wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:57 PM BST

PDB ID	:	4PT2
EMDB ID:	:	EMD-5917
Title	:	Myxococcus xanthus encpasulin protein (EncA)
Authors	:	Fontana, J.; Aksyuk, A.A.; Steven, A.C.; Hoiczyk, E.
Deposited on	:	2014-03-10
Resolution	:	4.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

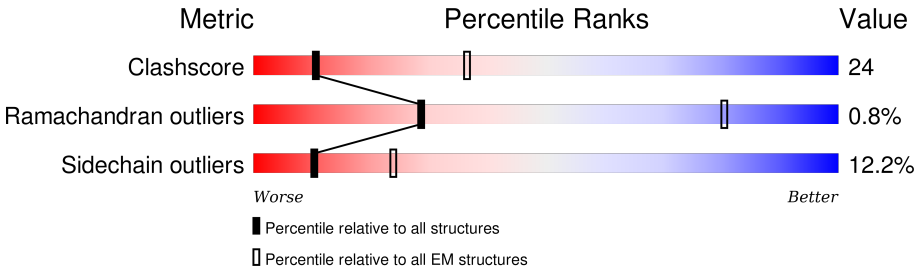
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	287	52% 35% 8%
1	B	287	52% 37% 7%
1	P	287	52% 36% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6462 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 Encapsulin protein.

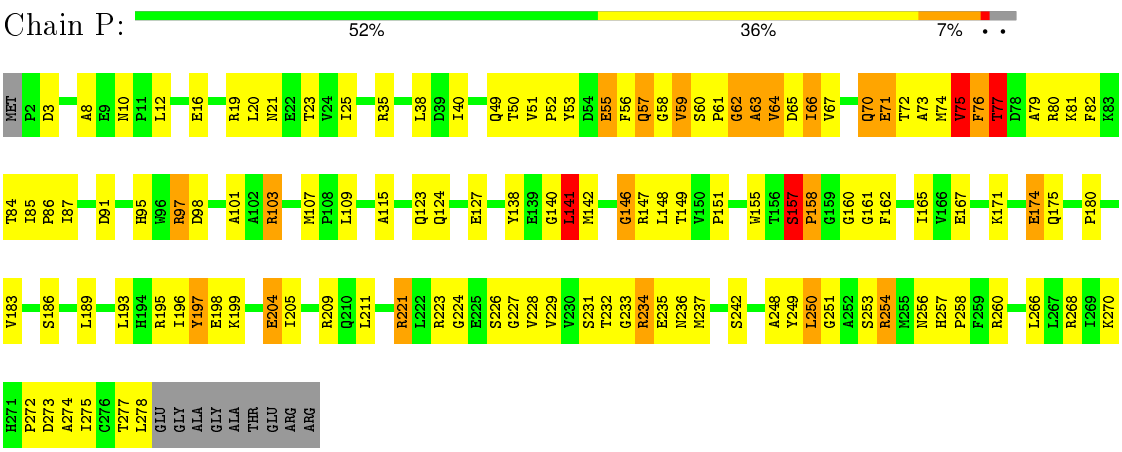
Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	277	Total	C	N	O	S	0	0
			2154	1361	382	402	9		
1	A	277	Total	C	N	O	S	0	0
			2154	1361	382	402	9		
1	B	277	Total	C	N	O	S	0	0
			2154	1361	382	402	9		

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.

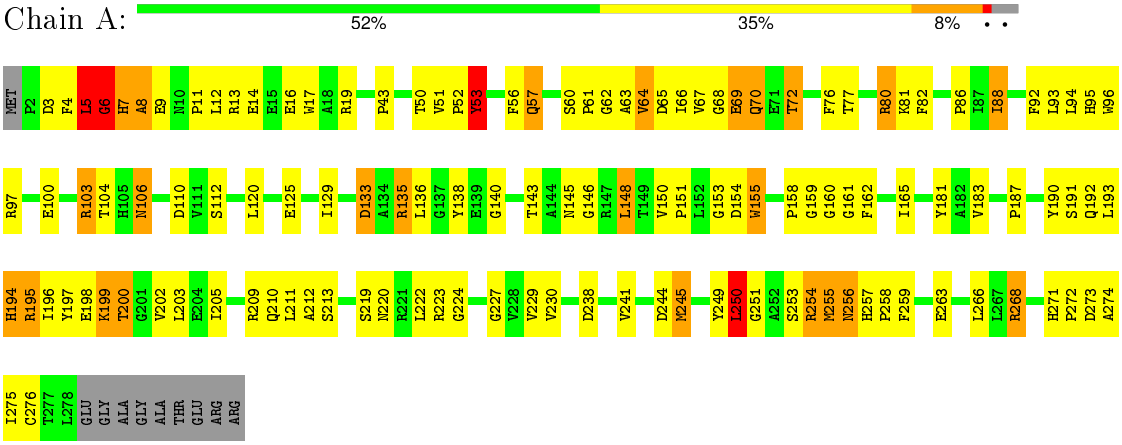
- Molecule 1: Encapsulin protein

Chain P:



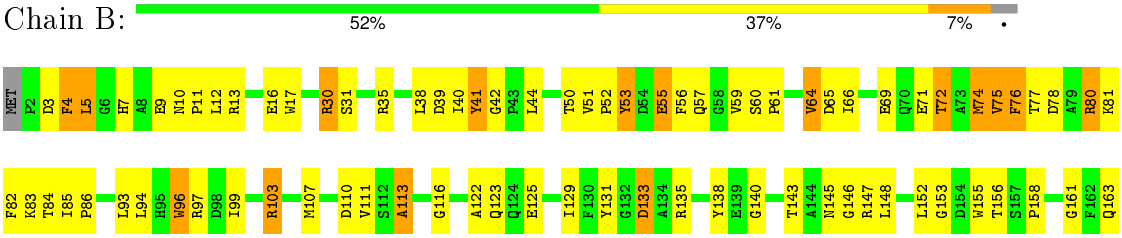
- Molecule 1: Encapsulin protein

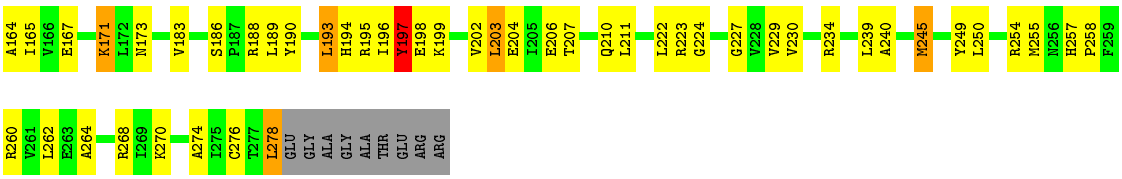
Chain A:



- Molecule 1: Encapsulin protein

Chain B:




A164 I165 Y166 E167 K171 L172 N173 V183 S186 P187 R188 L189 Y190 L193 H194 R195 I196 Y197 E198 K199 V202 L203 E204 I205 E206 T207 Q210 L211 L222 R223 G224 G227 Y228 V229 V230 R234 L239 A240 M245 Y249 L250 R254 M255 N256 H257 P258 F259
R260 V261 L262 E263 A264 R268 I269 K270 A274 I275 C276 T277 L278 GLU GLY ALA GLY ALA THR GLU ARG ARG

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	14000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1650	Depositor
Magnification	59000	Depositor
Image detector	Not provided	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	0.32	0/2198	0.79	4/2982 (0.1%)
1	B	0.33	0/2198	0.82	3/2982 (0.1%)
1	P	0.35	0/2198	0.86	10/2982 (0.3%)
All	All	0.33	0/6594	0.83	17/8946 (0.2%)

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	9
1	B	0	3
1	P	0	7
All	All	0	19

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	62	GLY	N-CA-C	10.48	139.29	113.10
1	P	157	SER	CB-CA-C	8.62	126.49	110.10
1	A	5	LEU	CA-CB-CG	8.40	134.63	115.30
1	A	6	GLY	N-CA-C	6.87	130.28	113.10
1	P	157	SER	C-N-CD	-6.43	106.45	120.60
1	P	157	SER	N-CA-CB	-6.22	101.17	110.50
1	A	250	LEU	CA-CB-CG	6.13	129.39	115.30
1	A	62	GLY	N-CA-C	-6.08	97.90	113.10
1	P	77	THR	N-CA-C	6.07	127.38	111.00
1	P	59	VAL	N-CA-C	6.04	127.30	111.00
1	P	75	VAL	C-N-CA	5.92	136.51	121.70
1	P	63	ALA	C-N-CA	5.83	136.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	140	GLY	N-CA-C	-5.75	98.72	113.10
1	B	197	TYR	CA-CB-CG	5.67	124.17	113.40
1	B	76	PHE	N-CA-C	5.47	125.78	111.00
1	B	53	TYR	N-CA-C	5.21	125.08	111.00
1	P	63	ALA	CA-C-N	5.14	128.52	117.20

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Peptide
1	A	194	HIS	Peptide
1	A	254	ARG	Peptide
1	A	5	LEU	Peptide
1	A	53	TYR	Peptide
1	A	6	GLY	Peptide
1	A	69	GLU	Peptide
1	A	72	THR	Peptide
1	A	8	ALA	Peptide
1	B	113	ALA	Peptide
1	B	254	ARG	Peptide
1	B	74	MET	Peptide
1	P	141	LEU	Peptide
1	P	57	GLN	Peptide
1	P	58	GLY	Peptide
1	P	70	GLN	Peptide
1	P	75	VAL	Peptide
1	P	76	PHE	Peptide
1	P	77	THR	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	2154	0	2136	112	0
1	B	2154	0	2136	110	0
1	P	2154	0	2136	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6462	0	6408	314	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 24.

All (314) 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:P:157:SER:HB2	1:P:158:PRO:HD2	1.42	1.01
1:A:6:GLY:HA2	1:A:8:ALA:HB2	1.43	1.00
1:P:157:SER:HB2	1:P:158:PRO:CD	1.99	0.92
1:P:77:THR:O	1:P:77:THR:HG22	1.69	0.91
1:A:69:GLU:HB2	1:A:70:GLN:HA	1.54	0.88
1:A:61:PRO:HG2	1:A:72:THR:H	1.41	0.86
1:B:145:ASN:O	1:B:147:ARG:HG3	1.76	0.86
1:A:220:ASN:ND2	1:B:173:ASN:O	2.10	0.85
1:B:31:SER:O	1:B:123:GLN:NE2	2.11	0.83
1:P:157:SER:CB	1:P:158:PRO:HD2	2.11	0.80
1:A:140:GLY:H	1:A:143:THR:HG22	1.44	0.80
1:P:158:PRO:HB3	1:P:196:ILE:HG12	1.60	0.80
1:B:16:GLU:OE1	1:B:103:ARG:NH1	2.15	0.79
1:A:8:ALA:HB3	1:A:11:PRO:HG3	1.61	0.79
1:P:71:GLU:HB3	1:P:72:THR:HA	1.64	0.79
1:P:86:PRO:HG3	1:P:138:TYR:HE2	1.48	0.78
1:P:148:LEU:HD12	1:P:171:LYS:HD2	1.65	0.77
1:P:189:LEU:HD12	1:P:226:SER:HB2	1.66	0.77
1:A:53:TYR:HE1	1:A:268:ARG:HB3	1.50	0.77
1:B:250:LEU:HB3	1:B:258:PRO:HG2	1.66	0.77
1:A:202:VAL:HG23	1:A:203:LEU:H	1.50	0.77
1:B:195:ARG:HA	1:B:196:ILE:HB	1.68	0.76
1:P:157:SER:CB	1:P:158:PRO:CD	2.59	0.74
1:B:9:GLU:HB3	1:B:10:ASN:C	2.08	0.74
1:P:75:VAL:HA	1:P:76:PHE:CG	2.23	0.73
1:B:152:LEU:HD13	1:B:278:LEU:HB2	1.70	0.72
1:A:93:LEU:HB2	1:B:76:PHE:CZ	2.24	0.72
1:P:73:ALA:N	1:P:74:MET:HA	2.04	0.72
1:B:72:THR:OG1	1:B:74:MET:N	2.18	0.71
1:A:8:ALA:O	1:A:11:PRO:HD3	1.91	0.71
1:A:76:PHE:HA	1:A:77:THR:HB	1.74	0.70
1:B:140:GLY:H	1:B:143:THR:HG22	1.57	0.70
1:P:228:VAL:HG12	1:P:277:THR:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:250:LEU:HB3	1:P:258:PRO:HG2	1.74	0.69
1:B:59:VAL:HG12	1:B:61:PRO:HD2	1.74	0.69
1:A:135:ARG:HD3	1:B:64:VAL:HG12	1.74	0.69
1:B:202:VAL:HG12	1:B:203:LEU:H	1.56	0.68
1:P:86:PRO:HG3	1:P:138:TYR:CE2	2.27	0.68
1:P:175:GLN:NE2	1:P:273:ASP:OD1	2.27	0.68
1:A:53:TYR:CE1	1:A:268:ARG:HB3	2.28	0.67
1:B:110:ASP:OD1	1:B:111:VAL:N	2.27	0.67
1:A:153:GLY:HA2	1:A:154:ASP:HB3	1.77	0.66
1:P:35:ARG:HH21	1:P:40:ILE:HG21	1.61	0.66
1:P:8:ALA:HB2	1:A:7:HIS:CD2	2.30	0.66
1:B:199:LYS:HZ3	1:B:202:VAL:H	1.43	0.65
1:A:245:MET:HG3	1:A:263:GLU:HG2	1.78	0.65
1:A:148:LEU:O	1:A:150:VAL:HG12	1.97	0.65
1:P:198:GLU:N	1:P:199:LYS:HA	2.12	0.65
1:P:103:ARG:CZ	1:P:103:ARG:HA	2.28	0.64
1:A:63:ALA:HB1	1:A:64:VAL:HB	1.79	0.64
1:B:197:TYR:HD1	1:B:198:GLU:HA	1.63	0.64
1:A:112:SER:HB3	1:B:270:LYS:HD3	1.78	0.63
1:A:7:HIS:CD2	1:A:9:GLU:H	2.16	0.63
1:A:88:ILE:HG12	1:A:263:GLU:HB2	1.80	0.62
1:B:195:ARG:HB2	1:B:204:GLU:HB2	1.82	0.62
1:P:75:VAL:HA	1:P:76:PHE:CD1	2.34	0.62
1:A:183:VAL:HG22	1:A:229:VAL:HG12	1.82	0.62
1:A:196:ILE:HG22	1:A:197:TYR:H	1.65	0.61
1:P:193:LEU:HB3	1:P:204:GLU:HG3	1.82	0.61
1:B:195:ARG:NH2	1:B:196:ILE:O	2.28	0.61
1:A:106:ASN:OD1	1:A:106:ASN:N	2.33	0.61
1:B:86:PRO:HG3	1:B:138:TYR:OH	2.01	0.60
1:P:77:THR:O	1:P:77:THR:CG2	2.41	0.60
1:B:222:LEU:HD21	1:B:227:GLY:HA2	1.82	0.60
1:A:56:PHE:CG	1:A:57:GLN:N	2.70	0.60
1:P:186:SER:N	1:P:226:SER:OG	2.34	0.60
1:B:52:PRO:HA	1:B:82:PHE:CD1	2.37	0.60
1:B:196:ILE:N	1:B:197:TYR:HA	2.16	0.59
1:B:77:THR:HA	1:B:78:ASP:CG	2.23	0.59
1:B:156:THR:O	1:B:195:ARG:NH1	2.36	0.59
1:A:158:PRO:N	1:A:159:GLY:HA2	2.17	0.59
1:B:81:LYS:O	1:B:83:LYS:NZ	2.25	0.59
1:B:12:LEU:HD12	1:B:17:TRP:HA	1.84	0.58
1:B:50:THR:HB	1:B:82:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:147:ARG:HG3	1:P:149:THR:H	1.68	0.58
1:B:96:TRP:CD2	1:B:97:ARG:HG3	2.39	0.58
1:A:256:ASN:O	1:A:257:HIS:ND1	2.36	0.58
1:A:52:PRO:HA	1:A:82:PHE:CE1	2.39	0.58
1:P:155:TRP:CE2	1:P:193:LEU:HD11	2.39	0.57
1:A:80:ARG:HB3	1:A:81:LYS:HA	1.86	0.57
1:A:3:ASP:O	1:A:4:PHE:HB3	2.04	0.57
1:P:50:THR:HB	1:P:82:PHE:HD2	1.68	0.57
1:P:253:SER:HB2	1:P:258:PRO:HG3	1.85	0.57
1:A:5:LEU:HG	1:A:6:GLY:N	2.20	0.57
1:P:223:ARG:CZ	1:P:224:GLY:H	2.18	0.57
1:B:75:VAL:HG22	1:B:77:THR:N	2.18	0.57
1:B:12:LEU:HB3	1:B:16:GLU:HB2	1.86	0.56
1:A:198:GLU:O	1:A:199:LYS:HG3	2.05	0.56
1:A:80:ARG:HB3	1:A:81:LYS:HD3	1.87	0.56
1:P:95:HIS:HB2	1:P:98:ASP:OD1	2.06	0.56
1:P:75:VAL:HG12	1:P:76:PHE:CE1	2.41	0.56
1:B:161:GLY:HA3	1:B:193:LEU:HD21	1.87	0.56
1:A:50:THR:HB	1:A:82:PHE:HD2	1.70	0.56
1:P:97:ARG:O	1:P:98:ASP:C	2.45	0.56
1:B:3:ASP:HA	1:B:4:PHE:HB3	1.88	0.56
1:P:49:GLN:HA	1:A:97:ARG:HH21	1.71	0.56
1:A:159:GLY:H	1:A:195:ARG:NH1	2.04	0.55
1:A:67:VAL:HG12	1:A:68:GLY:H	1.71	0.55
1:B:152:LEU:HG	1:B:153:GLY:H	1.71	0.55
1:P:23:THR:HG22	1:P:115:ALA:HB2	1.88	0.55
1:P:71:GLU:HB3	1:P:72:THR:CA	2.34	0.55
1:P:87:ILE:HD11	1:A:97:ARG:HD2	1.87	0.55
1:A:120:LEU:HD22	1:B:60:SER:HA	1.88	0.55
1:B:74:MET:HG3	1:B:75:VAL:H	1.71	0.55
1:P:103:ARG:NH1	1:P:103:ARG:HA	2.22	0.55
1:B:195:ARG:HD2	1:B:196:ILE:HB	1.87	0.55
1:P:16:GLU:HB3	1:P:109:LEU:HD22	1.89	0.55
1:A:65:ASP:OD1	1:A:66:ILE:N	2.26	0.54
1:A:69:GLU:HB2	1:A:70:GLN:CA	2.33	0.54
1:A:195:ARG:HG3	1:A:196:ILE:H	1.72	0.54
1:B:50:THR:HB	1:B:82:PHE:CD2	2.43	0.54
1:B:197:TYR:CD1	1:B:198:GLU:HA	2.41	0.54
1:B:145:ASN:C	1:B:147:ARG:HG3	2.27	0.54
1:B:99:ILE:HD12	1:B:257:HIS:HD2	1.73	0.54
1:B:80:ARG:CB	1:B:81:LYS:HA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HG22	1:B:229:VAL:HG12	1.88	0.54
1:P:256:ASN:O	1:P:257:HIS:ND1	2.41	0.54
1:B:50:THR:HB	1:B:82:PHE:HD2	1.73	0.54
1:P:56:PHE:CG	1:P:57:GLN:N	2.67	0.54
1:B:76:PHE:N	1:B:77:THR:OG1	2.41	0.54
1:P:165:ILE:HD12	1:P:211:LEU:HD23	1.90	0.53
1:P:127:GLU:HB2	1:P:221:ARG:HG2	1.89	0.53
1:A:194:HIS:ND1	1:A:194:HIS:O	2.42	0.53
1:B:190:TYR:O	1:B:194:HIS:N	2.41	0.53
1:B:197:TYR:H	1:B:198:GLU:HA	1.72	0.53
1:P:84:THR:HB	1:B:81:LYS:HE2	1.92	0.52
1:A:202:VAL:HG23	1:A:203:LEU:N	2.20	0.52
1:P:157:SER:HB2	1:P:158:PRO:HD3	1.86	0.52
1:A:11:PRO:HG2	1:A:257:HIS:CE1	2.45	0.52
1:A:81:LYS:HG3	1:A:82:PHE:H	1.73	0.52
1:B:204:GLU:HA	1:B:207:THR:HG22	1.92	0.52
1:A:13:ARG:HG3	1:A:14:GLU:H	1.74	0.52
1:P:65:ASP:OD1	1:P:66:ILE:HG13	2.10	0.52
1:A:220:ASN:HD21	1:B:173:ASN:C	2.10	0.51
1:P:72:THR:HB	1:P:73:ALA:C	2.30	0.51
1:B:245:MET:SD	1:B:245:MET:N	2.82	0.51
1:B:13:ARG:HB2	1:B:103:ARG:NH1	2.25	0.51
1:A:110:ASP:OD1	1:A:112:SER:OG	2.29	0.51
1:A:61:PRO:HG2	1:A:72:THR:N	2.20	0.51
1:B:75:VAL:HG13	1:B:77:THR:OG1	2.11	0.51
1:B:94:LEU:HD23	1:B:99:ILE:HD11	1.93	0.51
1:B:113:ALA:O	1:B:116:GLY:N	2.43	0.50
1:A:238:ASP:HB2	1:A:268:ARG:HD3	1.93	0.50
1:P:254:ARG:HB3	1:P:254:ARG:CZ	2.40	0.50
1:A:255:MET:HG2	1:A:256:ASN:H	1.75	0.50
1:A:250:LEU:HB3	1:A:258:PRO:HG2	1.92	0.50
1:P:174:GLU:O	1:P:175:GLN:HB2	2.11	0.50
1:B:81:LYS:CG	1:B:82:PHE:H	2.23	0.50
1:P:141:LEU:HD12	1:P:275:ILE:HG12	1.92	0.50
1:B:85:ILE:HG12	1:B:264:ALA:HB1	1.92	0.50
1:A:249:TYR:HE1	1:A:257:HIS:HB3	1.77	0.50
1:A:93:LEU:HB2	1:B:76:PHE:HZ	1.74	0.50
1:A:86:PRO:HG3	1:A:138:TYR:OH	2.12	0.50
1:A:253:SER:N	1:A:255:MET:O	2.45	0.49
1:P:55:GLU:CD	1:P:56:PHE:H	2.14	0.49
1:B:41:TYR:HD1	1:B:42:GLY:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:63:ALA:CB	1:P:64:VAL:HA	2.43	0.49
1:B:56:PHE:CG	1:B:57:GLN:N	2.78	0.49
1:A:13:ARG:N	1:A:16:GLU:OE1	2.45	0.49
1:B:9:GLU:HB3	1:B:11:PRO:N	2.27	0.49
1:B:195:ARG:HA	1:B:196:ILE:CB	2.41	0.49
1:P:52:PRO:HA	1:P:82:PHE:CE1	2.47	0.49
1:P:87:ILE:HD13	1:A:96:TRP:HE1	1.78	0.49
1:P:50:THR:CG2	1:B:81:LYS:HG2	2.43	0.49
1:P:81:LYS:HE3	1:B:84:THR:HB	1.95	0.49
1:B:189:LEU:O	1:B:193:LEU:HB2	2.13	0.49
1:A:133:ASP:HB2	1:A:138:TYR:HD2	1.78	0.49
1:A:155:TRP:HE1	1:A:161:GLY:HA2	1.77	0.49
1:P:183:VAL:HG22	1:P:229:VAL:HG12	1.95	0.49
1:A:181:TYR:HB2	1:A:212:ALA:HA	1.94	0.48
1:B:55:GLU:HB2	1:B:270:LYS:CG	2.43	0.48
1:B:193:LEU:O	1:B:195:ARG:HG2	2.13	0.48
1:A:81:LYS:HD2	1:A:82:PHE:CD1	2.49	0.48
1:B:4:PHE:N	1:B:5:LEU:HB2	2.28	0.48
1:P:248:ALA:HB3	1:P:260:ARG:HG3	1.96	0.48
1:P:72:THR:H	1:P:73:ALA:HA	1.77	0.48
1:B:64:VAL:HG21	1:B:69:GLU:HB2	1.96	0.48
1:P:52:PRO:HA	1:P:82:PHE:CD1	2.48	0.48
1:P:189:LEU:CD1	1:P:226:SER:HB2	2.42	0.48
1:A:191:SER:HA	1:A:194:HIS:HB2	1.95	0.48
1:B:165:ILE:HD12	1:B:211:LEU:HD23	1.96	0.47
1:A:81:LYS:CG	1:A:82:PHE:H	2.27	0.47
1:B:260:ARG:HD3	1:B:262:LEU:HD21	1.95	0.47
1:P:85:ILE:HG13	1:P:86:PRO:HD2	1.94	0.47
1:A:160:GLY:H	1:A:198:GLU:HG2	1.78	0.47
1:A:251:GLY:O	1:A:258:PRO:HD2	2.14	0.47
1:A:205:ILE:HG23	1:A:209:ARG:HH21	1.78	0.47
1:A:145:ASN:ND2	1:A:146:GLY:H	2.11	0.47
1:B:71:GLU:OE1	1:B:72:THR:HA	2.14	0.47
1:P:272:PRO:HA	1:P:275:ILE:HD13	1.94	0.47
1:A:210:GLN:O	1:A:213:SER:OG	2.32	0.47
1:A:272:PRO:HA	1:A:275:ILE:HD13	1.96	0.47
1:P:62:GLY:O	1:P:64:VAL:HG22	2.15	0.47
1:P:3:ASP:OD1	1:P:3:ASP:N	2.35	0.47
1:P:197:TYR:C	1:P:199:LYS:HA	2.35	0.47
1:B:9:GLU:OE2	1:B:9:GLU:N	2.47	0.47
1:A:223:ARG:CZ	1:A:224:GLY:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD21	1:A:227:GLY:HA2	1.97	0.46
1:A:5:LEU:HD13	1:A:100:GLU:OE1	2.14	0.46
1:P:91:ASP:OD2	1:P:260:ARG:HB3	2.15	0.46
1:P:71:GLU:CB	1:P:72:THR:HA	2.35	0.46
1:A:4:PHE:CG	1:A:4:PHE:O	2.69	0.46
1:P:77:THR:O	1:P:79:ALA:N	2.49	0.46
1:P:123:GLN:HG3	1:P:221:ARG:HH21	1.81	0.46
1:P:85:ILE:HD13	1:P:242:SER:HB2	1.96	0.46
1:B:80:ARG:HB3	1:B:81:LYS:HA	1.97	0.46
1:A:81:LYS:HD3	1:A:81:LYS:HA	1.72	0.46
1:P:142:MET:O	1:P:147:ARG:NH1	2.37	0.46
1:A:150:VAL:HG23	1:A:151:PRO:HD2	1.98	0.46
1:P:98:ASP:O	1:P:101:ALA:N	2.49	0.46
1:P:235:GLU:HA	1:P:270:LYS:HD2	1.98	0.46
1:B:163:GLN:O	1:B:167:GLU:HG2	2.16	0.46
1:A:60:SER:HA	1:A:61:PRO:HD3	1.65	0.46
1:P:142:MET:C	1:P:147:ARG:HH22	2.19	0.46
1:B:229:VAL:HG22	1:B:276:CYS:HB2	1.96	0.46
1:B:153:GLY:HA3	1:B:164:ALA:HB2	1.97	0.45
1:A:92:PHE:HA	1:B:74:MET:HB3	1.97	0.45
1:P:60:SER:HA	1:P:61:PRO:HD3	1.81	0.45
1:A:6:GLY:CA	1:A:8:ALA:HB2	2.30	0.45
1:A:145:ASN:CG	1:A:146:GLY:H	2.19	0.45
1:B:148:LEU:HD13	1:B:171:LYS:HB3	1.99	0.45
1:B:140:GLY:H	1:B:143:THR:CG2	2.28	0.45
1:P:50:THR:HB	1:P:82:PHE:CD2	2.48	0.45
1:B:133:ASP:HB2	1:B:138:TYR:HD2	1.81	0.45
1:B:51:VAL:HG11	1:B:240:ALA:HB1	1.99	0.45
1:B:230:VAL:HA	1:B:274:ALA:O	2.17	0.45
1:A:13:ARG:HE	1:A:103:ARG:HE	1.63	0.45
1:B:122:ALA:O	1:B:125:GLU:HB3	2.16	0.45
1:B:93:LEU:HA	1:B:258:PRO:HA	1.97	0.45
1:P:161:GLY:HA2	1:P:193:LEU:HD22	1.96	0.45
1:A:256:ASN:O	1:A:257:HIS:CG	2.69	0.45
1:A:198:GLU:OE1	1:A:200:THR:OG1	2.22	0.45
1:A:13:ARG:HH21	1:A:103:ARG:HE	1.64	0.44
1:A:165:ILE:HD12	1:A:211:LEU:HD23	2.00	0.44
1:P:151:PRO:HD2	1:P:167:GLU:OE2	2.17	0.44
1:B:55:GLU:HB2	1:B:270:LYS:HG2	1.99	0.44
1:B:7:HIS:ND1	1:B:7:HIS:O	2.50	0.44
1:A:135:ARG:NH1	1:A:135:ARG:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD11	1:B:56:PHE:HE1	1.83	0.44
1:P:63:ALA:HB3	1:P:64:VAL:HG13	1.99	0.44
1:B:158:PRO:HA	1:B:195:ARG:HH22	1.83	0.44
1:P:199:LYS:HB3	1:P:199:LYS:HE3	1.83	0.44
1:P:155:TRP:CD2	1:P:193:LEU:HD11	2.53	0.44
1:A:50:THR:HB	1:A:82:PHE:CD2	2.51	0.44
1:B:4:PHE:H	1:B:5:LEU:HB2	1.82	0.44
1:P:65:ASP:OD1	1:P:66:ILE:N	2.51	0.43
1:B:202:VAL:HG11	1:B:206:GLU:HG3	1.99	0.43
1:P:254:ARG:NH1	1:P:254:ARG:HB3	2.33	0.43
1:P:249:TYR:HB3	1:P:251:GLY:HA2	2.00	0.43
1:B:206:GLU:O	1:B:210:GLN:HB2	2.19	0.43
1:P:160:GLY:HA2	1:P:161:GLY:HA3	1.69	0.43
1:A:209:ARG:O	1:A:213:SER:HA	2.19	0.43
1:A:125:GLU:O	1:A:129:ILE:HG13	2.19	0.43
1:B:75:VAL:C	1:B:76:PHE:CD1	2.92	0.43
1:A:88:ILE:CG1	1:A:263:GLU:HB2	2.47	0.43
1:B:223:ARG:CZ	1:B:224:GLY:H	2.31	0.43
1:P:85:ILE:HA	1:P:86:PRO:HD3	1.78	0.43
1:B:81:LYS:HG3	1:B:82:PHE:H	1.83	0.43
1:P:146:GLY:HA3	1:P:272:PRO:O	2.19	0.43
1:A:190:TYR:O	1:A:194:HIS:N	2.53	0.42
1:B:30:ARG:HA	1:B:30:ARG:HH11	1.84	0.42
1:A:94:LEU:HB2	1:A:259:PHE:CE1	2.54	0.42
1:A:159:GLY:H	1:A:195:ARG:CZ	2.32	0.42
1:P:124:GLN:HG2	1:P:124:GLN:O	2.18	0.42
1:A:43:PRO:HA	1:A:241:VAL:O	2.20	0.42
1:P:75:VAL:HA	1:P:76:PHE:CD2	2.54	0.42
1:P:82:PHE:CD1	1:P:82:PHE:N	2.85	0.42
1:P:66:ILE:HG22	1:P:67:VAL:H	1.85	0.42
1:B:195:ARG:HB3	1:B:196:ILE:C	2.40	0.42
1:B:64:VAL:HG23	1:B:65:ASP:H	1.85	0.42
1:P:234:ARG:HB3	1:P:234:ARG:NH1	2.34	0.42
1:P:205:ILE:HG23	1:P:209:ARG:HH21	1.85	0.42
1:A:230:VAL:HA	1:A:274:ALA:O	2.20	0.42
1:P:233:GLY:O	1:P:236:ASN:HB3	2.19	0.42
1:A:249:TYR:CE1	1:A:257:HIS:HB3	2.54	0.42
1:P:51:VAL:HG21	1:P:266:LEU:HD12	2.02	0.42
1:B:38:LEU:HD23	1:B:239:LEU:HB2	2.01	0.42
1:P:10:ASN:O	1:P:12:LEU:N	2.53	0.42
1:B:35:ARG:HH21	1:B:40:ILE:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PRO:HD3	1:A:219:SER:O	2.19	0.42
1:B:59:VAL:HG12	1:B:61:PRO:CD	2.46	0.41
1:A:159:GLY:HA3	1:A:160:GLY:HA2	1.77	0.41
1:A:56:PHE:CD1	1:A:272:PRO:HD2	2.55	0.41
1:P:197:TYR:CD1	1:P:197:TYR:N	2.87	0.41
1:P:275:ILE:HD12	1:P:275:ILE:N	2.35	0.41
1:B:131:TYR:OH	1:B:223:ARG:HD2	2.20	0.41
1:A:155:TRP:NE1	1:A:161:GLY:HA2	2.35	0.41
1:A:197:TYR:HA	1:A:202:VAL:O	2.20	0.41
1:P:38:LEU:HD11	1:P:237:MET:O	2.20	0.41
1:P:180:PRO:HG2	1:P:232:THR:CG2	2.51	0.41
1:B:161:GLY:O	1:B:165:ILE:HG12	2.20	0.41
1:A:12:LEU:HD12	1:A:17:TRP:HE3	1.86	0.41
1:A:271:HIS:CD2	1:A:273:ASP:HB2	2.55	0.41
1:P:227:GLY:O	1:P:277:THR:HA	2.20	0.41
1:B:82:PHE:CD1	1:B:82:PHE:N	2.85	0.41
1:A:103:ARG:N	1:A:104:THR:HA	2.36	0.41
1:A:5:LEU:CG	1:A:6:GLY:N	2.84	0.41
1:A:76:PHE:HA	1:A:77:THR:CB	2.43	0.41
1:B:186:SER:OG	1:B:223:ARG:O	2.39	0.41
1:P:12:LEU:HD11	1:P:20:LEU:HD22	2.01	0.41
1:P:226:SER:O	1:P:278:LEU:HD13	2.21	0.41
1:B:55:GLU:HB2	1:B:270:LYS:HG3	2.03	0.41
1:P:236:ASN:HD21	1:P:274:ALA:HB2	1.85	0.41
1:P:21:ASN:O	1:P:25:ILE:HG23	2.21	0.41
1:A:255:MET:SD	1:A:255:MET:N	2.94	0.40
1:A:64:VAL:HG13	1:A:65:ASP:N	2.35	0.40
1:A:51:VAL:HG21	1:A:266:LEU:HD12	2.03	0.40
1:B:11:PRO:HB3	1:B:257:HIS:CD2	2.56	0.40
1:P:197:TYR:CG	1:P:199:LYS:HG3	2.56	0.40
1:P:50:THR:HB	1:P:82:PHE:HB2	2.03	0.40
1:B:211:LEU:HA	1:B:211:LEU:HD12	1.92	0.40
1:B:74:MET:SD	1:B:75:VAL:HG12	2.61	0.40
1:P:55:GLU:HB2	1:P:270:LYS:HG3	2.02	0.40
1:P:8:ALA:HB2	1:A:7:HIS:CG	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	275/287 (96%)	238 (86%)	37 (14%)	0	100 100
1	B	275/287 (96%)	233 (85%)	39 (14%)	3 (1%)	17 64
1	P	275/287 (96%)	231 (84%)	40 (14%)	4 (2%)	13 58
All	All	825/861 (96%)	702 (85%)	116 (14%)	7 (1%)	29 69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	157	SER
1	B	75	VAL
1	P	66	ILE
1	P	158	PRO
1	B	66	ILE
1	P	146	GLY
1	B	146	GLY

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	224/230 (97%)	194 (87%)	30 (13%)	5 29
1	B	224/230 (97%)	195 (87%)	29 (13%)	5 30
1	P	224/230 (97%)	201 (90%)	23 (10%)	9 40
All	All	672/690 (97%)	590 (88%)	82 (12%)	10 32

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	19	ARG
1	P	53	TYR
1	P	55	GLU
1	P	59	VAL
1	P	64	VAL
1	P	70	GLN
1	P	71	GLU
1	P	80	ARG
1	P	97	ARG
1	P	103	ARG
1	P	107	MET
1	P	141	LEU
1	P	162	PHE
1	P	174	GLU
1	P	195	ARG
1	P	197	TYR
1	P	204	GLU
1	P	221	ARG
1	P	231	SER
1	P	234	ARG
1	P	250	LEU
1	P	254	ARG
1	P	268	ARG
1	A	5	LEU
1	A	7	HIS
1	A	19	ARG
1	A	53	TYR
1	A	57	GLN
1	A	64	VAL
1	A	70	GLN
1	A	80	ARG
1	A	88	ILE
1	A	95	HIS
1	A	106	ASN
1	A	133	ASP
1	A	135	ARG
1	A	136	LEU
1	A	148	LEU
1	A	155	TRP
1	A	162	PHE
1	A	192	GLN
1	A	193	LEU

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Mol	Chain	Res	Type
1	A	195	ARG
1	A	199	LYS
1	A	200	THR
1	A	244	ASP
1	A	245	MET
1	A	250	LEU
1	A	254	ARG
1	A	255	MET
1	A	256	ASN
1	A	268	ARG
1	A	276	CYS
1	B	4	PHE
1	B	5	LEU
1	B	30	ARG
1	B	39	ASP
1	B	41	TYR
1	B	44	LEU
1	B	53	TYR
1	B	55	GLU
1	B	64	VAL
1	B	72	THR
1	B	80	ARG
1	B	96	TRP
1	B	103	ARG
1	B	107	MET
1	B	129	ILE
1	B	133	ASP
1	B	135	ARG
1	B	155	TRP
1	B	171	LYS
1	B	188	ARG
1	B	193	LEU
1	B	197	TYR
1	B	203	LEU
1	B	234	ARG
1	B	245	MET
1	B	249	TYR
1	B	255	MET
1	B	268	ARG
1	B	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	105	HIS
1	P	124	GLN
1	P	220	ASN
1	P	236	ASN
1	P	271	HIS
1	A	145	ASN

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.