4:D:93:SER:N	2.21	0.56
2:B:441:PHE:O	2:B:445:PHE:CB	2.46	0.56
3:C:35:LEU:HA	3:C:124:SER:HB2	1.86	0.56
1:A:62:CYS:SG	1:A:180:ILE:HD12	2.46	0.56
2:B:177:PHE:HA	2:B:180:ILE:HD12	1.86	0.56
3:C:176:VAL:HG11	3:C:228:ALA:HB1	1.88	0.56
2:B:171:LEU:HD12	2:B:210:MET:CG	2.35	0.55
1:A:634:ALA:O	1:A:638:SER:N	2.40	0.55
2:B:171:LEU:HD12	2:B:210:MET:HG3	1.87	0.55
2:B:208:VAL:HG23	2:B:225:TYR:CZ	2.42	0.55
3:C:113:SER:OG	3:C:116:GLN:N	2.39	0.55
2:B:92:CYS:HB3	2:B:386:PHE:CE1	2.41	0.55
1:A:662:LEU:HD13	3:C:149:ILE:HB	1.89	0.55
2:B:96:VAL:O	2:B:100:ILE:HD12	2.07	0.55
2:B:175:PHE:CE2	2:B:203:TRP:HA	2.42	0.54
3:C:134:VAL:HG22	3:C:138:LEU:HB2	1.88	0.54
1:A:40:ILE:CG1	3:C:147:VAL:HG22	2.37	0.54
1:A:275:VAL:HG12	1:A:324:ASN:HB3	1.90	0.54
1:A:183:LEU:HD12	1:A:189:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:PRO:HB3	4:D:36:TRP:CE2	2.42	0.54
3:C:174:TRP:O	3:C:178:PHE:N	2.41	0.54
2:B:466:TYR:CD1	3:C:163:LEU:HD23	2.41	0.54
3:C:173:PHE:CG	3:C:225:GLY:HA2	2.43	0.54
3:C:31:ARG:HA	3:C:34:ILE:HD12	1.90	0.54
1:A:480:VAL:HG12	1:A:519:THR:HG21	1.89	0.53
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.90	0.53
1:A:260:LEU:HD22	1:A:312:LEU:HD13	1.90	0.53
2:B:395:LYS:O	2:B:399:THR:HG23	2.09	0.53
3:C:42:TRP:CH2	3:C:46:LEU:HD13	2.44	0.53
3:C:17:ALA:HB1	3:C:127:ILE:HD11	1.90	0.53
2:B:417:GLY:HA3	2:B:438:SER:CB	2.39	0.52
2:B:82:VAL:HG11	2:B:422:LEU:HG	1.90	0.52
1:A:247:VAL:O	1:A:248:CYS:HB2	2.08	0.52
2:B:224:ALA:O	2:B:227:ILE:HG12	2.09	0.52
3:C:174:TRP:CH2	3:C:197:HIS:HA	2.44	0.52
2:B:390:SER:O	2:B:393:VAL:HG12	2.10	0.51
1:A:49:PRO:HB3	1:A:181:PHE:CZ	2.45	0.51
2:B:223:GLN:HA	2:B:226:LEU:HD12	1.91	0.51
3:C:127:ILE:HG22	3:C:128:ILE:N	2.25	0.51
1:A:385:GLN:O	1:A:391:ARG:HB2	2.10	0.51
1:A:280:THR:OG1	1:A:305:GLN:NE2	2.44	0.51
1:A:656:ILE:HD12	1:A:657:ARG:HA	1.92	0.51
3:C:173:PHE:CD1	3:C:225:GLY:HA2	2.47	0.50
1:A:456:ILE:N	1:A:456:ILE:HD12	2.26	0.50
2:B:403:ASP:O	2:B:404:TRP:C	2.50	0.50
3:C:227:TRP:O	3:C:231:THR:HG23	2.11	0.50
3:C:200:THR:O	3:C:204:THR:HG23	2.12	0.50
2:B:195:TYR:HA	4:D:94:PHE:HB2	1.93	0.49
3:C:39:ALA:N	3:C:124:SER:OG	2.45	0.49
1:A:338:ILE:HD12	1:A:339:GLY:N	2.27	0.49
3:C:106:GLU:N	3:C:107:ASP:HA	2.27	0.49
1:A:635:PHE:CZ	1:A:649:THR:HG23	2.47	0.49
2:B:385:ASP:OD1	2:B:385:ASP:N	2.46	0.49
2:B:207:VAL:HG11	4:D:26:LEU:HD21	1.94	0.49
2:B:225:TYR:O	2:B:229:ILE:HG12	2.13	0.49
3:C:176:VAL:CG1	3:C:228:ALA:HB1	2.43	0.49
1:A:200:ASN:O	1:A:201:LEU:HD13	2.13	0.49
1:A:282:LEU:HD12	1:A:302:PHE:CD2	2.48	0.49
2:B:381:LEU:H	2:B:382:GLY:HA3	1.76	0.48
2:B:241:LEU:HD22	2:B:243:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:TRP:CE3	3:C:128:ILE:HG23	2.49	0.48
3:C:78:VAL:HG12	3:C:82:LEU:HD22	1.96	0.48
3:C:25:VAL:HG12	3:C:32:VAL:HG22	1.96	0.48
2:B:171:LEU:HD23	2:B:171:LEU:C	2.34	0.48
2:B:174:LEU:C	2:B:174:LEU:HD23	2.34	0.48
2:B:194:ASP:HB3	4:D:78:PHE:CZ	2.48	0.48
1:A:111:LEU:HD21	1:A:118:ILE:HD13	1.96	0.48
1:A:227:THR:HG21	1:A:647:THR:HB	1.95	0.47
1:A:40:ILE:HG13	3:C:147:VAL:HG22	1.97	0.47
2:B:89:VAL:HA	2:B:386:PHE:CZ	2.50	0.47
2:B:207:VAL:HG11	4:D:26:LEU:CD2	2.43	0.47
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.49	0.47
1:A:183:LEU:CD1	1:A:189:THR:HG22	2.45	0.47
1:A:555:ILE:O	1:A:555:ILE:HG22	2.15	0.47
3:C:170:LEU:HD22	3:C:221:THR:CG2	2.40	0.47
1:A:690:ILE:O	1:A:694:ALA:N	2.47	0.47
3:C:17:ALA:HB1	3:C:127:ILE:CD1	2.44	0.47
1:A:335:PHE:O	1:A:338:ILE:HG23	2.15	0.47
1:A:223:ALA:HB3	1:A:651:SER:HB2	1.97	0.47
2:B:103:VAL:HG11	2:B:106:TYR:CD2	2.49	0.47
2:B:241:LEU:HB2	2:B:242:PRO:C	2.36	0.46
1:A:86:LEU:O	1:A:117:ARG:NE	2.48	0.46
2:B:467:ILE:HD11	3:C:79:SER:OG	2.14	0.46
1:A:338:ILE:HG22	1:A:646:SER:OG	2.15	0.46
2:B:92:CYS:SG	2:B:230:SER:OG	2.69	0.46
1:A:425:SER:O	1:A:426:SER:C	2.54	0.46
2:B:465:PHE:CZ	3:C:72:LEU:HD22	2.50	0.46
3:C:136:ASN:N	3:C:136:ASN:HD22	2.14	0.46
3:C:215:LEU:N	3:C:216:PRO:CD	2.79	0.46
2:B:383:LEU:HD22	2:B:384:GLY:N	2.31	0.45
1:A:421:PRO:O	1:A:422:LEU:HB2	2.16	0.45
3:C:170:LEU:HD12	3:C:174:TRP:CE2	2.51	0.45
3:C:209:TRP:O	3:C:212:ALA:HB3	2.17	0.45
2:B:226:LEU:CD1	2:B:380:LYS:HG3	2.46	0.45
1:A:626:ARG:O	1:A:627:LEU:HD23	2.17	0.45
4:D:34:ILE:O	4:D:38:PHE:CB	2.62	0.45
1:A:182:LEU:HD22	1:A:288:PHE:CG	2.51	0.45
1:A:84:TRP:CD1	1:A:85:VAL:N	2.85	0.45
2:B:200:LEU:HD23	2:B:201:LEU:HD12	1.99	0.45
2:B:177:PHE:CE1	2:B:236:VAL:HG23	2.51	0.45
3:C:127:ILE:CG2	3:C:128:ILE:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:LEU:HD12	3:C:174:TRP:CZ2	2.51	0.44
1:A:212:LEU:O	1:A:662:LEU:HA	2.17	0.44
3:C:196:SER:O	3:C:200:THR:HG23	2.17	0.44
1:A:396:ASP:O	1:A:400:THR:HG23	2.17	0.44
1:A:260:LEU:HD13	1:A:312:LEU:HD12	2.00	0.44
2:B:241:LEU:HD13	2:B:243:GLU:HA	2.00	0.44
1:A:363:VAL:HA	1:A:439:VAL:O	2.18	0.44
1:A:164:TRP:CZ2	1:A:423:PRO:HA	2.52	0.44
1:A:541:ASP:OD1	1:A:541:ASP:N	2.51	0.44
2:B:173:LEU:HD23	2:B:173:LEU:C	2.38	0.44
2:B:211:ILE:HD12	2:B:212:SER:N	2.32	0.44
2:B:224:ALA:HA	2:B:227:ILE:HG12	1.99	0.44
1:A:280:THR:HG22	1:A:281:ARG:O	2.18	0.44
1:A:50:CYS:SG	1:A:180:ILE:HD12	2.58	0.44
2:B:200:LEU:CD2	2:B:201:LEU:HD12	2.48	0.44
3:C:80:VAL:HG11	3:C:198:LEU:HG	1.99	0.44
1:A:631:LEU:HD23	1:A:635:PHE:HB2	1.99	0.43
4:D:98:LEU:O	4:D:100:THR:N	2.49	0.43
1:A:633:PRO:HG2	1:A:645:TYR:CD1	2.53	0.43
1:A:147:VAL:HG11	1:A:431:LEU:HB3	2.01	0.43
2:B:410:CYS:SG	2:B:446:TYR:HB2	2.59	0.43
1:A:450:ASN:C	1:A:450:ASN:HD22	2.21	0.43
1:A:182:LEU:HD22	1:A:288:PHE:CB	2.48	0.43
1:A:280:THR:HG21	1:A:302:PHE:HA	2.01	0.43
1:A:374:LEU:HD23	1:A:374:LEU:N	2.33	0.43
1:A:49:PRO:HB2	1:A:50:CYS:O	2.19	0.43
2:B:208:VAL:HA	2:B:211:ILE:HG13	2.00	0.43
2:B:254:SER:HB2	2:B:439:ILE:CD1	2.49	0.43
3:C:14:PHE:O	3:C:15:GLY:C	2.56	0.43
1:A:121:LEU:HD23	1:A:121:LEU:N	2.34	0.43
1:A:197:GLN:O	1:A:201:LEU:HD21	2.18	0.43
2:B:209:GLY:O	2:B:213:ILE:HG12	2.19	0.43
2:B:88:PRO:HA	2:B:91:LEU:HG	2.00	0.43
1:A:497:ALA:O	1:A:501:LEU:HD23	2.19	0.43
2:B:171:LEU:HD23	2:B:172:LEU:N	2.33	0.43
2:B:465:PHE:CG	3:C:205:PHE:HD1	2.37	0.43
4:D:77:ILE:O	4:D:81:TYR:N	2.46	0.43
1:A:223:ALA:HB2	1:A:247:VAL:CG2	2.48	0.43
1:A:247:VAL:HA	1:A:652:ARG:HG2	2.00	0.43
1:A:152:TYR:CE2	1:A:383:VAL:HG11	2.54	0.42
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:CYS:SG	1:A:62:CYS:N	2.91	0.42
1:A:120:GLY:C	1:A:121:LEU:HD23	2.38	0.42
1:A:258:SER:CB	1:A:571:LEU:HD21	2.49	0.42
2:B:416:ILE:CG1	3:C:40:PHE:CB	2.97	0.42
3:C:77:ALA:O	3:C:81:LEU:HG	2.19	0.42
2:B:403:ASP:O	2:B:406:THR:N	2.53	0.42
2:B:80:LYS:O	2:B:83:ILE:HG22	2.19	0.42
1:A:578:VAL:HG22	1:A:579:VAL:H	1.85	0.42
3:C:80:VAL:HG13	3:C:197:HIS:CE1	2.54	0.42
1:A:299:VAL:HA	1:A:302:PHE:CZ	2.54	0.42
2:B:241:LEU:CD2	2:B:246:ALA:HB3	2.36	0.42
1:A:323:ARG:HB2	1:A:502:ALA:HA	2.01	0.41
1:A:86:LEU:O	1:A:117:ARG:CD	2.68	0.41
4:D:37:PHE:N	4:D:37:PHE:CD1	2.88	0.41
1:A:300:ALA:O	1:A:304:THR:HG23	2.20	0.41
1:A:279:ALA:HA	1:A:328:VAL:HG13	2.00	0.41
1:A:282:LEU:HD22	1:A:329:PHE:CB	2.50	0.41
1:A:397:LEU:O	1:A:400:THR:OG1	2.25	0.41
2:B:234:ALA:O	2:B:238:ILE:HD12	2.20	0.41
1:A:599:LEU:O	1:A:600:TYR:CD2	2.74	0.41
1:A:210:PHE:CG	1:A:665:SER:HB3	2.55	0.41
1:A:264:ASN:HA	1:A:599:LEU:HG	2.01	0.41
1:A:217:LEU:HD12	1:A:658:ALA:CB	2.51	0.41
2:B:247:TRP:CZ2	2:B:443:LEU:HD11	2.55	0.41
2:B:465:PHE:CE1	3:C:72:LEU:HD22	2.54	0.41
1:A:53:LEU:HD12	1:A:53:LEU:N	2.35	0.41
2:B:83:ILE:HG12	3:C:29:PRO:HB2	2.03	0.41
3:C:170:LEU:HG	3:C:174:TRP:CH2	2.56	0.41
1:A:286:SER:OG	1:A:291:VAL:O	2.36	0.41
2:B:203:TRP:O	2:B:207:VAL:HG23	2.20	0.41
2:B:92:CYS:HG	2:B:230:SER:HG	1.66	0.41
3:C:49:ALA:HB2	3:C:79:SER:HA	2.02	0.41
1:A:415:ARG:HB3	1:A:416:PRO:HD2	2.02	0.41
1:A:301:SER:O	1:A:304:THR:OG1	2.29	0.41
1:A:421:PRO:O	1:A:422:LEU:CB	2.69	0.40
1:A:457:TYR:O	1:A:459:THR:N	2.54	0.40
3:C:97:ALA:O	3:C:101:LEU:N	2.35	0.40
1:A:246:ILE:O	1:A:246:ILE:HG22	2.21	0.40
1:A:282:LEU:HD12	1:A:302:PHE:CG	2.56	0.40
1:A:480:VAL:HG12	1:A:519:THR:CG2	2.50	0.40
2:B:233:MET:HB3	2:B:387:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:THR:HB	3:C:138:LEU:HD21	2.02	0.40
2:B:463:HIS:CE1	3:C:72:LEU:HD11	2.56	0.40
2:B:379:VAL:HG12	2:B:380:LYS:HD3	2.04	0.40
2:B:466:TYR:CE1	3:C:163:LEU:HD23	2.56	0.40
3:C:202:GLY:HA2	3:C:205:PHE:CD2	2.57	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	663/709 (94%)	527 (80%)	96 (14%)	40 (6%)	2 27
2	B	215/467 (46%)	195 (91%)	17 (8%)	3 (1%)	14 59
3	C	241/265 (91%)	219 (91%)	17 (7%)	5 (2%)	9 52
4	D	90/101 (89%)	78 (87%)	8 (9%)	4 (4%)	3 34
All	All	1209/1542 (78%)	1019 (84%)	138 (11%)	52 (4%)	6 35

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	A	333	GLU
1	A	336	ASP
1	A	422	LEU
1	A	472	SER
1	A	632	SER
1	A	655	ASP
3	C	243	LEU
1	A	89	GLY
1	A	103	PHE

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Mol	Chain	Res	Type
1	A	268	THR
1	A	289	TRP
1	A	436	ILE
1	A	446	GLY
1	A	458	ASP
1	A	460	ALA
1	A	530	ASN
2	B	401	SER
3	C	15	GLY
3	C	111	PRO
1	A	239	THR
1	A	473	PRO
1	A	594	SER
1	A	631	LEU
2	B	216	LYS
3	C	213	SER
1	A	243	ASN
1	A	358	ASN
1	A	371	ARG
1	A	561	THR
1	A	646	SER
3	C	113	SER
4	D	20	LEU
4	D	86	GLY
1	A	225	ILE
1	A	316	PRO
1	A	559	SER
1	A	580	ASN
1	A	589	PRO
4	D	7	SER
1	A	257	TRP
1	A	421	PRO
1	A	451	LYS
2	B	102	SER
4	D	98	LEU
1	A	210	PHE
1	A	503	GLY
1	A	244	PRO
1	A	332	GLY
1	A	66	ILE
1	A	267	GLY
1	A	412	ILE

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	583/612 (95%)	513 (88%)	70 (12%)	6 33
2	B	183/408 (45%)	153 (84%)	30 (16%)	3 21
3	C	192/214 (90%)	158 (82%)	34 (18%)	2 17
4	D	85/89 (96%)	78 (92%)	7 (8%)	14 51
All	All	1043/1323 (79%)	902 (86%)	141 (14%)	9 29

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	64	SER
1	A	69	ASP
1	A	70	THR
1	A	84	TRP
1	A	86	LEU
1	A	107	LEU
1	A	114	ARG
1	A	121	LEU
1	A	129	SER
1	A	134	PHE
1	A	139	GLN
1	A	152	TYR
1	A	177	SER
1	A	190	LYS
1	A	201	LEU
1	A	202	SER
1	A	210	PHE
1	A	218	PHE
1	A	233	ARG
1	A	237	GLN
1	A	250	PRO
1	A	256	VAL
1	A	264	ASN

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	272	ASP
1	A	285	ARG
1	A	296	GLU
1	A	333	GLU
1	A	343	MET
1	A	344	VAL
1	A	370	LEU
1	A	374	LEU
1	A	396	ASP
1	A	425	SER
1	A	437	SER
1	A	450	ASN
1	A	464	ASN
1	A	472	SER
1	A	474	GLU
1	A	512	GLN
1	A	520	ARG
1	A	522	LEU
1	A	531	ASN
1	A	537	ILE
1	A	539	ARG
1	A	541	ASP
1	A	543	ARG
1	A	551	LEU
1	A	561	THR
1	A	565	TYR
1	A	566	VAL
1	A	574	LEU
1	A	586	CYS
1	A	587	GLN
1	A	604	TRP
1	A	605	VAL
1	A	610	HIS
1	A	631	LEU
1	A	636	GLU
1	A	637	LEU
1	A	638	SER
1	A	643	THR
1	A	644	GLU
1	A	649	THR
1	A	653	TRP

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Mol	Chain	Res	Type
1	A	659	ARG
1	A	666	LYS
1	A	677	PHE
1	A	698	PHE
2	B	81	HIS
2	B	83	ILE
2	B	91	LEU
2	B	93	MET
2	B	99	THR
2	B	101	LYS
2	B	105	PHE
2	B	171	LEU
2	B	172	LEU
2	B	179	PHE
2	B	184	GLU
2	B	194	ASP
2	B	195	TYR
2	B	202	ILE
2	B	210	MET
2	B	236	VAL
2	B	383	LEU
2	B	385	ASP
2	B	386	PHE
2	B	392	LEU
2	B	393	VAL
2	B	411	PHE
2	B	415	LEU
2	B	416	ILE
2	B	422	LEU
2	B	428	PHE
2	B	429	LYS
2	B	438	SER
2	B	446	TYR
2	B	458	ASP
3	C	22	LEU
3	C	40	PHE
3	C	45	SER
3	C	46	LEU
3	C	63	SER
3	C	64	ASP
3	C	66	ARG
3	C	68	GLN

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Mol	Chain	Res	Type
3	C	71	LEU
3	C	72	LEU
3	C	74	PHE
3	C	82	LEU
3	C	91	TYR
3	C	93	LEU
3	C	109	ARG
3	C	112	ILE
3	C	120	VAL
3	C	123	LEU
3	C	127	ILE
3	C	134	VAL
3	C	142	LEU
3	C	152	ASP
3	C	160	SER
3	C	162	PHE
3	C	170	LEU
3	C	180	ASP
3	C	183	GLU
3	C	192	LEU
3	C	206	LEU
3	C	218	TYR
3	C	224	MET
3	C	226	LEU
3	C	227	TRP
3	C	243	LEU
4	D	8	ASN
4	D	26	LEU
4	D	37	PHE
4	D	40	GLU
4	D	50	GLN
4	D	64	PHE
4	D	91	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	150	ASN
1	A	305	GLN
1	A	331	GLN
1	A	450	ASN

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Mol	Chain	Res	Type
1	A	454	GLN
1	A	535	GLN
2	B	223	GLN
3	C	136	ASN
3	C	171	HIS
4	D	50	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 carbohydrates 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

There are no chain breaks in this entry.