



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 04:36 PM EDT

PDB ID : 5LII
EMDB ID: : EMD-4053
Title : bacteriophage phi812K1-420 major capsid protein
Authors : Novacek, J.; Siborova, M.; Benesik, M.; Pantucek, R.; Doskar, J.; Plevka, P.
Deposited on : unknown
Resolution : 3.80 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 ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

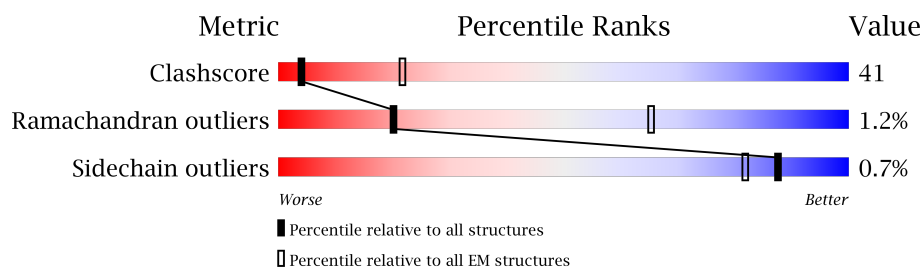
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	P	463	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3098 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 Major capsid protein.

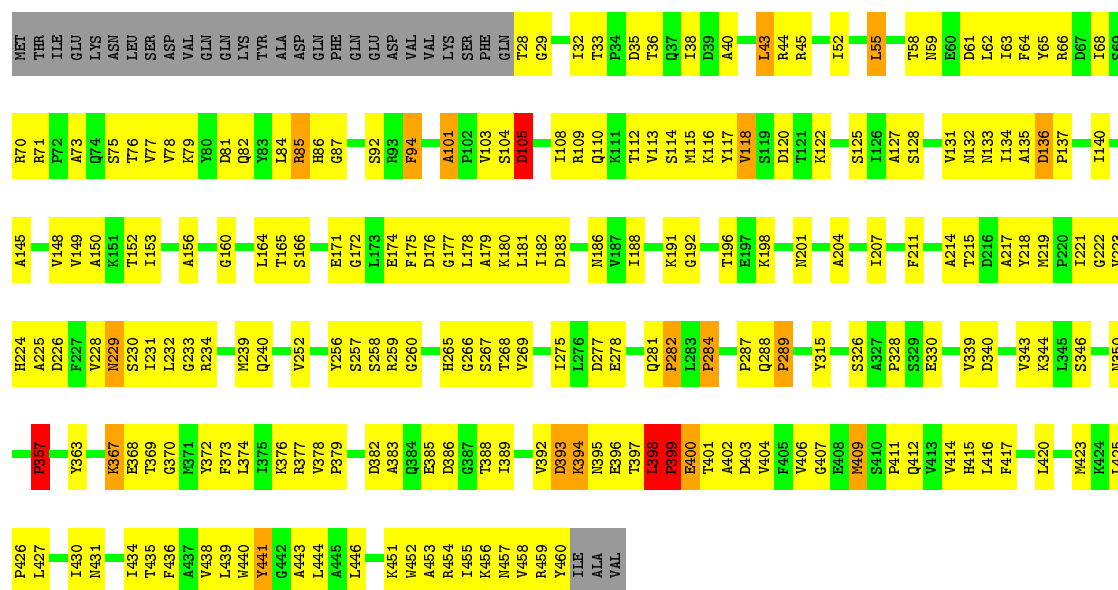
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	P	433	3098	1947	545	595	11	0	0

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 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: Major capsid protein

Chain P: 



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	12018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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	P	0.69	2/3148 (0.1%)	1.18	21/4286 (0.5%)

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	P	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	101	ALA	C-N	-10.76	1.13	1.34
1	P	409	MET	CA-CB	-5.24	1.42	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	399	PRO	N-CA-CB	-31.12	65.95	103.30
1	P	399	PRO	N-CA-C	19.37	162.47	112.10
1	P	398	LEU	C-N-CD	-16.31	84.72	120.60
1	P	399	PRO	N-CD-CG	-15.58	79.83	103.20
1	P	118	VAL	N-CA-CB	-15.16	78.16	111.50
1	P	398	LEU	N-CA-C	14.20	149.33	111.00
1	P	398	LEU	CB-CA-C	-7.27	96.38	110.20
1	P	328	PRO	N-CA-CB	6.86	111.53	103.30
1	P	289	PRO	N-CA-CB	6.81	111.47	103.30
1	P	357	PRO	N-CA-CB	6.69	111.33	103.30
1	P	229	ASN	CB-CA-C	-6.28	97.85	110.40
1	P	105	ASP	C-N-CD	6.18	141.39	128.40
1	P	287	PRO	N-CA-CB	5.94	110.43	103.30
1	P	282	PRO	N-CA-CB	5.90	110.38	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	400	GLU	N-CA-CB	-5.85	100.08	110.60
1	P	284	PRO	N-CA-CB	5.80	110.26	103.30
1	P	133	ASN	N-CA-C	5.66	126.28	111.00
1	P	55	LEU	CA-CB-CG	5.63	128.25	115.30
1	P	43	LEU	CA-CB-CG	5.20	127.26	115.30
1	P	393	ASP	C-N-CA	-5.07	109.02	121.70
1	P	441	TYR	CA-CB-CG	-5.04	103.83	113.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	105	ASP	Peptide
1	P	136	ASP	Peptide
1	P	175	PHE	Peptide
1	P	357	PRO	Peptide
1	P	367	LYS	Peptide
1	P	385	GLU	Peptide
1	P	394	LYS	Peptide
1	P	398	LEU	Peptide
1	P	82	GLN	Peptide
1	P	85	ARG	Peptide
1	P	94	PHE	Peptide

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	P	3098	0	2832	241	0
All	All	3098	0	2832	241	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 41.

All (241) 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:117:TYR:CE2	1:P:152:THR:HG21	1.20	1.66
1:P:379:PRO:CB	1:P:398:LEU:HD11	1.41	1.47
1:P:117:TYR:CE2	1:P:152:THR:CG2	1.99	1.41
1:P:117:TYR:CZ	1:P:152:THR:HG21	1.55	1.41
1:P:379:PRO:HB3	1:P:398:LEU:CD1	1.63	1.27
1:P:394:LYS:NZ	1:P:398:LEU:CD1	2.16	1.09
1:P:118:VAL:HG12	1:P:439:LEU:HA	1.33	1.07
1:P:379:PRO:CG	1:P:398:LEU:HD11	1.86	1.05
1:P:397:THR:O	1:P:397:THR:HG23	1.62	0.99
1:P:117:TYR:HE2	1:P:152:THR:HG21	1.17	0.96
1:P:394:LYS:HZ2	1:P:398:LEU:HD12	1.31	0.96
1:P:229:ASN:O	1:P:229:ASN:OD1	1.85	0.92
1:P:117:TYR:HE2	1:P:152:THR:CG2	1.66	0.89
1:P:394:LYS:NZ	1:P:398:LEU:HD12	1.82	0.89
1:P:379:PRO:HB3	1:P:398:LEU:HD11	0.88	0.88
1:P:397:THR:HA	1:P:457:ASN:HD21	1.37	0.88
1:P:117:TYR:HE2	1:P:152:THR:CB	1.86	0.87
1:P:118:VAL:CG1	1:P:439:LEU:HA	2.04	0.86
1:P:233:GLY:O	1:P:234:ARG:NH1	2.08	0.86
1:P:379:PRO:CB	1:P:398:LEU:CD1	2.36	0.86
1:P:122:LYS:HB2	1:P:436:PHE:HB3	1.57	0.85
1:P:394:LYS:HZ1	1:P:398:LEU:CD1	1.85	0.85
1:P:118:VAL:HG12	1:P:439:LEU:CA	2.07	0.83
1:P:394:LYS:HZ2	1:P:398:LEU:CD1	1.86	0.81
1:P:32:ILE:HG22	1:P:43:LEU:HD23	1.61	0.81
1:P:379:PRO:HB3	1:P:398:LEU:CG	2.11	0.81
1:P:79:LYS:NZ	1:P:112:THR:O	2.15	0.80
1:P:394:LYS:HZ1	1:P:398:LEU:HD13	1.45	0.79
1:P:377:ARG:HG3	1:P:399:PRO:O	1.83	0.77
1:P:117:TYR:CD2	1:P:117:TYR:O	2.37	0.77
1:P:115:MET:HG3	1:P:174:GLU:HA	1.67	0.77
1:P:116:LYS:HG2	1:P:440:TRP:HE1	1.47	0.76
1:P:117:TYR:O	1:P:117:TYR:CG	2.38	0.75
1:P:180:LYS:HZ1	1:P:446:LEU:HD12	1.49	0.75
1:P:458:VAL:HG12	1:P:459:ARG:H	1.52	0.75
1:P:397:THR:CG2	1:P:398:LEU:HG	2.16	0.74
1:P:379:PRO:HG3	1:P:398:LEU:HD11	1.67	0.74
1:P:120:ASP:OD2	1:P:438:VAL:N	2.15	0.74
1:P:35:ASP:O	1:P:45:ARG:NH2	2.19	0.74
1:P:407:GLY:HA3	1:P:452:TRP:CE3	2.23	0.74
1:P:63:ILE:HG22	1:P:66:ARG:HH12	1.53	0.72
1:P:368:GLU:HG3	1:P:369:THR:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:258:SER:OG	1:P:259:ARG:NH1	2.23	0.71
1:P:101:ALA:O	1:P:103:VAL:N	2.24	0.70
1:P:397:THR:HG23	1:P:398:LEU:HG	1.72	0.69
1:P:165:THR:HG22	1:P:166:SER:H	1.57	0.69
1:P:222:GLY:O	1:P:460:TYR:HA	1.91	0.69
1:P:75:SER:OG	1:P:78:VAL:O	2.09	0.69
1:P:117:TYR:CZ	1:P:152:THR:CG2	2.50	0.68
1:P:435:THR:HG22	1:P:436:PHE:H	1.59	0.67
1:P:58:THR:HG22	1:P:59:ASN:H	1.58	0.67
1:P:267:SER:HB3	1:P:269:VAL:HG22	1.76	0.67
1:P:218:TYR:CE2	1:P:409:MET:HE1	2.30	0.67
1:P:388:THR:HG22	1:P:389:ILE:H	1.58	0.67
1:P:394:LYS:NZ	1:P:398:LEU:HD13	2.02	0.67
1:P:73:ALA:HB2	1:P:417:PHE:CD1	2.29	0.67
1:P:278:GLU:O	1:P:281:GLN:N	2.27	0.66
1:P:131:VAL:HG22	1:P:132:ASN:H	1.60	0.65
1:P:117:TYR:CE2	1:P:152:THR:HG22	2.22	0.65
1:P:402:ALA:HB1	1:P:457:ASN:H	1.62	0.65
1:P:183:ASP:OD1	1:P:183:ASP:N	2.27	0.64
1:P:394:LYS:CE	1:P:398:LEU:HD12	2.28	0.64
1:P:379:PRO:HG3	1:P:398:LEU:CD1	2.27	0.63
1:P:191:LYS:HZ2	1:P:340:ASP:H	1.45	0.63
1:P:134:ILE:HG22	1:P:135:ALA:N	2.14	0.62
1:P:137:PRO:O	1:P:140:ILE:N	2.32	0.62
1:P:201:ASN:OD1	1:P:257:SER:OG	2.17	0.62
1:P:117:TYR:HE2	1:P:152:THR:HB	1.65	0.62
1:P:116:LYS:HG2	1:P:440:TRP:NE1	2.15	0.62
1:P:218:TYR:HE2	1:P:409:MET:HE1	1.65	0.61
1:P:71:ARG:HB2	1:P:415:HIS:CE1	2.35	0.60
1:P:232:LEU:HG	1:P:233:GLY:H	1.67	0.60
1:P:61:ASP:OD2	1:P:268:THR:OG1	2.20	0.60
1:P:75:SER:OG	1:P:76:THR:N	2.33	0.60
1:P:394:LYS:CE	1:P:398:LEU:CD1	2.80	0.59
1:P:43:LEU:HD12	1:P:44:ARG:H	1.68	0.59
1:P:379:PRO:HG3	1:P:394:LYS:HZ1	1.68	0.59
1:P:186:ASN:HA	1:P:454:ARG:O	2.02	0.59
1:P:403:ASP:N	1:P:403:ASP:OD1	2.35	0.59
1:P:379:PRO:CG	1:P:398:LEU:CD1	2.71	0.58
1:P:117:TYR:OH	1:P:152:THR:HG21	1.98	0.57
1:P:397:THR:HG22	1:P:398:LEU:HG	1.86	0.57
1:P:73:ALA:HB2	1:P:417:PHE:HD1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:79:LYS:NZ	1:P:112:THR:HG23	2.20	0.57
1:P:33:THR:N	1:P:35:ASP:OD2	2.37	0.57
1:P:397:THR:HA	1:P:457:ASN:ND2	2.14	0.57
1:P:174:GLU:OE2	1:P:443:ALA:HA	2.05	0.57
1:P:215:THR:N	1:P:407:GLY:O	2.37	0.56
1:P:79:LYS:HE3	1:P:417:PHE:CE2	2.40	0.56
1:P:181:LEU:CD1	1:P:452:TRP:HB3	2.36	0.56
1:P:71:ARG:HB2	1:P:415:HIS:HE1	1.71	0.56
1:P:177:GLY:HA2	1:P:444:LEU:HD22	1.89	0.55
1:P:179:ALA:O	1:P:182:ILE:HG12	2.06	0.55
1:P:226:ASP:O	1:P:230:SER:OG	2.21	0.55
1:P:79:LYS:HE3	1:P:417:PHE:CD2	2.41	0.55
1:P:118:VAL:HG23	1:P:118:VAL:O	2.06	0.55
1:P:256:TYR:CB	1:P:260:GLY:HA2	2.36	0.55
1:P:367:LYS:CB	1:P:398:LEU:HD13	2.37	0.55
1:P:134:ILE:O	1:P:135:ALA:C	2.44	0.54
1:P:211:PHE:O	1:P:451:LYS:HE2	2.07	0.54
1:P:191:LYS:HZ3	1:P:339:VAL:HA	1.72	0.54
1:P:430:ILE:HG13	1:P:431:ASN:N	2.21	0.54
1:P:346:SER:O	1:P:393:ASP:HA	2.08	0.54
1:P:86:HIS:CG	1:P:87:GLY:H	2.27	0.53
1:P:122:LYS:HE2	1:P:145:ALA:HB2	1.90	0.53
1:P:188:ILE:HG13	1:P:456:LYS:HZ2	1.73	0.53
1:P:420:LEU:HG	1:P:440:TRP:HB2	1.91	0.53
1:P:38:ILE:C	1:P:40:ALA:H	2.12	0.53
1:P:396:GLU:O	1:P:397:THR:HG22	2.09	0.52
1:P:160:GLY:C	1:P:176:ASP:HB2	2.30	0.52
1:P:369:THR:HB	1:P:374:LEU:HA	1.91	0.52
1:P:149:VAL:O	1:P:152:THR:N	2.43	0.52
1:P:180:LYS:HZ3	1:P:446:LEU:HB2	1.75	0.52
1:P:160:GLY:O	1:P:176:ASP:HB2	2.09	0.52
1:P:118:VAL:HG12	1:P:439:LEU:C	2.29	0.52
1:P:84:LEU:HD23	1:P:85:ARG:N	2.25	0.52
1:P:171:GLU:CD	1:P:172:GLY:H	2.13	0.52
1:P:104:SER:OG	1:P:105:ASP:OD1	2.22	0.52
1:P:196:THR:C	1:P:198:LYS:H	2.13	0.51
1:P:423:MET:O	1:P:438:VAL:HA	2.10	0.51
1:P:29:GLY:N	1:P:43:LEU:HD13	2.26	0.51
1:P:116:LYS:CG	1:P:440:TRP:HE1	2.18	0.51
1:P:122:LYS:HG3	1:P:436:PHE:HD2	1.74	0.51
1:P:181:LEU:HD11	1:P:452:TRP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:81:ASP:HB3	1:P:110:GLN:O	2.11	0.50
1:P:118:VAL:HG11	1:P:439:LEU:HD23	1.94	0.50
1:P:372:TYR:CD2	1:P:372:TYR:N	2.79	0.50
1:P:367:LYS:H	1:P:379:PRO:CD	2.25	0.50
1:P:92:SER:O	1:P:94:PHE:N	2.45	0.50
1:P:458:VAL:HG12	1:P:459:ARG:N	2.24	0.50
1:P:420:LEU:HD13	1:P:423:MET:CE	2.42	0.50
1:P:171:GLU:OE1	1:P:172:GLY:N	2.45	0.49
1:P:192:GLY:HA2	1:P:457:ASN:O	2.12	0.49
1:P:411:PRO:O	1:P:415:HIS:HD2	1.94	0.49
1:P:378:VAL:O	1:P:378:VAL:HG13	2.12	0.49
1:P:28:THR:C	1:P:43:LEU:HD13	2.33	0.49
1:P:401:THR:OG1	1:P:460:TYR:HB3	2.12	0.49
1:P:256:TYR:HB3	1:P:260:GLY:HA2	1.95	0.49
1:P:219:MET:O	1:P:265:HIS:CE1	2.66	0.49
1:P:414:VAL:HG22	1:P:446:LEU:CD2	2.42	0.49
1:P:131:VAL:HG13	1:P:132:ASN:O	2.13	0.49
1:P:434:ILE:HG22	1:P:435:THR:O	2.13	0.48
1:P:36:THR:HG23	1:P:38:ILE:HG13	1.96	0.48
1:P:223:VAL:O	1:P:226:ASP:N	2.46	0.48
1:P:125:SER:O	1:P:128:SER:N	2.47	0.48
1:P:439:LEU:HD22	1:P:440:TRP:CZ3	2.48	0.48
1:P:92:SER:C	1:P:94:PHE:H	2.15	0.48
1:P:344:LYS:CB	1:P:395:ASN:H	2.26	0.48
1:P:388:THR:HG22	1:P:389:ILE:HD12	1.95	0.48
1:P:370:GLY:HA2	1:P:399:PRO:CG	2.44	0.48
1:P:207:ILE:O	1:P:207:ILE:HG12	2.14	0.48
1:P:406:VAL:HG23	1:P:453:ALA:HB3	1.96	0.48
1:P:223:VAL:HG13	1:P:224:HIS:H	1.79	0.48
1:P:427:LEU:HD22	1:P:435:THR:HG21	1.95	0.47
1:P:223:VAL:HG13	1:P:224:HIS:N	2.29	0.47
1:P:230:SER:OG	1:P:231:ILE:HG12	2.14	0.47
1:P:153:ILE:O	1:P:156:ALA:N	2.47	0.47
1:P:233:GLY:C	1:P:234:ARG:HH11	2.13	0.47
1:P:392:VAL:HG12	1:P:393:ASP:O	2.14	0.47
1:P:256:TYR:HB2	1:P:260:GLY:HA2	1.95	0.47
1:P:32:ILE:HG13	1:P:33:THR:HB	1.96	0.47
1:P:343:VAL:O	1:P:395:ASN:HB2	2.15	0.47
1:P:414:VAL:HG22	1:P:446:LEU:HD21	1.96	0.47
1:P:149:VAL:HG13	1:P:150:ALA:N	2.30	0.47
1:P:420:LEU:CD1	1:P:440:TRP:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:426:PRO:C	1:P:427:LEU:HD12	2.36	0.46
1:P:75:SER:OG	1:P:76:THR:O	2.32	0.46
1:P:204:ALA:HA	1:P:207:ILE:HG22	1.96	0.46
1:P:420:LEU:HD13	1:P:423:MET:HE3	1.97	0.46
1:P:225:ALA:O	1:P:228:VAL:N	2.26	0.46
1:P:131:VAL:HG22	1:P:132:ASN:N	2.30	0.46
1:P:229:ASN:C	1:P:229:ASN:OD1	2.52	0.46
1:P:350:ASN:O	1:P:389:ILE:HG23	2.15	0.46
1:P:58:THR:HG22	1:P:59:ASN:N	2.28	0.46
1:P:108:ILE:HG22	1:P:109:ARG:N	2.31	0.46
1:P:326:SER:O	1:P:363:TYR:HA	2.15	0.46
1:P:164:LEU:O	1:P:383:ALA:HB1	2.16	0.46
1:P:71:ARG:NE	1:P:415:HIS:NE2	2.64	0.45
1:P:368:GLU:HG3	1:P:369:THR:N	2.28	0.45
1:P:420:LEU:HD12	1:P:420:LEU:O	2.17	0.45
1:P:70:ARG:HG2	1:P:416:LEU:HB3	1.97	0.45
1:P:177:GLY:O	1:P:178:LEU:HD23	2.17	0.45
1:P:315:TYR:HA	1:P:330:GLU:CB	2.47	0.45
1:P:76:THR:HG22	1:P:77:VAL:H	1.81	0.45
1:P:379:PRO:HA	1:P:397:THR:HG21	1.99	0.44
1:P:218:TYR:O	1:P:404:VAL:HG23	2.17	0.44
1:P:370:GLY:HA2	1:P:399:PRO:HG3	1.99	0.44
1:P:372:TYR:CG	1:P:373:PHE:N	2.86	0.44
1:P:217:ALA:HB2	1:P:406:VAL:HG12	1.98	0.44
1:P:435:THR:HG22	1:P:436:PHE:N	2.31	0.44
1:P:64:PHE:O	1:P:68:ILE:HG12	2.18	0.44
1:P:258:SER:C	1:P:259:ARG:HG3	2.38	0.44
1:P:79:LYS:HZ3	1:P:112:THR:HG23	1.82	0.44
1:P:367:LYS:H	1:P:379:PRO:HD3	1.83	0.44
1:P:178:LEU:HD13	1:P:452:TRP:HE1	1.83	0.44
1:P:118:VAL:CG1	1:P:439:LEU:CA	2.84	0.43
1:P:180:LYS:NZ	1:P:446:LEU:HD12	2.25	0.43
1:P:113:VAL:HG22	1:P:114:SER:O	2.18	0.43
1:P:62:LEU:HA	1:P:62:LEU:HD23	1.65	0.43
1:P:224:HIS:HE1	1:P:252:VAL:O	2.01	0.43
1:P:439:LEU:HB3	1:P:440:TRP:H	1.51	0.43
1:P:137:PRO:O	1:P:140:ILE:HG22	2.18	0.43
1:P:64:PHE:CZ	1:P:68:ILE:HD11	2.52	0.43
1:P:134:ILE:O	1:P:136:ASP:HB2	2.18	0.43
1:P:224:HIS:O	1:P:224:HIS:CG	2.72	0.43
1:P:412:GLN:OE1	1:P:412:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:55:LEU:HD12	1:P:55:LEU:O	2.19	0.43
1:P:181:LEU:HD13	1:P:452:TRP:HD1	1.84	0.43
1:P:134:ILE:CG2	1:P:135:ALA:N	2.81	0.42
1:P:221:ILE:HG12	1:P:221:ILE:O	2.20	0.42
1:P:239:MET:HG3	1:P:240:GLN:N	2.35	0.42
1:P:386:ASP:HB3	1:P:388:THR:O	2.20	0.42
1:P:35:ASP:HB2	1:P:45:ARG:NH2	2.35	0.42
1:P:265:HIS:HD1	1:P:266:GLY:H	1.65	0.41
1:P:394:LYS:HG2	1:P:395:ASN:HA	2.02	0.41
1:P:63:ILE:O	1:P:66:ARG:N	2.46	0.41
1:P:207:ILE:HG21	1:P:214:ALA:HB2	2.01	0.41
1:P:275:ILE:C	1:P:277:ASP:H	2.24	0.41
1:P:32:ILE:O	1:P:33:THR:HG22	2.21	0.41
1:P:28:THR:O	1:P:43:LEU:HD22	2.21	0.41
1:P:368:GLU:C	1:P:370:GLY:H	2.23	0.41
1:P:65:TYR:HE1	1:P:441:TYR:OH	2.04	0.41
1:P:386:ASP:HB3	1:P:388:THR:H	1.85	0.41
1:P:108:ILE:HG22	1:P:109:ARG:H	1.86	0.41
1:P:369:THR:HG23	1:P:376:LYS:NZ	2.36	0.41
1:P:377:ARG:HG3	1:P:399:PRO:HB2	2.03	0.41
1:P:153:ILE:HD11	1:P:441:TYR:CB	2.51	0.41
1:P:394:LYS:HE3	1:P:398:LEU:HD12	1.99	0.41
1:P:28:THR:N	1:P:43:LEU:HB2	2.35	0.41
1:P:218:TYR:CZ	1:P:409:MET:HE1	2.55	0.41
1:P:125:SER:OG	1:P:127:ALA:HB3	2.21	0.41
1:P:145:ALA:O	1:P:148:VAL:N	2.54	0.41
1:P:377:ARG:NH1	1:P:400:GLU:HA	2.36	0.41
1:P:379:PRO:HB3	1:P:398:LEU:CD2	2.51	0.41
1:P:43:LEU:HG	1:P:44:ARG:N	2.36	0.41
1:P:455:ILE:HG21	1:P:455:ILE:HD13	1.69	0.41
1:P:382:ASP:N	1:P:382:ASP:OD1	2.48	0.40
1:P:153:ILE:HA	1:P:153:ILE:HD13	1.60	0.40
1:P:425:LEU:HD12	1:P:425:LEU:O	2.21	0.40
1:P:68:ILE:HG23	1:P:68:ILE:HD12	1.80	0.40
1:P:191:LYS:NZ	1:P:339:VAL:HA	2.33	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	P	431/463 (93%)	353 (82%)	73 (17%)	5 (1%)	15 58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	282	PRO
1	P	357	PRO
1	P	284	PRO
1	P	289	PRO
1	P	288	GLN

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	P	283/395 (72%)	281 (99%)	2 (1%)	87 94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	52	ILE
1	P	399	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	224	HIS
1	P	229	ASN
1	P	395	ASN
1	P	457	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	101:ALA	C	102:PRO	N	1.13