Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 11:53 pm BST

PDB ID	:	3TX7
Title	:	Crystal structure of LRH-1/beta-catenin complex
Authors	:	Yumoto, F.; Fletterick, R.
Deposited on	:	2011-09-22
Resolution	:	2.76 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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.
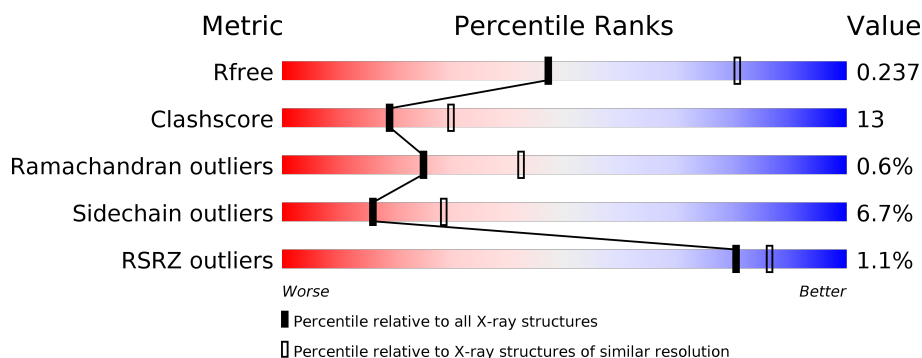
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	69% 24% · ·
2	B	352	41% 19% · 38%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5644 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total 3841	C 2417	N 697	O 702	S 25	0	0	0

There is a discrepancy between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	137	SER	-	EXPRESSION TAG	UNP P35222

- Molecule 2 is a protein called Nuclear receptor subfamily 5 group A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total 1752	C 1125	N 290	O 324	S 13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	SER	-	EXPRESSION TAG	UNP O00482

- Molecule 3 is (2S)-3-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-2-[(6E)-HEXADEC-6-ENOYLOXY]PROPYL (8E)-OCTADEC-8-ENOATE (three-letter code: P6L) (formula: $C_{40}H_{75}O_{10}P$).

P6L
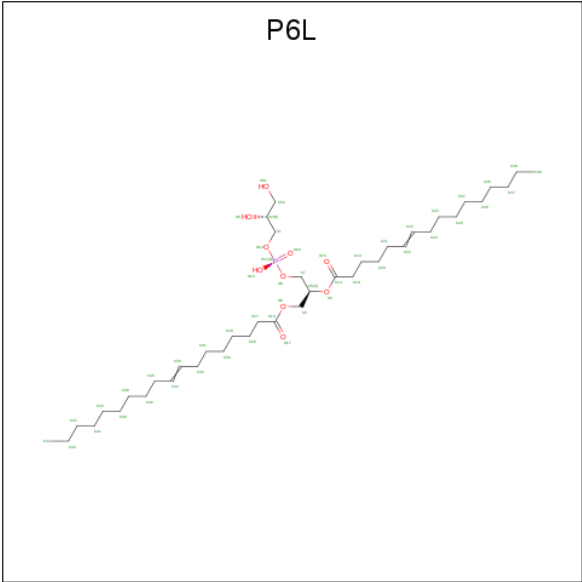
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			51	40	10	1		

3 Residue-property plots ⓘ

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Catenin beta-1
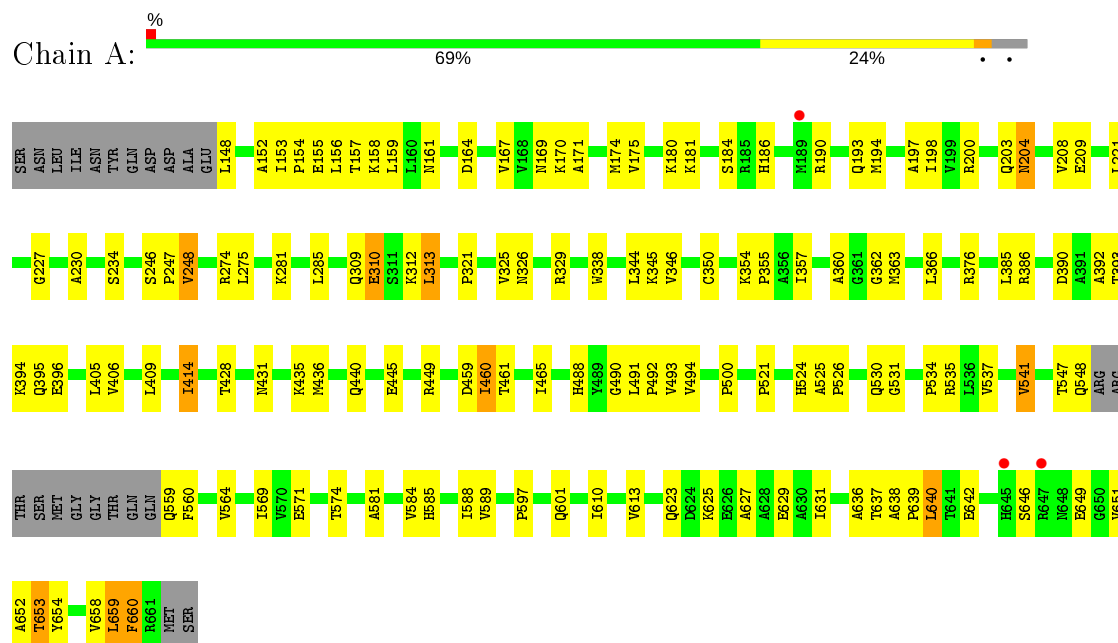
- Molecule 2: Nuclear receptor subfamily 5 group A member 2
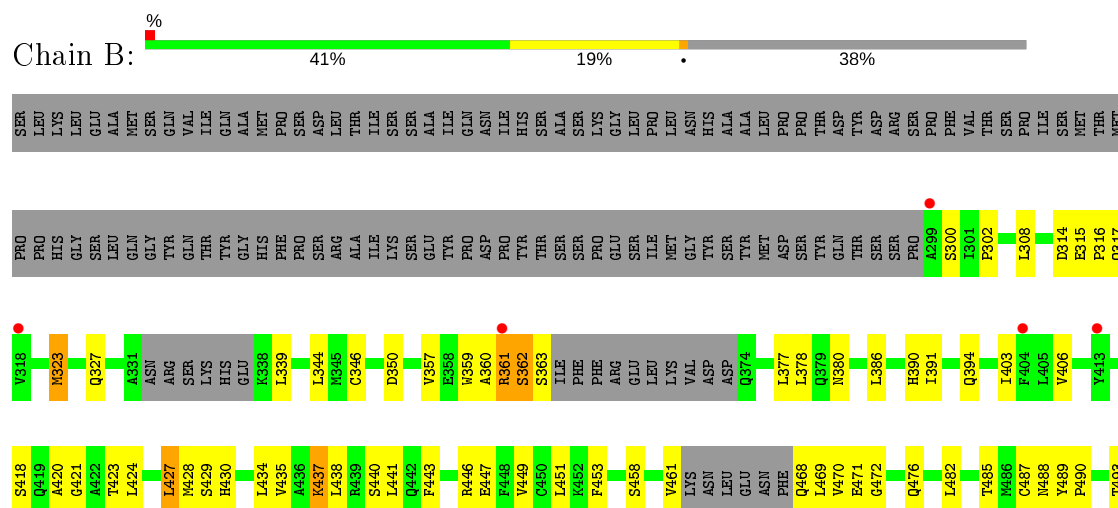
E494 Q498 L501 R502 L503 P504 I509 Q512 N530 L531 A538 LYS ARG ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.82Å 151.60Å 76.13Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	47.02 – 2.76 49.46 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.02-2.76) 99.8 (49.46-2.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.09 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.199 , 0.243 0.195 , 0.237	Depositor DCC
R_{free} test set	1467 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.9	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5644	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:
P6L

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	0.43	0/3895	0.58	0/5287
2	B	0.41	0/1781	0.52	0/2405
All	All	0.42	0/5676	0.57	0/7692

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 (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	3841	0	3992	103	0
2	B	1752	0	1764	45	0
3	B	51	0	74	11	0
All	All	5644	0	5830	149	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (149) 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:468:GLN:HG3	2:B:469:LEU:H	1.37	0.90
1:A:155:GLU:O	1:A:158:LYS:HG2	1.75	0.86
1:A:559:GLN:HG2	1:A:560:PHE:H	1.50	0.77
1:A:394:LYS:HG3	1:A:395:GLN:HE21	1.50	0.77
1:A:445:GLU:HG2	1:A:449:ARG:NH2	2.00	0.76
1:A:363:MET:HE1	1:A:392:ALA:HB1	1.67	0.76
1:A:640:LEU:HD23	1:A:659:LEU:HD13	1.72	0.72
2:B:377:LEU:HD23	2:B:461:VAL:HG11	1.72	0.72
1:A:414:ILE:HD12	1:A:460:ILE:HD11	1.71	0.71
1:A:386:ARG:NH2	2:B:493:THR:HB	2.06	0.70
1:A:393:THR:HA	1:A:431:ASN:HD22	1.58	0.69
1:A:445:GLU:CD	1:A:449:ARG:HH22	1.97	0.67
1:A:209:GLU:HA	1:A:209:GLU:OE1	1.94	0.67
1:A:445:GLU:CG	1:A:449:ARG:HH22	2.09	0.66
1:A:625:LYS:HE3	1:A:629:GLU:OE2	1.97	0.65
1:A:531:GLY:O	1:A:534:PRO:HD2	1.98	0.64
1:A:386:ARG:HH22	2:B:493:THR:HB	1.64	0.63
1:A:156:LEU:HD21	1:A:174:MET:HG2	1.80	0.62
1:A:654:TYR:O	1:A:658:VAL:HG23	2.00	0.61
1:A:274:ARG:HH22	1:A:310:GLU:HG2	1.64	0.61
1:A:414:ILE:HD12	1:A:460:ILE:CD1	2.31	0.61
2:B:424:LEU:HD22	3:B:100:P6L:H181	1.83	0.60
1:A:649:GLU:O	1:A:653:THR:HG23	2.00	0.60
2:B:438:LEU:HD21	2:B:502:ARG:HG3	1.84	0.60
2:B:472:GLY:O	2:B:476:GLN:HG3	2.02	0.60
1:A:525:ALA:HB3	1:A:526:PRO:HD3	1.84	0.58
1:A:537:VAL:O	1:A:541:VAL:HG12	2.04	0.58
1:A:354:LYS:HB3	1:A:355:PRO:HD3	1.85	0.58
1:A:152:ALA:O	1:A:155:GLU:HB2	2.04	0.58
3:B:100:P6L:H311	3:B:100:P6L:H192	1.86	0.57
2:B:323:MET:O	2:B:327:GLN:HG2	2.05	0.57
1:A:363:MET:HG2	1:A:385:LEU:HD23	1.87	0.57
2:B:482:LEU:HD23	2:B:482:LEU:O	2.05	0.56
1:A:194:MET:O	1:A:198:ILE:HG13	2.05	0.56
1:A:221:LEU:O	1:A:227:GLY:HA3	2.06	0.56
2:B:468:GLN:CG	2:B:469:LEU:H	2.16	0.56
1:A:171:ALA:O	1:A:175:VAL:HG23	2.05	0.56
1:A:157:THR:O	1:A:161:ASN:ND2	2.40	0.55
1:A:394:LYS:HE2	1:A:395:GLN:NE2	2.21	0.55
1:A:636:ALA:O	1:A:640:LEU:HB2	2.07	0.54
1:A:445:GLU:HG2	1:A:449:ARG:HH22	1.66	0.54
1:A:325:VAL:HG11	1:A:360:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD23	1:A:148:LEU:C	2.28	0.54
1:A:274:ARG:HH12	1:A:310:GLU:HG2	1.72	0.54
2:B:447:GLU:OE2	2:B:485:THR:HG22	2.08	0.54
1:A:461:THR:O	1:A:465:ILE:HG12	2.09	0.53
1:A:312:LYS:HE2	1:A:346:VAL:HG13	1.91	0.53
2:B:468:GLN:HG3	2:B:469:LEU:N	2.16	0.53
2:B:350:ASP:OD1	2:B:531:LEU:N	2.41	0.53
1:A:428:THR:O	1:A:435:LYS:HE2	2.09	0.53
1:A:521:PRO:HA	1:A:524:HIS:ND1	2.23	0.53
2:B:421:GLY:HA3	3:B:100:P6L:H11	1.91	0.53
1:A:200:ARG:O	1:A:204:ASN:ND2	2.42	0.52
1:A:186:HIS:HB3	1:A:190:ARG:NH1	2.24	0.52
1:A:394:LYS:HE2	1:A:395:GLN:HE21	1.75	0.52
2:B:308:LEU:HD22	2:B:453:PHE:CE1	2.44	0.52
1:A:491:LEU:HB2	1:A:492:PRO:HD3	1.92	0.52
1:A:491:LEU:HD12	1:A:526:PRO:HB2	1.92	0.51
1:A:344:LEU:HD23	1:A:357:ILE:HD13	1.92	0.51
2:B:315:GLU:HB3	2:B:316:PRO:HD3	1.93	0.50
2:B:420:ALA:CB	2:B:424:LEU:HD23	2.41	0.50
1:A:571:GLU:HB2	1:A:610:ILE:HD13	1.91	0.50
1:A:547:THR:HG22	1:A:547:THR:O	2.12	0.50
1:A:597:PRO:O	1:A:601:GLN:HG2	2.12	0.50
3:B:100:P6L:H443	3:B:100:P6L:H261	1.94	0.49
1:A:274:ARG:NH2	1:A:310:GLU:HG2	2.28	0.49
2:B:406:VAL:HG22	2:B:406:VAL:O	2.13	0.49
1:A:230:ALA:O	1:A:234:SER:HB3	2.12	0.49
1:A:156:LEU:CD2	1:A:174:MET:HG2	2.42	0.49
1:A:246:SER:OG	1:A:248:VAL:HG13	2.13	0.49
1:A:585:HIS:O	1:A:588:ILE:HG13	2.13	0.48
1:A:445:GLU:HG3	1:A:488:HIS:CD2	2.48	0.48
1:A:436:MET:O	1:A:440:GLN:HG3	2.14	0.48
3:B:100:P6L:H311	3:B:100:P6L:C19	2.44	0.48
1:A:281:LYS:O	1:A:285:LEU:HG	2.13	0.47
2:B:420:ALA:HB1	2:B:424:LEU:HD23	1.95	0.47
1:A:148:LEU:CD2	1:A:148:LEU:C	2.83	0.47
1:A:640:LEU:HD21	1:A:658:VAL:CG1	2.45	0.47
2:B:394:GLN:HB2	2:B:435:VAL:HG21	1.97	0.47
1:A:627:ALA:O	1:A:631:ILE:HG13	2.14	0.47
1:A:660:PHE:C	1:A:660:PHE:CD2	2.89	0.47
1:A:445:GLU:CG	1:A:449:ARG:NH2	2.69	0.47
2:B:423:THR:HB	3:B:100:P6L:O3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:SER:O	2:B:363:SER:C	2.53	0.46
2:B:428:MET:SD	3:B:100:P6L:H492	2.55	0.46
2:B:430:HIS:HB3	2:B:509:ILE:CD1	2.46	0.46
2:B:390:HIS:CD2	3:B:100:P6L:H493	2.50	0.46
2:B:488:ASN:C	2:B:490:PRO:HD3	2.36	0.46
2:B:482:LEU:HD23	2:B:482:LEU:C	2.36	0.46
1:A:197:ALA:HA	1:A:200:ARG:NH2	2.30	0.46
1:A:326:ASN:OD1	1:A:329:ARG:NH2	2.49	0.46
1:A:321:PRO:HB3	1:A:357:ILE:HG12	1.98	0.46
1:A:646:SER:OG	1:A:651:VAL:HG21	2.16	0.45
1:A:338:TRP:CD1	1:A:376:ARG:HG3	2.51	0.45
1:A:175:VAL:HG21	1:A:194:MET:HE3	1.98	0.45
2:B:427:LEU:HD11	2:B:512:GLN:HB3	1.98	0.45
1:A:169:ASN:OD1	1:A:169:ASN:C	2.55	0.45
2:B:443:PHE:CZ	2:B:451:LEU:HD12	2.52	0.45
1:A:170:LYS:HA	1:A:170:LYS:HD2	1.67	0.45
1:A:584:VAL:O	1:A:588:ILE:HG23	2.17	0.44
2:B:359:TRP:C	2:B:361:ARG:H	2.20	0.44
2:B:489:TYR:N	2:B:490:PRO:HD3	2.32	0.44
2:B:501:LEU:O	2:B:504:PRO:HD2	2.17	0.44
2:B:424:LEU:HG	2:B:424:LEU:O	2.18	0.44
1:A:180:LYS:HA	1:A:180:LYS:HD2	1.64	0.44
1:A:493:VAL:HG13	1:A:494:VAL:N	2.32	0.44
1:A:362:GLY:O	1:A:366:LEU:HG	2.18	0.44
1:A:493:VAL:CG1	1:A:494:VAL:N	2.80	0.44
1:A:275:LEU:HA	1:A:275:LEU:HD12	1.81	0.43
1:A:500:PRO:HD3	1:A:535:ARG:NH2	2.34	0.43
1:A:640:LEU:HA	1:A:640:LEU:HD12	1.77	0.43
1:A:574:THR:HG22	1:A:613:VAL:HB	2.01	0.43
3:B:100:P6L:H361	3:B:100:P6L:H471	1.99	0.43
2:B:427:LEU:HD11	2:B:512:GLN:CB	2.49	0.43
1:A:274:ARG:NH1	1:A:310:GLU:HG2	2.33	0.43
1:A:640:LEU:HD21	1:A:658:VAL:HB	2.00	0.43
2:B:428:MET:HE3	3:B:100:P6L:H312	2.00	0.43
1:A:564:VAL:HG11	1:A:569:ILE:HD11	2.00	0.43
2:B:391:ILE:HD13	2:B:434:LEU:HB3	2.01	0.42
1:A:153:ILE:HG22	1:A:154:PRO:N	2.34	0.42
2:B:458:SER:O	2:B:470:VAL:HG11	2.19	0.42
1:A:171:ALA:O	1:A:174:MET:HB3	2.19	0.42
1:A:406:VAL:O	1:A:409:LEU:HB2	2.19	0.42
1:A:651:VAL:HG23	1:A:652:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LYS:HE3	2:B:487:CYS:SG	2.60	0.42
2:B:437:LYS:HA	2:B:437:LYS:HD3	1.66	0.42
1:A:164:ASP:O	1:A:167:VAL:N	2.53	0.42
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.86	0.42
1:A:158:LYS:HG3	1:A:159:LEU:HD12	2.00	0.41
1:A:537:VAL:O	1:A:541:VAL:CG1	2.68	0.41
2:B:346:CYS:O	2:B:350:ASP:HB2	2.19	0.41
1:A:159:LEU:HB3	1:A:171:ALA:HB2	2.02	0.41
2:B:430:HIS:HB3	2:B:509:ILE:HD11	2.01	0.41
2:B:441:LEU:HD11	2:B:498:GLN:HB3	2.01	0.41
1:A:363:MET:HE1	1:A:392:ALA:CB	2.45	0.41
1:A:638:ALA:N	1:A:639:PRO:HD2	2.36	0.41
1:A:585:HIS:O	1:A:589:VAL:HG23	2.21	0.41
2:B:357:VAL:HG12	2:B:378:LEU:HD13	2.03	0.41
1:A:492:PRO:HG3	1:A:530:GLN:NE2	2.36	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.94	0.41
1:A:571:GLU:HB2	1:A:610:ILE:CD1	2.51	0.41
1:A:193:GLN:HG3	1:A:194:MET:N	2.37	0.40
1:A:246:SER:HA	1:A:247:PRO:HD3	1.86	0.40
2:B:386:LEU:HB3	3:B:100:P6L:H391	2.04	0.40
1:A:313:LEU:HA	1:A:313:LEU:HD22	1.96	0.40
1:A:490:GLY:O	1:A:493:VAL:HG12	2.20	0.40
1:A:312:LYS:HE2	1:A:346:VAL:CG1	2.51	0.40
2:B:314:ASP:HB3	2:B:317:GLN:HB3	2.03	0.40
1:A:638:ALA:HB3	1:A:639:PRO:CD	2.52	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 X-ray entries followed by that with respect to entries of similar resolution.

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	500/527 (95%)	475 (95%)	23 (5%)	2 (0%)	34	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	210/352 (60%)	200 (95%)	8 (4%)	2 (1%)	15	27
All	All	710/879 (81%)	675 (95%)	31 (4%)	4 (1%)	25	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	581	ALA
2	B	360	ALA
2	B	302	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	417/437 (95%)	394 (94%)	23 (6%)	21	37
2	B	194/315 (62%)	176 (91%)	18 (9%)	9	15
All	All	611/752 (81%)	570 (93%)	41 (7%)	16	28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	LYS
1	A	184	SER
1	A	204	ASN
1	A	208	VAL
1	A	248	VAL
1	A	309	GLN
1	A	310	GLU
1	A	313	LEU
1	A	350	CYS
1	A	390	ASP
1	A	396	GLU
1	A	414	ILE

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Mol	Chain	Res	Type
1	A	459	ASP
1	A	460	ILE
1	A	541	VAL
1	A	548	GLN
1	A	623	GLN
1	A	637	THR
1	A	640	LEU
1	A	642	GLU
1	A	653	THR
1	A	659	LEU
1	A	660	PHE
2	B	300	SER
2	B	323	MET
2	B	339	LEU
2	B	344	LEU
2	B	361	ARG
2	B	362	SER
2	B	380	ASN
2	B	403	ILE
2	B	418	SER
2	B	427	LEU
2	B	429	SER
2	B	437	LYS
2	B	440	SER
2	B	446	ARG
2	B	449	VAL
2	B	471	GLU
2	B	494	GLU
2	B	530	ASN

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

Mol	Chain	Res	Type
1	A	204	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)

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	$\#|Z| > 2$
3	P6L	B	100	-	50,50,50	2.03	9 (18%)	53,56,56	1.60	7 (13%)

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	P6L	B	100	-	-	29/55/55/55	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	100	P6L	O17-C16	6.60	1.42	1.22
3	B	100	P6L	O15-C14	6.58	1.42	1.22
3	B	100	P6L	C34-C33	4.34	1.56	1.31
3	B	100	P6L	C23-C22	4.05	1.55	1.31
3	B	100	P6L	P11-O10	3.56	1.63	1.50
3	B	100	P6L	O8-C16	3.40	1.43	1.33
3	B	100	P6L	C18-C14	2.74	1.58	1.50
3	B	100	P6L	O4-C14	2.38	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	100	P6L	C27-C16	2.20	1.57	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	100	P6L	O4-C14-O15	-6.03	109.14	123.70
3	B	100	P6L	O8-C16-O17	-4.96	111.08	123.59
3	B	100	P6L	O15-C14-C18	-3.60	109.70	123.73
3	B	100	P6L	O4-C14-C18	2.35	116.57	111.50
3	B	100	P6L	O8-C6-C5	2.19	114.82	108.43
3	B	100	P6L	C28-C27-C16	2.03	120.99	113.62
3	B	100	P6L	C5-O4-C14	2.02	122.77	117.79

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	100	P6L	C1-C2-C50-O51
3	B	100	P6L	O15-C14-O4-C5
3	B	100	P6L	C18-C14-O4-C5
3	B	100	P6L	C1-O12-P11-O9
3	B	100	P6L	C1-O12-P11-O10
3	B	100	P6L	O12-C1-C2-O3
3	B	100	P6L	C38-C39-C40-C41
3	B	100	P6L	C40-C41-C42-C43
3	B	100	P6L	C32-C33-C34-C35
3	B	100	P6L	C29-C30-C31-C32
3	B	100	P6L	C25-C26-C37-C45
3	B	100	P6L	C21-C22-C23-C24
3	B	100	P6L	C22-C23-C24-C25
3	B	100	P6L	C37-C45-C46-C47
3	B	100	P6L	C33-C34-C35-C36
3	B	100	P6L	O4-C5-C6-O8
3	B	100	P6L	C46-C47-C48-C49
3	B	100	P6L	O4-C5-C7-O9
3	B	100	P6L	C30-C31-C32-C33
3	B	100	P6L	C6-C5-C7-O9
3	B	100	P6L	O12-C1-C2-C50
3	B	100	P6L	C36-C38-C39-C40
3	B	100	P6L	C7-O9-P11-O12
3	B	100	P6L	C24-C25-C26-C37
3	B	100	P6L	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
3	B	100	P6L	C41-C42-C43-C44
3	B	100	P6L	O17-C16-O8-C6
3	B	100	P6L	O17-C16-C27-C28
3	B	100	P6L	C19-C20-C21-C22

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	100	P6L	11	0

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 P6L B 100

Bond lengths

Bond angles

Torsions

Rings
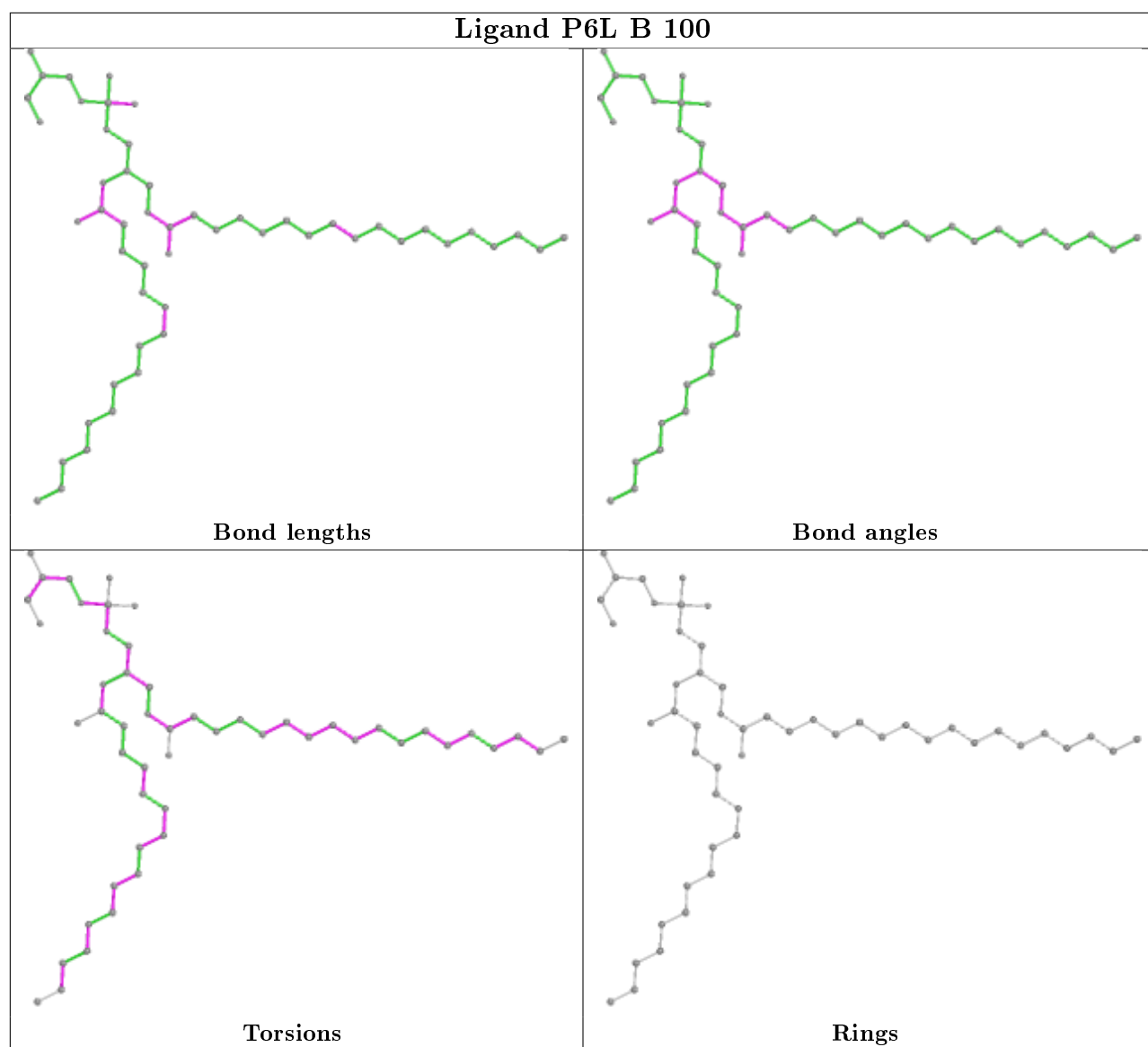
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	504/527 (95%)	0.08	3 (0%)	89	92	43, 64, 104, 130	0
2	B	218/352 (61%)	0.16	5 (2%)	60	69	52, 77, 115, 122	0
All	All	722/879 (82%)	0.11	8 (1%)	80	86	43, 68, 107, 130	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	299	ALA	2.7
2	B	361	ARG	2.4
2	B	404	PHE	2.3
1	A	647	ARG	2.3
2	B	413	TYR	2.3
1	A	645	HIS	2.2
1	A	189	MET	2.2
2	B	318	VAL	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

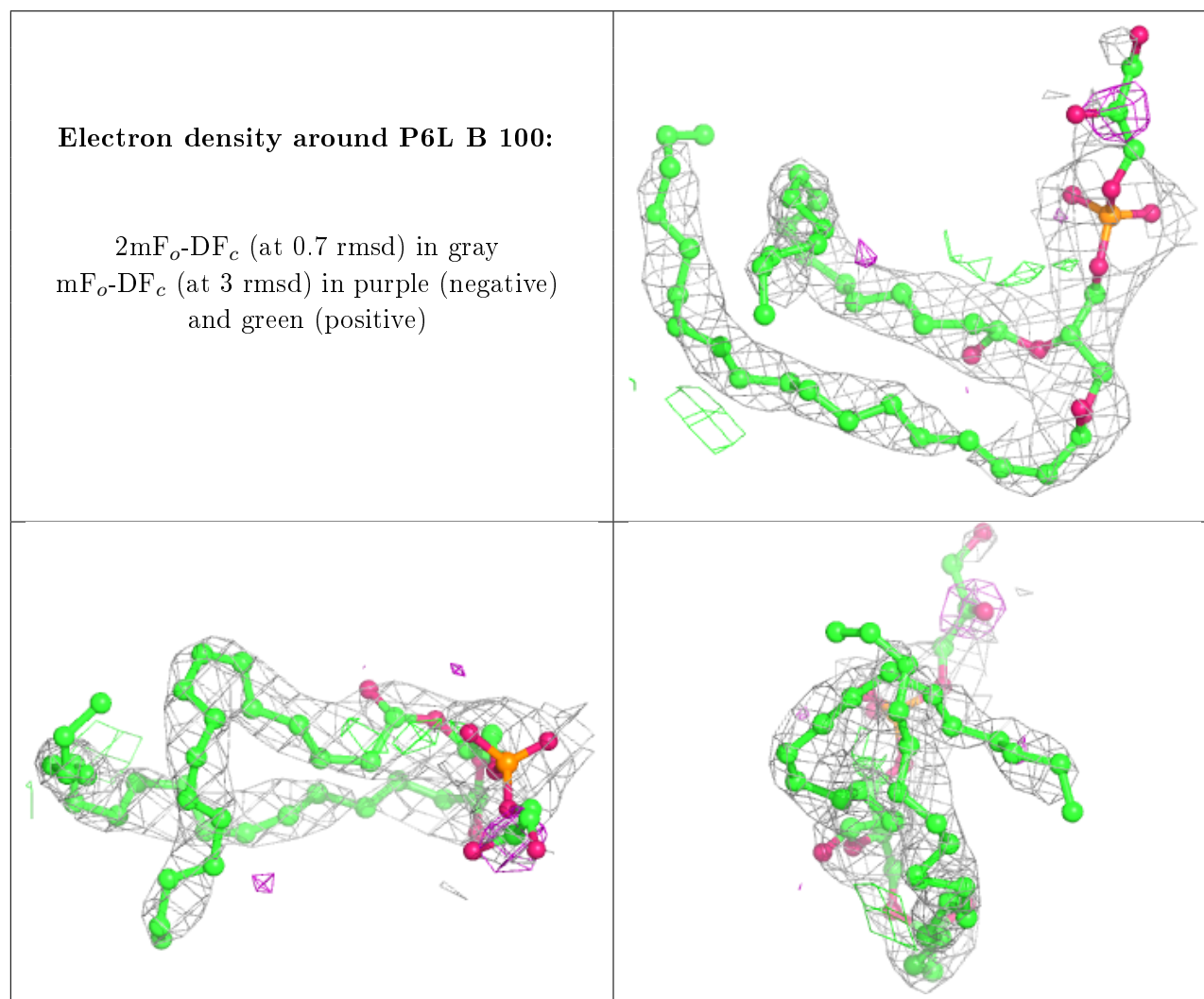## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P6L	B	100	51/51	0.92	0.37	57,76,96,103	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6L B 100:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.