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

Sep 3, 2019 – 01:28 PM EDT

PDB ID	:	6OXL
EMDB ID:	:	EMD-20220
Title	:	CRYO-EM STRUCTURE OF PHOSPHORYLATED AP-2 (mu E302K) BOUND TO NECAP IN THE PRESENCE OF SS DNA
Authors	:	Partlow, E.A.; Baker, R.W.; Beacham, G.M.; Chappie, J.; Leschziner, A.E.; Hollopeter, G.
Deposited on	:	2019-05-13
Resolution	:	3.50 Å(reported)
Based on PDB ID	:	1TQZ, 2VGL

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
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

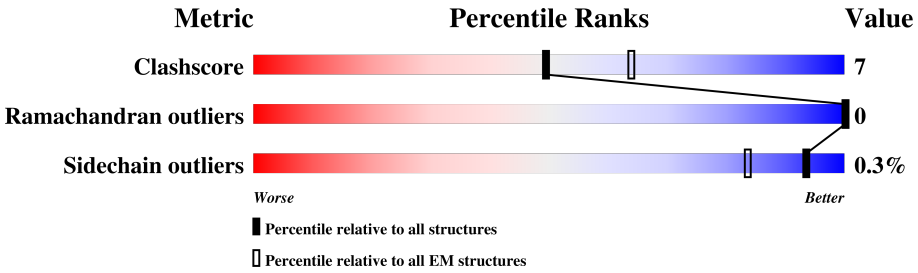
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 3.50 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	621	80% 15% 5%
2	B	591	80% 16% 5%
3	M	435	72% 17% 10%
4	S	142	82% 18% .
5	N	266	39% 8% 53%
6	n	7	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14413 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 AP-2 complex subunit alpha-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	589	4629	2958	785	865	21	0	0

- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	564	4465	2848	740	852	25	0	0

- Molecule 3 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
3	M	390	3118	2010	540	548	1	19	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	302	LYS	GLU	engineered mutation	UNP P84091

- Molecule 4 is a protein called AP-2 complex subunit sigma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S	141	1190	773	199	211	7	0	0

- Molecule 5 is a protein called Adaptin ear-binding coat-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	124	975	626	164	183	2	0	0

- Molecule 6 is a protein called Unknown region of Adaptin ear-binding coat-associated protein

2 Ex-domain.

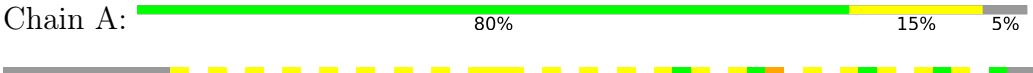
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	n	7	36	21	7	8	0	0

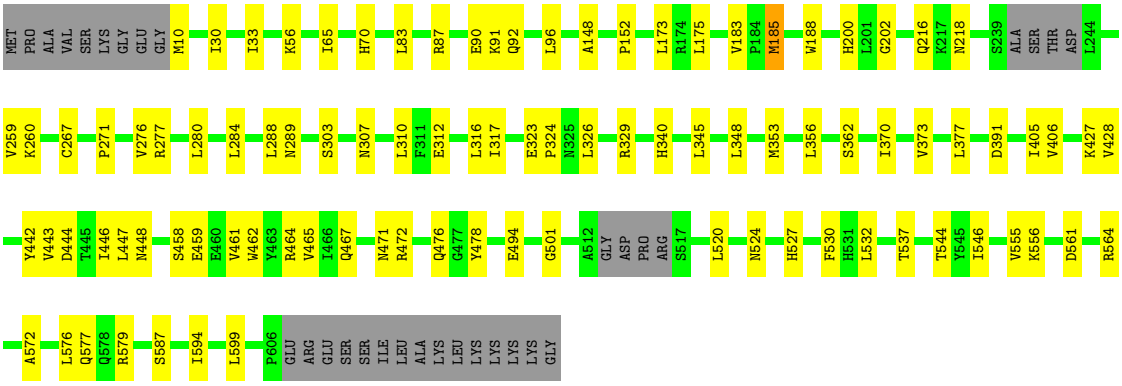
3 Residue-property plots (i)

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: AP-2 complex subunit alpha-2

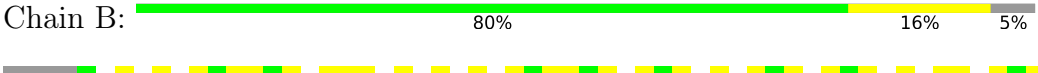
Chain A:

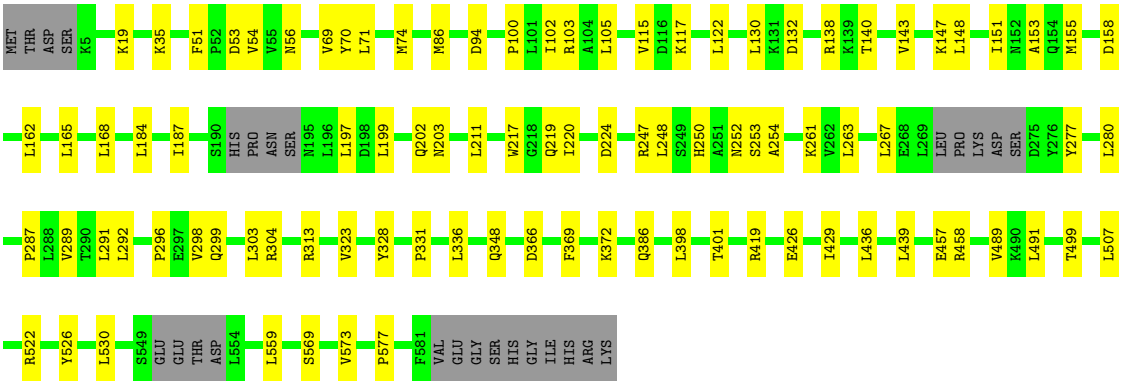




- Molecule 2: AP-2 complex subunit beta

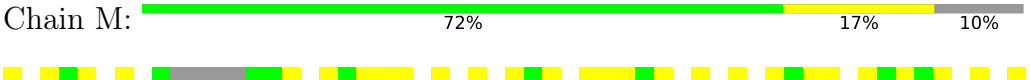
Chain B:

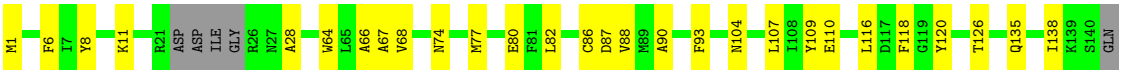


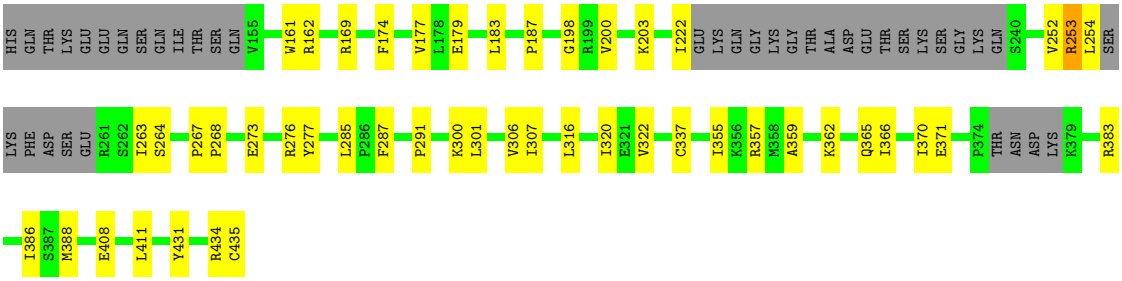


- Molecule 3: AP-2 complex subunit mu

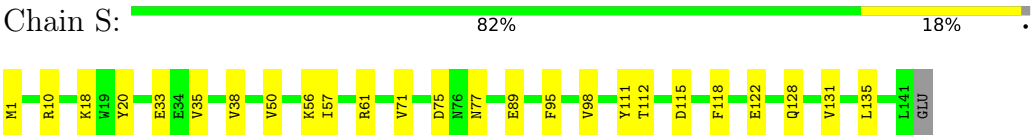
Chain M:



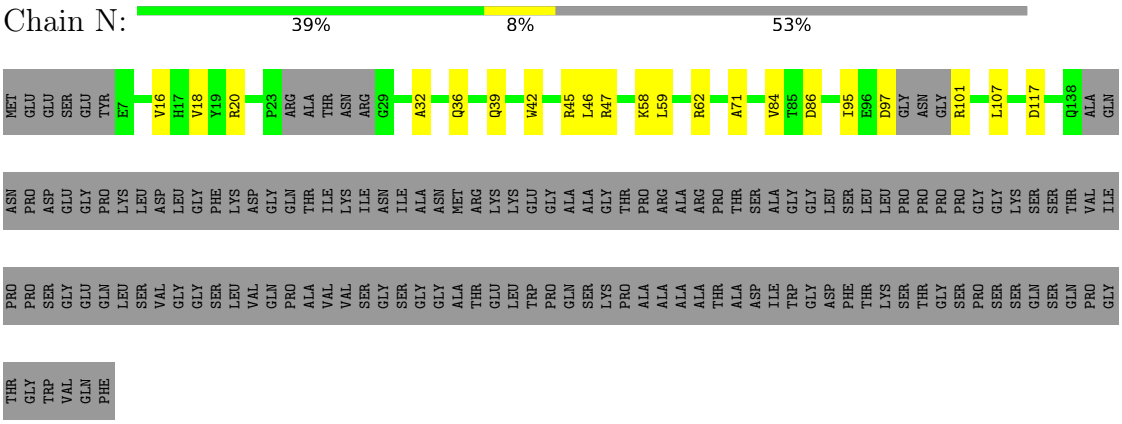




• Molecule 4: AP-2 complex subunit sigma



• Molecule 5: Adaptin ear-binding coat-associated protein 2



• Molecule 6: Unknown region of Adaptin ear-binding coat-associated protein 2 Ex-domain

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	324922	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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	0.45	0/4711	0.57	2/6394 (0.0%)
2	B	0.45	0/4531	0.59	2/6144 (0.0%)
3	M	0.50	0/3167	0.58	1/4265 (0.0%)
4	S	0.56	0/1214	0.60	0/1638
5	N	0.43	0/999	0.59	0/1353
All	All	0.47	0/14622	0.58	5/19794 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	532	LEU	CA-CB-CG	6.60	130.49	115.30
2	B	507	LEU	CA-CB-CG	5.47	127.87	115.30
3	M	116	LEU	CA-CB-CG	5.37	127.65	115.30
2	B	291	LEU	CB-CG-CD1	-5.14	102.27	111.00
1	A	594	ILE	CG1-CB-CG2	-5.12	100.13	111.40

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	4629	0	4703	69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4465	0	4566	62	0
3	M	3118	0	3194	49	0
4	S	1190	0	1189	15	0
5	N	975	0	917	12	0
6	n	36	0	10	0	0
All	All	14413	0	14579	190	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 7.

All (190) 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:252:ASN:OD1	3:M:80:GLU:HG2	1.33	1.27
1:A:459:GLU:HG2	1:A:462:TRP:CH2	1.70	1.25
1:A:175:LEU:CD2	1:A:183:VAL:CG2	2.38	1.02
2:B:247:ARG:NH2	2:B:250:HIS:CD2	2.29	0.99
2:B:247:ARG:HH22	2:B:250:HIS:CD2	1.79	0.98
1:A:175:LEU:CD2	1:A:183:VAL:HG21	1.95	0.96
3:M:222:ILE:HG21	3:M:254:LEU:HD21	1.46	0.96
1:A:459:GLU:HG2	1:A:462:TRP:CZ2	2.04	0.93
1:A:459:GLU:CG	1:A:462:TRP:CH2	2.58	0.85
1:A:175:LEU:HD22	1:A:183:VAL:HG21	1.58	0.84
2:B:253:SER:OG	2:B:298:VAL:HG11	1.79	0.82
3:M:253:ARG:HG3	3:M:264:SER:O	1.80	0.82
1:A:443:VAL:O	1:A:447:LEU:HG	1.81	0.80
1:A:459:GLU:HG2	1:A:462:TRP:CZ3	2.18	0.78
1:A:175:LEU:HD23	1:A:183:VAL:CG2	2.16	0.74
1:A:446:ILE:HG21	1:A:465:VAL:CG2	2.18	0.73
1:A:175:LEU:CD2	1:A:183:VAL:HG23	2.19	0.71
2:B:247:ARG:HH22	2:B:250:HIS:HD2	1.40	0.70
3:M:222:ILE:HG21	3:M:254:LEU:CD2	2.19	0.70
2:B:247:ARG:NH2	2:B:250:HIS:HD2	1.87	0.69
2:B:348:GLN:NE2	2:B:386:GLN:OE1	2.27	0.67
4:S:10:ARG:HH22	4:S:61:ARG:HH21	1.44	0.66
3:M:253:ARG:CG	3:M:264:SER:O	2.44	0.65
3:M:252:VAL:HG13	3:M:263:ILE:HG23	1.79	0.63
3:M:8:TYR:HB2	3:M:64:TRP:HB2	1.81	0.62
1:A:175:LEU:HD23	1:A:183:VAL:HG23	1.79	0.62
1:A:464:ARG:HA	1:A:467:GLN:HG2	1.80	0.62
1:A:260:LYS:HE3	4:S:122:GLU:OE2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:71:ALA:HB2	5:N:95:ILE:HD13	1.82	0.61
3:M:306:VAL:HG22	3:M:365:GLN:HG2	1.82	0.61
3:M:222:ILE:CG2	3:M:254:LEU:HD21	2.27	0.61
3:M:6:PHE:HB2	3:M:66:ALA:HB3	1.83	0.61
2:B:336:LEU:HD22	2:B:372:LYS:HD2	1.82	0.60
1:A:185:MET:SD	1:A:218:ASN:ND2	2.75	0.59
3:M:162:ARG:NH1	3:M:267:PRO:O	2.35	0.59
1:A:443:VAL:HG12	1:A:447:LEU:HD11	1.85	0.59
2:B:162:LEU:HD21	2:B:187:ILE:HD13	1.82	0.59
1:A:175:LEU:HD21	1:A:183:VAL:CG2	2.33	0.58
2:B:132:ASP:O	2:B:138:ARG:NH1	2.36	0.58
4:S:18:LYS:NZ	4:S:115:ASP:OD1	2.36	0.58
3:M:359:ALA:HB3	3:M:362:LYS:HE2	1.85	0.57
1:A:10:MET:SD	1:A:56:LYS:NZ	2.78	0.57
1:A:92:GLN:NE2	4:S:112:THR:OG1	2.38	0.56
2:B:491:LEU:HG	2:B:499:THR:HG21	1.86	0.56
1:A:467:GLN:O	1:A:471:ASN:ND2	2.38	0.56
3:M:174:PHE:HB2	3:M:203:LYS:HB2	1.86	0.56
3:M:301:LEU:HB3	3:M:370:ILE:HB	1.87	0.56
1:A:284:LEU:HD11	1:A:316:LEU:HD23	1.88	0.56
2:B:197:LEU:O	2:B:203:ASN:ND2	2.38	0.56
3:M:179:GLU:OE2	3:M:277:TYR:OH	2.24	0.56
1:A:87:ARG:NH2	1:A:90:GLU:OE2	2.39	0.55
2:B:219:GLN:OE1	2:B:247:ARG:NH2	2.39	0.55
2:B:254:ALA:HB2	3:M:77:MET:HA	1.88	0.55
1:A:216:GLN:NE2	1:A:267:CYS:SG	2.79	0.55
1:A:348:LEU:HD21	4:S:77:ASN:HD21	1.71	0.55
1:A:459:GLU:CG	1:A:462:TRP:CZ2	2.85	0.55
2:B:252:ASN:CG	3:M:80:GLU:HG2	2.22	0.55
3:M:287:PHE:O	3:M:431:TYR:OH	2.26	0.54
5:N:47:ARG:HB3	5:N:58:LYS:HB2	1.89	0.54
2:B:457:GLU:HG3	2:B:458:ARG:HG3	1.88	0.54
2:B:115:VAL:HG12	2:B:117:LYS:H	1.73	0.54
2:B:155:MET:HG3	2:B:158:ASP:H	1.72	0.54
1:A:577:GLN:OE1	2:B:419:ARG:NH2	2.37	0.54
1:A:303:SER:O	1:A:307:ASN:ND2	2.40	0.54
2:B:263:LEU:HD22	2:B:280:LEU:HD21	1.89	0.54
1:A:442:TYR:O	1:A:446:ILE:HG12	2.07	0.54
3:M:320:ILE:HB	3:M:355:ILE:HG23	1.90	0.54
5:N:97:ASP:O	5:N:101:ARG:N	2.41	0.53
5:N:18:VAL:HB	5:N:42:TRP:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:45:ARG:NH2	5:N:62:ARG:O	2.42	0.53
1:A:30:ILE:HG12	1:A:70:HIS:HE1	1.73	0.53
3:M:28:ALA:HB1	3:M:68:VAL:HG11	1.90	0.53
1:A:446:ILE:CG2	1:A:465:VAL:CG2	2.87	0.53
1:A:520:LEU:O	1:A:524:ASN:ND2	2.42	0.52
2:B:328:TYR:OH	5:N:117:ASP:OD1	2.27	0.52
2:B:35:LYS:HE2	3:M:135:GLN:HE22	1.74	0.52
5:N:59:LEU:HD11	5:N:107:LEU:HD11	1.92	0.52
1:A:494:GLU:OE2	1:A:537:THR:OG1	2.24	0.52
3:M:87:ASP:OD1	3:M:87:ASP:O	2.27	0.52
3:M:291:PRO:HB3	3:M:386:ILE:HD12	1.92	0.52
1:A:472:ARG:O	1:A:476:GLN:NE2	2.42	0.51
4:S:38:VAL:HG11	4:S:50:VAL:HG11	1.93	0.51
1:A:271:PRO:O	1:A:277:ARG:NH1	2.43	0.51
1:A:317:ILE:HD13	1:A:326:LEU:HB3	1.93	0.51
2:B:289:VAL:HG13	2:B:323:VAL:HG11	1.93	0.51
2:B:54:VAL:HG12	2:B:69:VAL:HG13	1.93	0.51
4:S:1:MET:N	4:S:75:ASP:OD2	2.41	0.50
3:M:67:ALA:HB2	3:M:82:LEU:HD21	1.93	0.50
1:A:83:LEU:O	1:A:91:LYS:NZ	2.43	0.50
3:M:11:LYS:NZ	4:S:33:GLU:OE1	2.45	0.50
2:B:489:VAL:HG13	2:B:530:LEU:HD11	1.94	0.50
5:N:16:VAL:HG11	5:N:46:LEU:HB2	1.92	0.50
5:N:84:VAL:HG12	5:N:86:ASP:H	1.76	0.50
1:A:175:LEU:HD23	1:A:183:VAL:HG21	1.78	0.49
1:A:391:ASP:OD1	1:A:427:LYS:NZ	2.42	0.49
1:A:200:HIS:HB3	1:A:202:GLY:H	1.78	0.49
3:M:307:ILE:HD11	3:M:322:VAL:HG21	1.94	0.49
3:M:300:LYS:NZ	3:M:371:GLU:OE2	2.46	0.49
1:A:446:ILE:HG21	1:A:465:VAL:HG22	1.94	0.49
1:A:546:ILE:HG23	1:A:599:LEU:HD21	1.94	0.49
1:A:356:LEU:O	1:A:362:SER:OG	2.31	0.49
3:M:222:ILE:CG2	3:M:254:LEU:CD2	2.90	0.48
1:A:406:VAL:HG13	1:A:428:VAL:HG13	1.94	0.48
1:A:148:ALA:HB1	1:A:183:VAL:HG22	1.95	0.48
1:A:96:LEU:HD21	4:S:111:TYR:HD2	1.78	0.48
4:S:89:GLU:OE1	4:S:128:GLN:NE2	2.35	0.48
1:A:288:LEU:HD23	1:A:310:LEU:HD11	1.94	0.48
2:B:70:TYR:OH	2:B:94:ASP:OD2	2.31	0.48
1:A:520:LEU:HD23	1:A:555:VAL:HG23	1.96	0.48
2:B:19:LYS:NZ	2:B:53:ASP:OD2	2.35	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:20:TYR:OH	4:S:118:PHE:O	2.29	0.48
1:A:276:VAL:O	1:A:280:LEU:N	2.43	0.47
2:B:211:LEU:HD12	2:B:219:GLN:HG2	1.96	0.47
2:B:267:LEU:HD21	2:B:280:LEU:HD23	1.97	0.47
2:B:426:GLU:HG2	2:B:429:ILE:HD12	1.97	0.47
5:N:20:ARG:NH1	5:N:36:GLN:OE1	2.48	0.46
3:M:187:PRO:HD3	3:M:434:ARG:HB3	1.97	0.46
1:A:556:LYS:HE3	1:A:587:SER:HB2	1.98	0.46
2:B:569:SER:HA	3:M:74:ASN:HA	1.97	0.46
2:B:70:TYR:O	2:B:74:MET:N	2.48	0.46
2:B:71:LEU:HD22	3:M:109:TYR:HB3	1.98	0.46
1:A:289:ASN:OD1	1:A:329:ARG:NH2	2.43	0.45
3:M:179:GLU:HG2	3:M:198:GLY:HA3	1.98	0.45
2:B:522:ARG:NH2	2:B:526:TYR:OH	2.50	0.45
2:B:71:LEU:HD11	3:M:110:GLU:HG3	1.99	0.45
4:S:56:LYS:N	4:S:71:VAL:O	2.49	0.45
1:A:33:ILE:HD12	1:A:65:ILE:HG12	1.98	0.45
2:B:130:LEU:HD22	2:B:168:LEU:HD11	1.99	0.45
2:B:366:ASP:HB3	2:B:369:PHE:HB3	1.99	0.45
2:B:224:ASP:OD1	2:B:261:LYS:NZ	2.44	0.45
3:M:183:LEU:HD22	3:M:285:LEU:HD22	1.99	0.44
3:M:383:ARG:HB3	3:M:435:CYS:HB3	1.99	0.44
2:B:292:LEU:O	2:B:299:GLN:NE2	2.51	0.44
4:S:95:PHE:HB2	4:S:98:VAL:HB	2.00	0.44
1:A:444:ASP:O	1:A:448:ASN:ND2	2.51	0.44
2:B:277:TYR:OH	2:B:313:ARG:NH1	2.51	0.44
3:M:273:GLU:OE2	3:M:276:ARG:NE	2.47	0.44
1:A:572:ALA:O	2:B:419:ARG:NH1	2.51	0.43
2:B:122:LEU:HD23	2:B:148:LEU:HD13	1.99	0.43
2:B:304:ARG:NE	2:B:573:VAL:O	2.42	0.43
1:A:152:PRO:HB3	1:A:188:TRP:CD1	2.53	0.43
3:M:104:ASN:HD21	3:M:138:ILE:H	1.66	0.43
3:M:388:MET:HB3	3:M:431:TYR:HD2	1.83	0.43
4:S:35:VAL:HG22	4:S:57:ILE:HD11	1.99	0.43
1:A:527:HIS:HA	1:A:530:PHE:HB2	2.00	0.43
2:B:165:LEU:HD23	2:B:168:LEU:HD12	2.00	0.43
3:M:86:CYS:O	3:M:90:ALA:N	2.44	0.43
1:A:561:ASP:OD1	1:A:564:ARG:NH2	2.51	0.43
5:N:36:GLN:HE22	5:N:39:GLN:HE21	1.66	0.43
1:A:340:HIS:CE1	1:A:345:LEU:HD12	2.54	0.43
1:A:576:LEU:HD23	1:A:576:LEU:HA	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:LEU:HD23	2:B:202:GLN:HB2	2.01	0.42
4:S:131:VAL:O	4:S:135:LEU:N	2.41	0.42
2:B:184:LEU:HA	2:B:187:ILE:HG22	2.00	0.42
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.83	0.42
2:B:151:ILE:O	2:B:153:ALA:N	2.52	0.42
2:B:217:TRP:HA	2:B:220:ILE:HD12	2.00	0.42
2:B:102:ILE:HA	2:B:105:LEU:HD12	2.01	0.42
2:B:267:LEU:HD23	2:B:267:LEU:HA	1.87	0.42
2:B:248:LEU:HB3	2:B:287:PRO:HG3	2.02	0.42
2:B:296:PRO:HB3	2:B:331:PRO:HG3	2.02	0.42
3:M:322:VAL:HG22	3:M:388:MET:HG3	2.02	0.42
3:M:316:LEU:HD21	3:M:357:ARG:HD2	2.00	0.42
3:M:337:CYS:HB3	3:M:366:ILE:HG13	2.00	0.42
2:B:140:THR:HA	2:B:143:VAL:HG12	2.02	0.42
1:A:443:VAL:HG12	1:A:447:LEU:CD1	2.48	0.42
3:M:93:PHE:HE1	3:M:107:LEU:HD23	1.83	0.42
1:A:444:ASP:OD1	1:A:478:TYR:OH	2.28	0.41
2:B:559:LEU:HD11	2:B:577:PRO:HD3	2.02	0.41
1:A:370:ILE:HD11	1:A:405:ILE:HG12	2.02	0.41
1:A:579:ARG:HH21	2:B:522:ARG:HH11	1.67	0.41
2:B:299:GLN:O	2:B:303:LEU:N	2.45	0.41
2:B:436:LEU:HD12	2:B:439:LEU:HD12	2.02	0.41
3:M:177:VAL:HG22	3:M:200:VAL:HG22	2.03	0.41
2:B:336:LEU:CD2	2:B:372:LYS:HD2	2.51	0.41
3:M:88:VAL:HG22	3:M:126:THR:HG22	2.02	0.41
1:A:323:GLU:HA	1:A:324:PRO:HD3	1.91	0.41
2:B:100:PRO:HB3	2:B:103:ARG:HD2	2.03	0.41
2:B:51:PHE:HE2	2:B:86:MET:HB2	1.86	0.41
3:M:408:GLU:OE1	3:M:411:LEU:N	2.54	0.41
1:A:259:VAL:HG13	1:A:312:GLU:HG3	2.03	0.41
1:A:373:VAL:O	1:A:377:LEU:N	2.54	0.41
1:A:458:SER:HB3	1:A:461:VAL:HG23	2.04	0.40
1:A:501:GLY:O	1:A:544:THR:OG1	2.29	0.40
3:M:161:TRP:CD1	3:M:268:PRO:HG3	2.56	0.40
1:A:353:MET:HA	1:A:356:LEU:HB3	2.04	0.40
5:N:32:ALA:HB2	5:N:84:VAL:HG11	2.02	0.40
2:B:147:LYS:HD3	3:M:118:PHE:HB2	2.04	0.40
2:B:398:LEU:O	2:B:401:THR:OG1	2.31	0.40
3:M:1:MET:HG3	3:M:120:TYR:CE1	2.56	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	583/621 (94%)	566 (97%)	17 (3%)	0	100	100
2	B	556/591 (94%)	521 (94%)	35 (6%)	0	100	100
3	M	377/435 (87%)	347 (92%)	30 (8%)	0	100	100
4	S	139/142 (98%)	132 (95%)	7 (5%)	0	100	100
5	N	118/266 (44%)	107 (91%)	11 (9%)	0	100	100
All	All	1773/2055 (86%)	1673 (94%)	100 (6%)	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	513/543 (94%)	512 (100%)	1 (0%)	94	98
2	B	503/532 (94%)	502 (100%)	1 (0%)	94	98
3	M	340/386 (88%)	338 (99%)	2 (1%)	87	95
4	S	130/131 (99%)	130 (100%)	0	100	100
5	N	100/212 (47%)	100 (100%)	0	100	100
All	All	1586/1804 (88%)	1582 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	MET
2	B	56	ASN
3	M	169	ARG
3	M	253	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	76	HIS
1	A	92	GLN
1	A	200	HIS
1	A	216	GLN
1	A	568	GLN
2	B	56	ASN
2	B	179	ASN
2	B	203	ASN
2	B	250	HIS
2	B	348	GLN
3	M	122	GLN
3	M	135	GLN
5	N	39	GLN
5	N	125	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	TPO	M	156	3	9,10,11	1.69	2 (22%)	11,14,16	1.34	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPO	M	156	3	-	3/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	156	TPO	P-O1P	3.25	1.61	1.50
3	M	156	TPO	P-OG1	2.16	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	156	TPO	CG2-CB-CA	-2.55	108.08	113.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	156	TPO	O-C-CA-CB
3	M	156	TPO	CG2-CB-OG1-P
3	M	156	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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)

There are no chain breaks in this entry.