WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Sep 18, 2021 – 08:03 am BST

PDB ID	:	7PEB
EMDB ID	:	EMD-13351
Title	:	cryo-EM structure of DEPTOR bound to human mTOR complex 1, focussed on one protomer
Authors	:	Waelchli, M.; Maier, T.
Deposited on	:	2021-08-09
Resolution	:	3.67 Å(reported)
Based on initial model	:	6BCX

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 3.67 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.
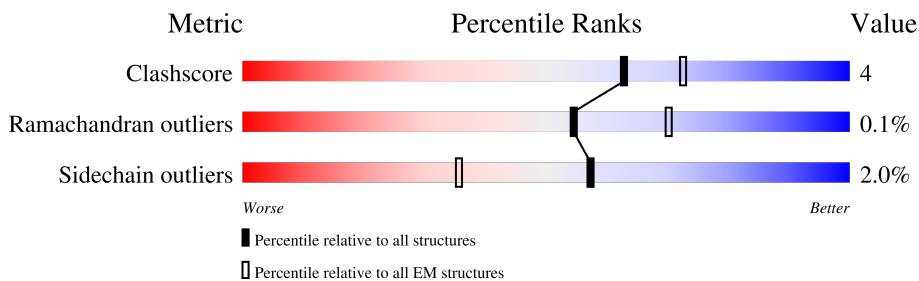
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	2549	75% 11% 14%
2	C	326	84% 12% ··
3	E	1396	66% 9% 25%
4	I	409	20% 6% 74%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29140 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2192	17468	11159	3060	3137	112	0	0

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	317	2456	1526	436	476	18	0	0

- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	1052	8385	5361	1450	1518	56	0	0

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-60	MET	-	initiating methionine	UNP Q8N122
E	-59	ALA	-	expression tag	UNP Q8N122
E	-58	HIS	-	expression tag	UNP Q8N122
E	-57	HIS	-	expression tag	UNP Q8N122
E	-56	HIS	-	expression tag	UNP Q8N122
E	-55	HIS	-	expression tag	UNP Q8N122
E	-54	HIS	-	expression tag	UNP Q8N122
E	-53	HIS	-	expression tag	UNP Q8N122
E	-52	HIS	-	expression tag	UNP Q8N122
E	-51	HIS	-	expression tag	UNP Q8N122
E	-50	HIS	-	expression tag	UNP Q8N122
E	-49	HIS	-	expression tag	UNP Q8N122
E	-48	GLY	-	expression tag	UNP Q8N122
E	-47	SER	-	expression tag	UNP Q8N122
E	-46	THR	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-45	SER	-	expression tag	UNP Q8N122
E	-44	GLY	-	expression tag	UNP Q8N122
E	-43	SER	-	expression tag	UNP Q8N122
E	-42	GLY	-	expression tag	UNP Q8N122
E	-41	GLU	-	expression tag	UNP Q8N122
E	-40	GLN	-	expression tag	UNP Q8N122
E	-39	LYS	-	expression tag	UNP Q8N122
E	-38	LEU	-	expression tag	UNP Q8N122
E	-37	ILE	-	expression tag	UNP Q8N122
E	-36	SER	-	expression tag	UNP Q8N122
E	-35	GLU	-	expression tag	UNP Q8N122
E	-34	GLU	-	expression tag	UNP Q8N122
E	-33	ASP	-	expression tag	UNP Q8N122
E	-32	LEU	-	expression tag	UNP Q8N122
E	-31	GLY	-	expression tag	UNP Q8N122
E	-30	SER	-	expression tag	UNP Q8N122
E	-29	THR	-	expression tag	UNP Q8N122
E	-28	SER	-	expression tag	UNP Q8N122
E	-27	GLY	-	expression tag	UNP Q8N122
E	-26	SER	-	expression tag	UNP Q8N122
E	-25	GLY	-	expression tag	UNP Q8N122
E	-24	ASP	-	expression tag	UNP Q8N122
E	-23	TYR	-	expression tag	UNP Q8N122
E	-22	LYS	-	expression tag	UNP Q8N122
E	-21	ASP	-	expression tag	UNP Q8N122
E	-20	ASP	-	expression tag	UNP Q8N122
E	-19	ASP	-	expression tag	UNP Q8N122
E	-18	ASP	-	expression tag	UNP Q8N122
E	-17	LYS	-	expression tag	UNP Q8N122
E	-16	LEU	-	expression tag	UNP Q8N122
E	-15	THR	-	expression tag	UNP Q8N122
E	-14	SER	-	expression tag	UNP Q8N122
E	-13	LEU	-	expression tag	UNP Q8N122
E	-12	TYR	-	expression tag	UNP Q8N122
E	-11	LYS	-	expression tag	UNP Q8N122
E	-10	LYS	-	expression tag	UNP Q8N122
E	-9	ALA	-	expression tag	UNP Q8N122
E	-8	GLY	-	expression tag	UNP Q8N122
E	-7	LEU	-	expression tag	UNP Q8N122
E	-6	GLU	-	expression tag	UNP Q8N122
E	-5	ASN	-	expression tag	UNP Q8N122
E	-4	LEU	-	expression tag	UNP Q8N122

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| Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	TYR	-	expression tag	UNP Q8N122
E	-2	PHE	-	expression tag	UNP Q8N122
E	-1	GLN	-	expression tag	UNP Q8N122
E	0	GLY	-	expression tag	UNP Q8N122

- Molecule 4 is a protein called DEP domain-containing mTOR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	106	795	504	138	146	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	204	SER	ASN	variant	UNP Q8TB45
I	389	ASN	SER	variant	UNP Q8TB45

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).
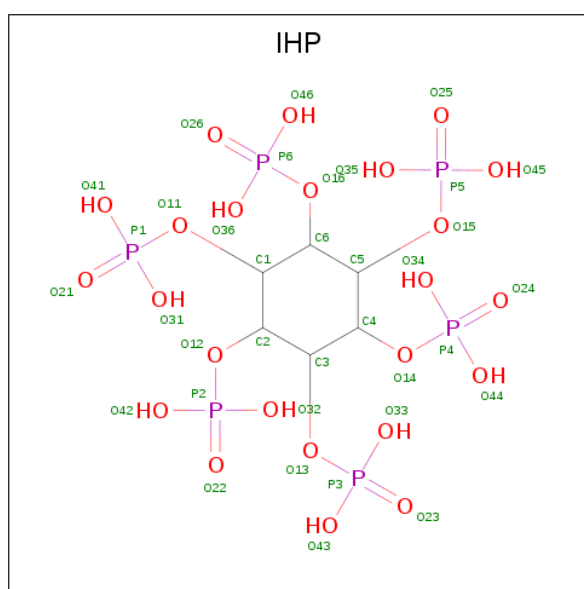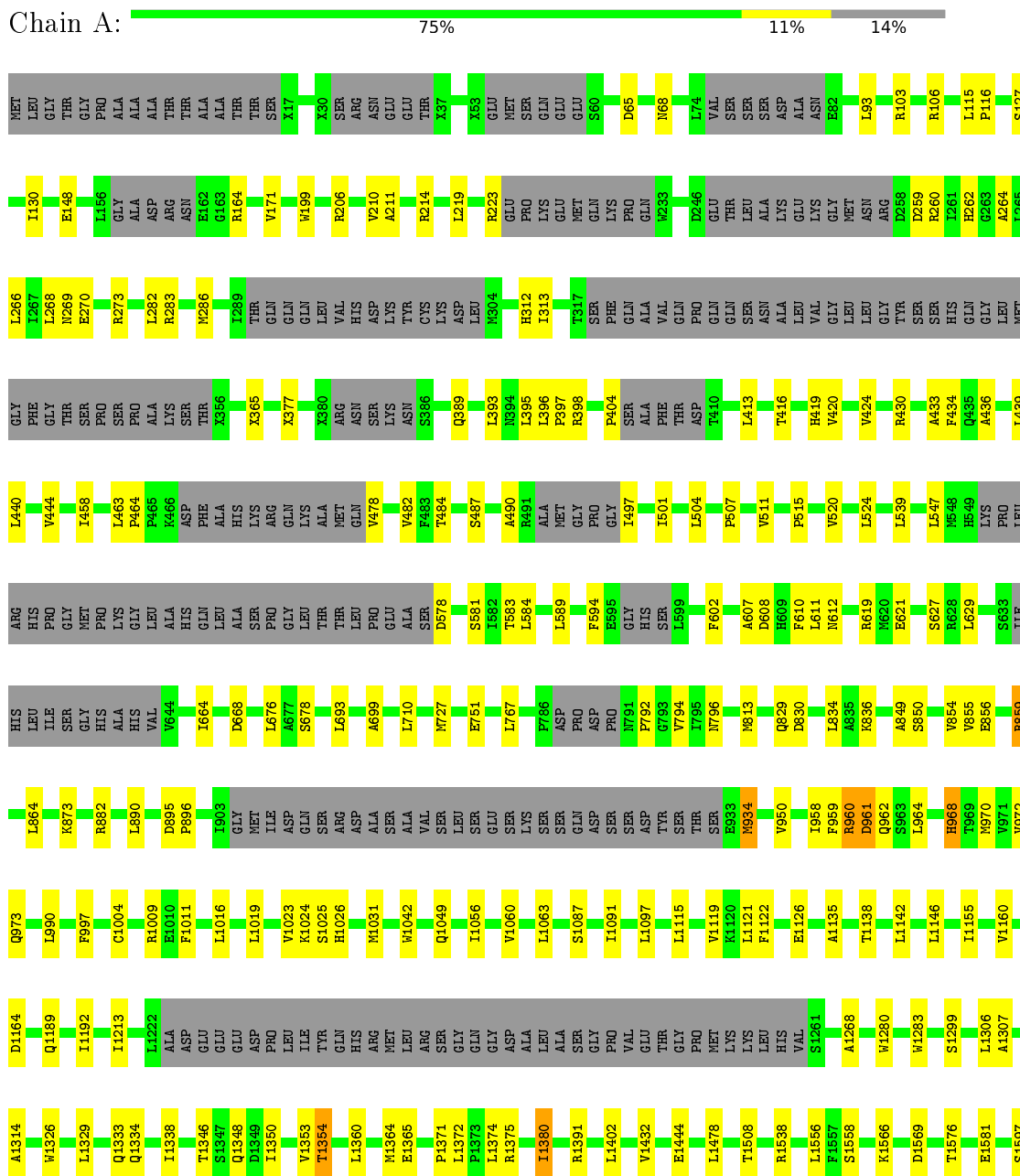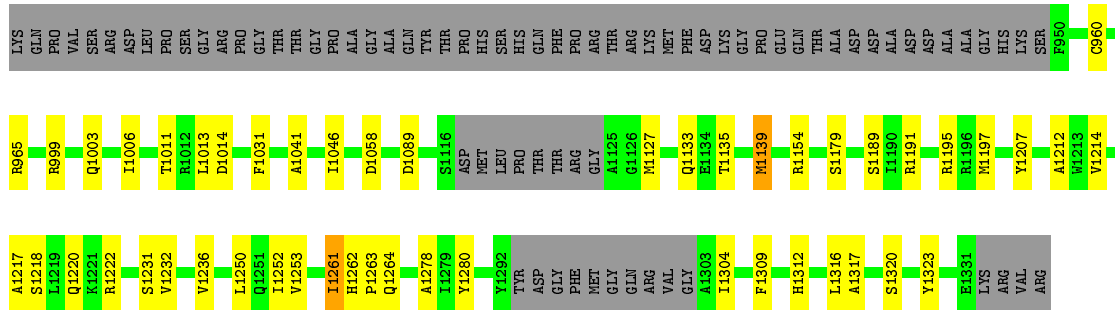

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
5	A	1	36	6	24	6	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein kinase mTOR

Chain A:

• Molecule 2: Target of rapamycin complex subunit LST8

Chain C:

84% 12%

• Molecule 3: Regulatory-associated protein of mTOR

Chain E:

66% 9% 25%

LYS GLN PRO VAL SER ARG ASP LEU PRO SER GLY ARG PRO GLY THR THR GLY PRO ALA GLY ALA GLN TYR THR PRO HIS SER HIS GLN PHE PRO ARG ARG THR ARG LYS MET PHE ASP LYS GLY PRO GLU GLN THR ALA ASP ASP ALA ASP ASP ALA ALA GLY HIS LYS SER F950 C960

R965 R999 Q1003 I1006 T1011 R1012 L1013 D1014 F1031 A1041 I1046 D1058 D1089 S1116 ASP MET LEU PRO THR THR ARG GLY A1125 G1126 M1127 Q1133 E1134 T1135 M1139 R1154 S1179 S1189 I1190 R1191 R1195 R1196 M1197 Y1207 A1212 W1213 V1214

A1217 S1218 L1219 Q1220 K1221 R1222 S1231 V1232 V1236 L1250 Q1251 I1252 V1253 I1261 H1262 P1263 Q1264 A1278 I1279 Y1280 Y1292 TYR ASP GLY PHE MET GLY GLN ARG VAL GLY A1303 I1304 F1309 H1312 L1316 A1317 S1320 Y1323 E1331 LYS ARG VAL ARG

• Molecule 4: DEP domain-containing mTOR-interacting protein

Chain I:

20%   6%   74%

MET GLU GLU GLY GLY SER THR GLY SER ALA GLY SER ASP SER SER GLY SER GLY SER GLY GLY ALA GLN GLN ALA ARG GLU LEU GLU ARG MET ALA GLU VAL LEU VAL THR GLY GLU GLN LEU ARG LEU HIS GLU LYS VAL ILE LYS ASP ARG ARG HIS HIS LEU LYS THR TYR

PRO ASN CYS PHE VAL ALA LYS GLU LEU ILE ASP TRP LEU ILE GLU HIS LYS GLU ALA SER ASP ARG GLU THR ALA ILE LYS LEU MET GLN LYS LEU ALA ASP ARG GLY ILE ILE HIS HIS VAL CYS ASP GLU HIS LYS GLU PHE LYS ASP VAL LYS LEU PHE TYR ARG PHE ARG LYS ASP

ASP GLY THR PHE PRO LEU ASP ASN GLU VAL LYS ALA PHE MET ARG GLY GLN ARG LEU TYR GLU LYS LEU MET SER PRO GLU ASN THR LEU LEU GLN PRO ARG GLU GLU GLY VAL LYS TYR GLU ARG THR PHE MET ALA SER GLU LEU PHE LEU ASP TRP LEU VAL GLN GLU GLY GLU ALA

THR THR ARG LYS GLU ALA GLU GLN LEU CYS HIS ARG LEU MET GLU HIS GLY ILE ILE GLN HIS VAL SER SER LYS LEU PRO PHE VAL ASP SER ASN LEU LEU TYR GLN PHE ARG MET ASN PHE ARG ARG ARG LEU MET GLU LEU LEU ASN GLU LYS SER PRO SER SER GLN GLU

THR HIS ASP SER PRO PHE CYS LEU ARG LYS GLN SER HIS ASP ASN ARG LYS SER THR SER PHE MET SER VAL SER PRO SER LYS GLU ILE LYS ILE VAL SER ALA VAL ARG ARG SER MET SER SER CYS GLY SER SER GLY TYR PHE SER SER SER PRO THR LEU SER SER SER PRO

PRO VAL LEU C304 A324 P325 Y326 F331 T332 I333 V334 G335 D336 A337 V338 G339 V343 K348 P349 C350 H351 I352 Q353 P360 A361 M366 Q370 F371 V372 V373 V380 L393 T398 M404 C409

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	850152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k 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:
IHP

The Z score for a bond length (or angle) is the number of standard deviations the observed value
is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an
outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or
angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	A	0.23	0/17538	0.45	0/23735
2	C	0.24	0/2514	0.49	0/3426
3	E	0.23	0/8585	0.47	0/11680
4	I	0.24	0/811	0.52	0/1104
All	All	0.23	0/29448	0.46	0/39945

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2　Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms
and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen
atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within
the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17468	0	17494	156	0
2	C	2456	0	2341	24	0
3	E	8385	0	8375	65	0
4	I	795	0	812	14	0
5	A	36	0	6	0	0
All	All	29140	0	29028	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 4.

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)
1:A:1338:ILE:HG23	1:A:1374:LEU:HD23	1.62	0.79
3:E:627:VAL:HG11	3:E:670:LEU:HD23	1.70	0.72
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.25	0.70
1:A:404:PRO:HB3	1:A:444:VAL:HG22	1.72	0.70
1:A:283:ARG:HG2	1:A:398:ARG:HH21	1.59	0.67
1:A:214:ARG:HE	1:A:273:ARG:HH22	1.42	0.67
1:A:1268:ALA:O	1:A:1283:TRP:NE1	2.25	0.66
3:E:1252:ILE:HG22	3:E:1253:VAL:HG23	1.77	0.66
3:E:141:ALA:HB1	3:E:144:GLU:HB2	1.77	0.66
2:C:63:GLN:HG2	2:C:85:ASN:HA	1.78	0.66
1:A:578:ASP:N	1:A:581:SER:HG	1.95	0.65
1:A:413:LEU:HD13	1:A:444:VAL:HG21	1.79	0.64
1:A:2018:ARG:NH1	1:A:2067:GLU:OE2	2.29	0.64
1:A:487:SER:HB3	1:A:520:VAL:HG13	1.79	0.64
1:A:1115:LEU:HD21	1:A:1155:ILE:HD11	1.78	0.64
1:A:396:LEU:HB3	1:A:416:THR:HG23	1.79	0.63
1:A:727:MET:HG3	1:A:767:LEU:HD23	1.81	0.63
1:A:1326:TRP:O	1:A:1334:GLN:NE2	2.31	0.63
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.80	0.63
1:A:1346:THR:OG1	1:A:1375:ARG:NH2	2.33	0.62
1:A:854:VAL:HG12	1:A:855:VAL:HG23	1.82	0.61
1:A:393:LEU:HG	1:A:419:HIS:HE1	1.65	0.61
1:A:1911:PHE:O	1:A:1950:ARG:NH1	2.33	0.61
1:A:266:LEU:HD23	1:A:395:LEU:HD21	1.83	0.61
3:E:480:LEU:HD23	3:E:491:LEU:HD13	1.82	0.61
1:A:873:LYS:NZ	1:A:1576:THR:O	2.34	0.60
1:A:2418:LEU:HA	1:A:2421:PHE:CE1	2.36	0.60
3:E:1262:HIS:CE1	3:E:1264:GLN:HB2	2.36	0.60
1:A:199:TRP:HA	1:A:206:ARG:HH21	1.65	0.60
3:E:188:SER:OG	3:E:189:PRO:HD3	2.01	0.60
4:I:324:ALA:HB3	4:I:325:PRO:HD3	1.83	0.60
3:E:681:VAL:HG21	3:E:808:TYR:HB2	1.84	0.59
1:A:1538:ARG:NH2	4:I:339:GLY:O	2.34	0.59
1:A:2170:ARG:HB2	1:A:2186:LEU:HB3	1.84	0.58
1:A:377:UNK:O	1:A:389:GLN:NE2	2.36	0.58
1:A:2282:GLN:HE21	2:C:316:VAL:HG11	1.69	0.58
3:E:268:THR:HG23	3:E:269:THR:HG23	1.84	0.58
1:A:1004:CYS:O	1:A:1009:ARG:NH2	2.37	0.57
1:A:850:SER:O	1:A:1611:ARG:NH2	2.38	0.57
1:A:65:ASP:OD2	1:A:106:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1041:ALA:HA	3:E:1046:ILE:HA	1.87	0.57
1:A:1781:GLU:OE2	1:A:1784:ARG:NH2	2.37	0.57
3:E:1304:ILE:HA	3:E:1320:SER:HA	1.86	0.56
1:A:1391:ARG:HD3	1:A:1581:GLU:HG3	1.88	0.56
1:A:393:LEU:HG	1:A:419:HIS:CE1	2.41	0.56
1:A:751:GLU:HB2	1:A:794:VAL:HG22	1.88	0.56
1:A:214:ARG:NE	1:A:273:ARG:HH22	2.04	0.56
1:A:676:LEU:HB3	1:A:710:LEU:HD23	1.87	0.56
1:A:2418:LEU:HA	1:A:2421:PHE:HE1	1.70	0.56
2:C:195:TYR:HE1	2:C:215:LYS:HE2	1.71	0.55
1:A:1280:TRP:HE1	1:A:1348:GLN:HB3	1.72	0.55
3:E:1189:SER:OG	3:E:1191:ARG:NH1	2.39	0.55
1:A:268:LEU:HD22	1:A:365:UNK:HA	1.89	0.55
1:A:266:LEU:O	1:A:270:GLU:HG2	2.08	0.54
1:A:515:PRO:HD3	1:A:584:LEU:HD11	1.89	0.54
2:C:285:ILE:HG23	2:C:297:TRP:HB2	1.88	0.54
4:I:333:ILE:HD11	4:I:360:PRO:HB2	1.89	0.54
1:A:607:ALA:HA	1:A:610:PHE:CE2	2.42	0.54
1:A:68:ASN:HD21	1:A:93:LEU:HD12	1.73	0.54
1:A:127:SER:HA	1:A:130:ILE:HD12	1.90	0.54
1:A:416:THR:HG21	1:A:440:LEU:HD21	1.90	0.54
3:E:1179:SER:HB3	3:E:1195:ARG:HG2	1.90	0.54
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.88	0.53
1:A:273:ARG:HH11	1:A:398:ARG:NH1	2.06	0.53
1:A:1556:LEU:HD11	4:I:393:LEU:HD22	1.89	0.53
1:A:2264:GLU:HG3	1:A:2294:THR:HG21	1.89	0.53
3:E:1212:ALA:HB3	3:E:1231:SER:HB2	1.91	0.53
1:A:589:LEU:HG	1:A:629:LEU:HD11	1.90	0.53
3:E:546:TYR:CZ	3:E:548:THR:HB	2.44	0.53
1:A:619:ARG:NH2	1:A:668:ASP:OD2	2.42	0.52
1:A:424:VAL:HG12	1:A:458:ILE:HG21	1.90	0.52
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.91	0.52
1:A:608:ASP:OD1	1:A:612:ASN:ND2	2.43	0.52
3:E:1214:VAL:HG11	3:E:1217:ALA:HB2	1.90	0.52
2:C:168:GLU:OE1	2:C:195:TYR:OH	2.28	0.52
2:C:223:ALA:HA	2:C:239:SER:HA	1.91	0.52
3:E:40:GLU:O	3:E:965:ARG:NH2	2.42	0.52
1:A:958:ILE:HD12	1:A:1306:LEU:HD21	1.92	0.51
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.91	0.51
1:A:206:ARG:NH1	1:A:259:ASP:O	2.42	0.51
1:A:664:ILE:HD11	1:A:699:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:ALA:HB1	1:A:1314:ALA:HB2	1.93	0.51
3:E:327:VAL:HG11	3:E:373:THR:HG22	1.92	0.51
3:E:485:ARG:HA	3:E:488:ARG:HG3	1.93	0.51
1:A:210:VAL:O	1:A:214:ARG:HG3	2.11	0.51
3:E:437:LEU:HD21	3:E:475:TYR:CE2	2.46	0.50
1:A:1598:GLU:O	1:A:1602:VAL:HG23	2.11	0.50
1:A:1119:VAL:HA	1:A:1122:PHE:CE2	2.47	0.50
1:A:856:GLU:HA	1:A:859:ARG:HE	1.77	0.50
1:A:2052:GLU:HG2	1:A:2053:PRO:HD3	1.93	0.50
2:C:89:ALA:N	2:C:103:GLY:O	2.45	0.50
2:C:248:ARG:HD2	2:C:251:ASN:HB2	1.93	0.50
1:A:2371:PHE:HB3	1:A:2542:TYR:HB2	1.93	0.50
1:A:2408:ARG:NH2	1:A:2524:GLN:OE1	2.45	0.49
3:E:55:MET:HB3	3:E:340:ASP:HB3	1.93	0.49
3:E:340:ASP:OD1	3:E:343:VAL:HB	2.12	0.49
4:I:334:VAL:HG23	4:I:398:THR:HG22	1.93	0.49
3:E:79:THR:HB	3:E:80:PRO:HD3	1.95	0.49
1:A:882:ARG:NH2	1:A:1569:ASP:OD2	2.45	0.49
1:A:312:HIS:CD2	1:A:313:ILE:HG12	2.48	0.49
1:A:1023:VAL:O	1:A:1024:LYS:HG2	2.13	0.49
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	1.94	0.49
1:A:420:VAL:O	1:A:424:VAL:HG23	2.12	0.49
1:A:1097:LEU:HD12	1:A:1138:THR:HG21	1.94	0.48
1:A:1478:LEU:HD11	1:A:1508:THR:HG23	1.94	0.48
1:A:1973:ILE:HD12	1:A:1974:TYR:H	1.78	0.48
3:E:78:THR:O	3:E:81:CYS:HB3	2.13	0.48
1:A:934:MET:HE2	1:A:950:VAL:HG21	1.94	0.48
3:E:1309:PHE:CE1	3:E:1316:LEU:HB2	2.48	0.48
1:A:1878:LEU:HD11	1:A:1918:ASP:HB2	1.95	0.48
3:E:1212:ALA:HB1	3:E:1232:VAL:HB	1.94	0.48
1:A:210:VAL:HG11	1:A:266:LEU:HD13	1.95	0.48
1:A:1380:ILE:HD11	1:A:1402:LEU:HD23	1.95	0.48
1:A:2405:GLU:HG2	1:A:2521:VAL:HG11	1.95	0.48
1:A:1023:VAL:HG13	1:A:1026:HIS:HB2	1.95	0.48
3:E:164:VAL:O	3:E:177:LEU:N	2.46	0.48
4:I:343:VAL:O	4:I:353:GLN:N	2.35	0.48
1:A:504:LEU:O	1:A:507:PRO:HD2	2.14	0.47
3:E:630:SER:O	3:E:633:ARG:HG2	2.14	0.47
1:A:199:TRP:HH2	1:A:264:ALA:HB2	1.78	0.47
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.97	0.47
3:E:683:LEU:HA	3:E:686:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HB2	1:A:602:PHE:HE1	1.79	0.47
1:A:2336:LEU:HG	1:A:2339:ARG:HD2	1.96	0.47
1:A:463:LEU:N	1:A:464:PRO:HD2	2.30	0.47
2:C:84:VAL:HG12	2:C:85:ASN:N	2.30	0.47
1:A:148:GLU:HB3	1:A:171:VAL:HG11	1.96	0.47
1:A:990:LEU:HD21	1:A:1023:VAL:HG21	1.97	0.47
1:A:2204:LEU:HD22	1:A:2417:VAL:HG21	1.97	0.47
1:A:1350:ILE:HG22	1:A:1353:VAL:H	1.81	0.46
1:A:1329:LEU:HB3	1:A:1333:GLN:HB2	1.97	0.46
3:E:1262:HIS:HD2	3:E:1263:PRO:HD2	1.80	0.46
1:A:1042:TRP:HE1	1:A:1049:GLN:HG2	1.79	0.46
3:E:26:LEU:HD22	3:E:1133:GLN:HG3	1.97	0.46
3:E:1031:PHE:CZ	3:E:1317:ALA:HB2	2.51	0.46
1:A:1538:ARG:NH1	4:I:336:ASP:OD2	2.48	0.46
2:C:74:ASN:N	2:C:75:PRO:HD3	2.30	0.46
3:E:156:PRO:HG2	3:E:165:TRP:CG	2.51	0.46
1:A:2548:PHE:HD1	1:A:2549:TRP:CD1	2.34	0.46
3:E:1262:HIS:HB2	3:E:1309:PHE:CG	2.51	0.46
1:A:1628:ARG:HB3	1:A:1659:LEU:HD21	1.98	0.46
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.98	0.46
2:C:150:GLY:HA2	2:C:173:ILE:HG23	1.98	0.46
3:E:628:GLY:O	3:E:673:GLN:NE2	2.49	0.46
1:A:211:ALA:HA	1:A:214:ARG:HD3	1.99	0.45
4:I:352:ILE:HD12	4:I:370:GLN:HB2	1.98	0.45
1:A:895:ASP:OD1	1:A:896:PRO:HD2	2.16	0.45
3:E:674:TYR:HB3	3:E:677:ASN:HB2	1.97	0.45
3:E:1218:SER:HB3	3:E:1261:ILE:HD12	1.98	0.45
1:A:2187:LYS:HG3	1:A:2237:ILE:HD12	1.98	0.45
3:E:660:ARG:NH1	3:E:821:ASP:OD2	2.49	0.45
1:A:424:VAL:HG22	1:A:433:ALA:HB1	1.98	0.45
1:A:693:LEU:HD12	1:A:693:LEU:HA	1.84	0.45
1:A:116:PRO:HB3	1:A:164:ARG:HH22	1.82	0.45
1:A:430:ARG:HH21	1:A:478:VAL:HG11	1.82	0.45
1:A:849:ALA:HB2	1:A:890:LEU:HD13	1.99	0.45
3:E:477:LEU:HD12	3:E:480:LEU:HD12	1.99	0.45
1:A:501:ILE:HA	1:A:504:LEU:HB2	1.99	0.45
1:A:2288:GLU:OE1	2:C:221:ARG:NH2	2.49	0.45
1:A:1364:MET:HG2	1:A:1372:LEU:HG	1.99	0.44
1:A:2034:ALA:HB1	1:A:2047:MET:HG2	1.98	0.44
2:C:254:LEU:HD21	2:C:257:GLU:HB2	1.98	0.44
3:E:539:LEU:HD13	3:E:558:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:GLN:O	1:A:830:ASP:HB2	2.17	0.44
1:A:792:PRO:HB3	1:A:834:LEU:HB3	1.98	0.44
3:E:616:ARG:NH2	3:E:1154:ARG:O	2.50	0.44
3:E:1236:VAL:HB	3:E:1250:LEU:HB2	1.98	0.44
1:A:2242:HIS:HA	1:A:2348:ARG:NH1	2.33	0.44
2:C:86:LYS:HB3	2:C:105:GLU:HB2	1.99	0.44
3:E:1003:GLN:HA	3:E:1006:ILE:HD12	2.00	0.44
3:E:1031:PHE:HZ	3:E:1317:ALA:HB2	1.82	0.44
1:A:1024:LYS:HG3	1:A:1025:SER:H	1.82	0.43
1:A:1122:PHE:HB3	1:A:1135:ALA:HB3	2.00	0.43
1:A:964:LEU:HD12	1:A:968:HIS:HA	2.01	0.43
1:A:1087:SER:OG	1:A:1091:ILE:HG13	2.19	0.43
3:E:168:ASN:HD21	3:E:172:THR:HG1	1.63	0.43
1:A:864:LEU:HD23	1:A:864:LEU:HA	1.85	0.43
2:C:86:LYS:O	2:C:87:ASN:HB2	2.18	0.43
3:E:242:GLN:HB2	3:E:367:SER:HB2	2.01	0.43
1:A:968:HIS:O	1:A:972:VAL:HG23	2.19	0.43
1:A:1896:ARG:HA	1:A:1896:ARG:HD2	1.81	0.43
1:A:463:LEU:HD22	1:A:511:VAL:HG21	2.00	0.43
1:A:610:PHE:CE1	1:A:611:LEU:HG	2.53	0.43
2:C:194:CYS:HB3	2:C:216:ILE:HB	2.00	0.43
1:A:1444:GLU:N	1:A:1444:GLU:OE1	2.52	0.42
1:A:2192:LEU:HD21	1:A:2237:ILE:HD11	2.00	0.42
3:E:319:ILE:HD13	3:E:382:TRP:HB2	2.01	0.42
3:E:147:LEU:HA	3:E:191:ILE:HG23	2.02	0.42
1:A:206:ARG:HB3	1:A:262:HIS:HE1	1.84	0.42
2:C:291:ASP:OD2	2:C:295:ARG:NH2	2.42	0.42
3:E:273:ILE:H	3:E:273:ILE:HG13	1.65	0.42
1:A:960:ARG:O	1:A:961:ASP:HB2	2.19	0.42
1:A:1189:GLN:HA	1:A:1192:ILE:HD12	2.01	0.42
1:A:1566:LYS:HD2	4:I:338:VAL:HG13	2.01	0.42
3:E:592:ARG:NH1	3:E:626:PHE:O	2.53	0.42
3:E:1197:MET:H	3:E:1197:MET:HG2	1.59	0.42
1:A:796:ASN:HD21	1:A:836:LYS:HG3	1.84	0.42
1:A:2300:ALA:HB2	1:A:2386:ALA:HA	2.01	0.42
1:A:199:TRP:HE3	1:A:260:ARG:HG2	1.83	0.42
1:A:283:ARG:HA	1:A:286:MET:HG2	2.02	0.42
1:A:539:LEU:HD22	1:A:594:PHE:HE1	1.85	0.42
3:E:450:LEU:HD12	3:E:487:LEU:HD22	2.02	0.42
3:E:1278:ALA:HB1	3:E:1280:TYR:CZ	2.55	0.42
1:A:890:LEU:HD23	1:A:1597:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:157:ARG:HG2	3:E:197:SER:OG	2.19	0.42
3:E:1220:GLN:OE1	3:E:1222:ARG:NH1	2.53	0.42
1:A:219:LEU:HB3	1:A:223:ARG:NH1	2.34	0.41
2:C:40:HIS:CE1	2:C:66:ARG:HD2	2.55	0.41
4:I:361:ALA:HB1	4:I:366:MET:HG2	2.01	0.41
3:E:60:VAL:HG13	3:E:147:LEU:HD23	2.01	0.41
3:E:583:ARG:HH21	3:E:960:CYS:HB3	1.85	0.41
1:A:115:LEU:HD21	1:A:130:ILE:HD11	2.02	0.41
4:I:326:TYR:CD2	4:I:404:MET:HG3	2.55	0.41
4:I:350:CYS:O	4:I:372:VAL:HG22	2.20	0.41
1:A:1797:ASN:O	1:A:1801:VAL:HG23	2.20	0.41
1:A:1365:GLU:HG2	1:A:1371:PRO:HG3	2.02	0.41
1:A:2245:THR:HA	1:A:2345:MET:HG2	2.01	0.41
3:E:633:ARG:HA	3:E:633:ARG:HD3	1.73	0.41
1:A:269:ASN:CB	1:A:395:LEU:HD22	2.50	0.41
1:A:1142:LEU:HB3	1:A:1146:LEU:HD12	2.01	0.41
1:A:2366:MET:HG2	1:A:2373:GLU:O	2.20	0.41
4:I:348:LYS:HB2	4:I:349:PRO:HD3	2.02	0.41
1:A:490:ALA:HA	1:A:497:ILE:HG13	2.02	0.41
1:A:997:PHE:HE1	1:A:1016:LEU:HB2	1.86	0.41
3:E:1139:MET:H	3:E:1139:MET:HG2	1.64	0.41
4:I:373:VAL:O	4:I:380:VAL:N	2.47	0.41
1:A:520:VAL:O	1:A:524:LEU:N	2.50	0.41
2:C:36:ARG:NH1	2:C:74:ASN:H	2.18	0.41
3:E:57:THR:HG21	3:E:342:LEU:HD23	2.02	0.41
3:E:509:LEU:HD13	3:E:542:ILE:HD11	2.02	0.41
1:A:269:ASN:CG	1:A:395:LEU:HD22	2.41	0.41
1:A:583:THR:HG23	1:A:621:GLU:HG3	2.01	0.41
1:A:1031:MET:HG2	1:A:1063:LEU:HD11	2.01	0.41
2:C:274:TRP:CZ2	2:C:316:VAL:HG22	2.56	0.41
1:A:397:PRO:HG3	1:A:436:ALA:HA	2.03	0.41
1:A:2214:THR:HG22	1:A:2218:LYS:HE3	2.03	0.41
1:A:434:PHE:CD2	1:A:482:VAL:HG22	2.56	0.40
1:A:2296:GLY:HA3	1:A:2381:ARG:NH1	2.35	0.40
3:E:72:PRO:HD2	3:E:77:LYS:HE3	2.03	0.40
3:E:1089:ASP:HA	3:E:1127:MET:HB2	2.03	0.40
1:A:973:GLN:HG3	1:A:1011:PHE:HZ	1.86	0.40
2:C:43:SER:OG	2:C:44:GLN:N	2.54	0.40
1:A:282:LEU:HD12	1:A:439:LEU:HD23	2.03	0.40
1:A:1752:LEU:HD22	1:A:1786:TRP:CH2	2.56	0.40
1:A:484:THR:O	1:A:487:SER:OG	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:SER:HB2	1:A:678:SER:HB2	2.03	0.40
1:A:1056:ILE:O	1:A:1060:VAL:HG23	2.22	0.40
1:A:2339:ARG:NH2	1:A:2343:ASN:HB3	2.37	0.40
3:E:457:LEU:HD22	3:E:464:VAL:HA	2.03	0.40
3:E:604:LEU:HD12	3:E:604:LEU:HA	1.85	0.40
1:A:65:ASP:OD1	1:A:103:ARG:NH1	2.55	0.40
1:A:1350:ILE:O	1:A:1354:THR:OG1	2.38	0.40
3:E:999:ARG:HG2	3:E:1312:HIS:CD2	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	2100/2549 (82%)	2025 (96%)	74 (4%)	1 (0%)	100	100
2	C	315/326 (97%)	288 (91%)	27 (9%)	0	100	100
3	E	1040/1396 (74%)	968 (93%)	72 (7%)	0	100	100
4	I	104/409 (25%)	95 (91%)	8 (8%)	1 (1%)	15	51
All	All	3559/4680 (76%)	3376 (95%)	181 (5%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	324	ALA
1	A	961	ASP

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	1876/2169 (86%)	1839 (98%)	37 (2%)	55	74
2	C	269/276 (98%)	264 (98%)	5 (2%)	57	76
3	E	928/1214 (76%)	909 (98%)	19 (2%)	55	74
4	I	89/364 (24%)	88 (99%)	1 (1%)	73	85
All	All	3162/4023 (79%)	3100 (98%)	62 (2%)	57	74

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	813	MET
1	A	859	ARG
1	A	934	MET
1	A	959	PHE
1	A	960	ARG
1	A	962	GLN
1	A	968	HIS
1	A	970	MET
1	A	1019	LEU
1	A	1121	LEU
1	A	1126	GLU
1	A	1160	VAL
1	A	1164	ASP
1	A	1213	ILE
1	A	1299	SER
1	A	1354	THR
1	A	1360	LEU
1	A	1380	ILE
1	A	1558	SER
1	A	1652	THR
1	A	1680	ASP
1	A	1701	MET
1	A	1780	THR
1	A	1959	GLN
1	A	1973	ILE
1	A	1988	HIS
1	A	2021	ILE
1	A	2138	LEU

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Mol	Chain	Res	Type
1	A	2161	GLN
1	A	2195	ASP
1	A	2298	ASP
1	A	2302	LEU
1	A	2344	LEU
1	A	2346	LEU
1	A	2493	LEU
1	A	2501	ILE
1	A	2548	PHE
2	C	108	THR
2	C	160	ASP
2	C	173	ILE
2	C	243	THR
2	C	274	TRP
3	E	133	LEU
3	E	164	VAL
3	E	268	THR
3	E	331	ASP
3	E	332	LEU
3	E	424	VAL
3	E	472	ILE
3	E	512	ASP
3	E	572	LEU
3	E	625	THR
3	E	1011	THR
3	E	1013	LEU
3	E	1014	ASP
3	E	1058	ASP
3	E	1135	THR
3	E	1139	MET
3	E	1207	TYR
3	E	1261	ILE
3	E	1323	TYR
4	I	331	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	527	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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	$\#|Z| > 2$
5	IHP	A	2601	-	36,36,36	0.80	2 (5%)	54,60,60	0.31	0

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
5	IHP	A	2601	-	-	3/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2601	IHP	P3-O13	3.00	1.65	1.59
5	A	2601	IHP	P1-O11	2.09	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C2-O12-P2-O22
5	A	2601	IHP	C3-O13-P3-O23
5	A	2601	IHP	C6-O16-P6-O36

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IHP A 2601

Bond lengths

Bond angles

Torsions

Rings
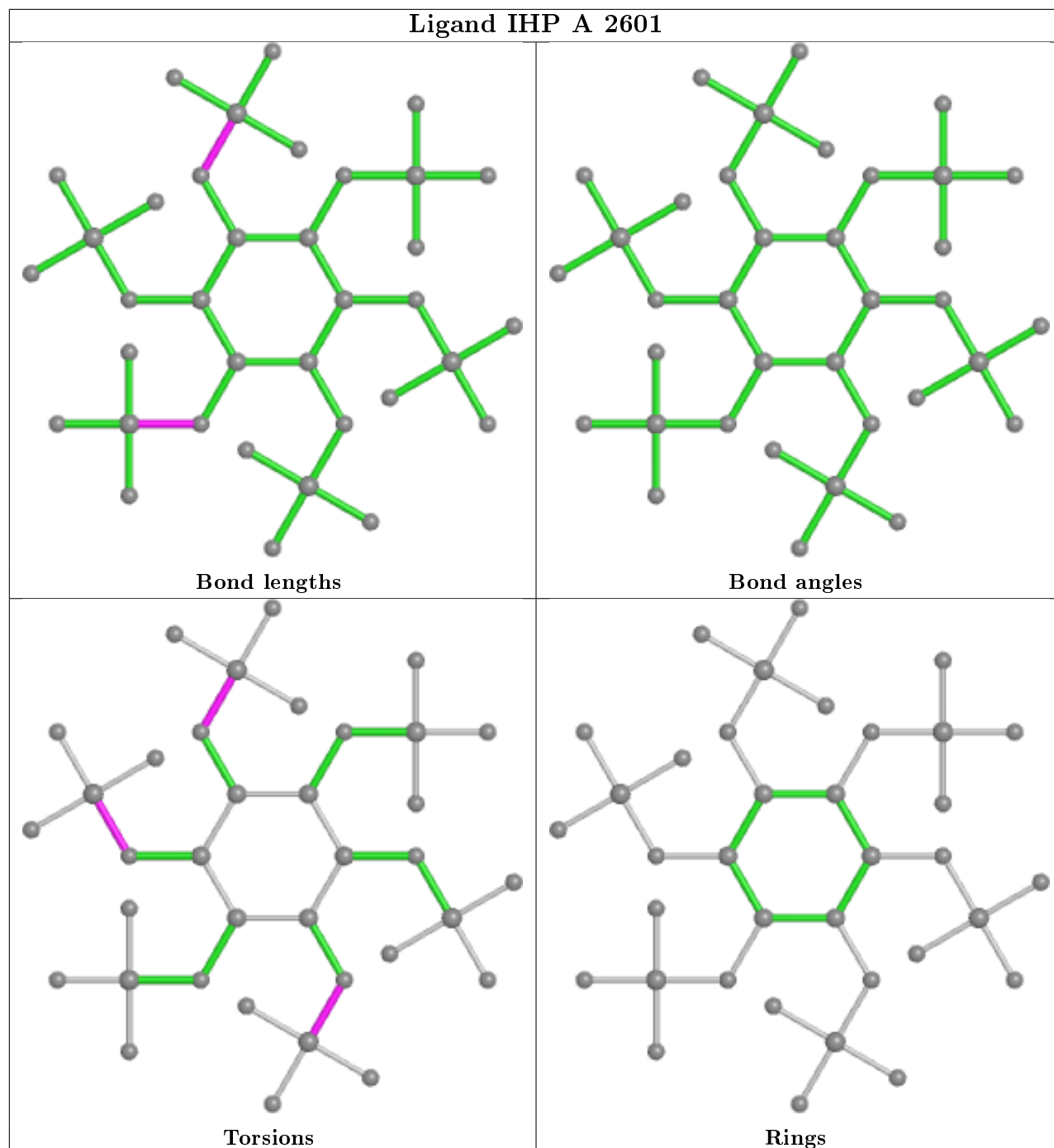
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.