



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:53 AM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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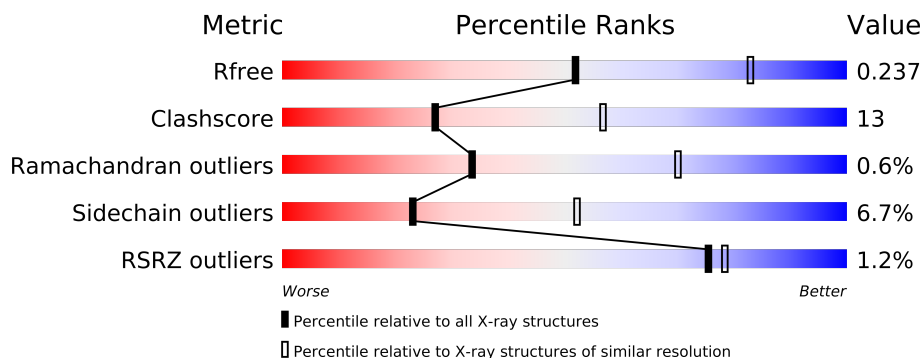
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	527	
2	B	352	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	P6L	B	100	-	X

## 2 Entry composition

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

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	C	N	O	S	0	0	0
			3841	2417	697	702	25			

There is a discrepancy between the modelled and reference sequences:

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

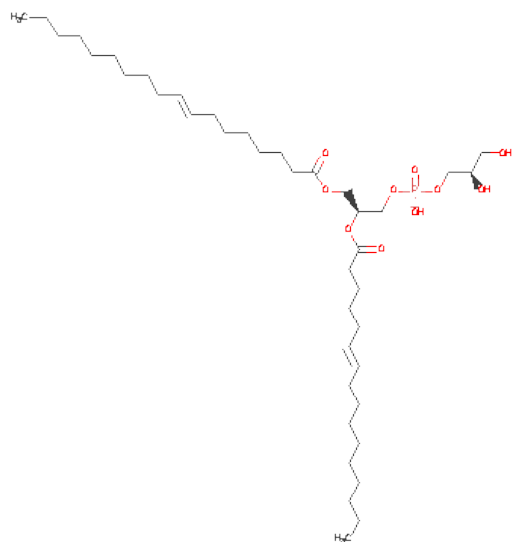
- Molecule 2 is a protein called Nuclear receptor subfamily 5 group A member 2.

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

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<sub>40</sub>H<sub>75</sub>O<sub>10</sub>P).



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28889 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (149) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:148:LEU:HD23	1:A:148:LEU:C	2.28	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:421:GLY:HA3	3:B:100:P6L:H11	1.91	0.53
1:A:521:PRO:HA	1:A:524:HIS:ND1	2.23	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:420:ALA:CB	2:B:424:LEU:HD23	2.41	0.50
2:B:315:GLU:HB3	2:B:316:PRO:HD3	1.93	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:640:LEU:HD21	1:A:658:VAL:CG1	2.45	0.47
1:A:148:LEU:CD2	1:A:148:LEU:C	2.83	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:362:SER:O	2:B:363:SER:C	2.53	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:321:PRO:HB3	1:A:357:ILE:HG12	1.98	0.46
1:A:326:ASN:OD1	1:A:329:ARG:NH2	2.49	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
2:B:443:PHE:CZ	2:B:451:LEU:HD12	2.52	0.45
1:A:169:ASN:OD1	1:A:169:ASN:C	2.55	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: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:359:TRP:C	2:B:361:ARG:H	2.20	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:493:VAL:CG1	1:A:494:VAL:N	2.80	0.44
1:A:362:GLY:O	1:A:366:LEU:HG	2.18	0.44
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.81	0.43
1:A:640:LEU:HA	1:A:640:LEU:HD12	1.77	0.43
1:A:500:PRO:HD3	1:A:535:ARG:NH2	2.34	0.43
3:B:100:P6L:H361	3:B:100:P6L:H471	1.99	0.43
1:A:574:THR:HG22	1:A:613:VAL:HB	2.01	0.43
2:B:427:LEU:HD11	2:B:512:GLN:CB	2.49	0.43
1:A:640:LEU:HD21	1:A:658:VAL:HB	2.00	0.43
1:A:274:ARG:NH1	1:A:310:GLU:HG2	2.33	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:651:VAL:HG23	1:A:652:ALA:N	2.35	0.42
1:A:406:VAL:O	1:A:409:LEU:HB2	2.19	0.42
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:571:GLU:HB2	1:A:610:ILE:CD1	2.51	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.94	0.41
1:A:193:GLN:HG3	1:A:194:MET:N	2.37	0.40
2:B:386:LEU:HB3	3:B:100:P6L:H391	2.04	0.40
1:A:246:SER:HA	1:A:247:PRO:HD3	1.86	0.40
1:A:490:GLY:O	1:A:493:VAL:HG12	2.20	0.40
1:A:313:LEU:HA	1:A:313:LEU:HD22	1.96	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

### 5.3.1 Protein backbone ⓘ

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%)	43	79
2	B	210/352 (60%)	200 (95%)	8 (4%)	2 (1%)	22	56
All	All	710/879 (81%)	675 (95%)	31 (4%)	4 (1%)	33	70

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 ⓘ

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%)	30	62
2	B	194/315 (62%)	176 (91%)	18 (9%)	13	33
All	All	611/752 (81%)	570 (93%)	41 (7%)	23	52

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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	2.02	9 (18%)	56,56,56	1.62	7 (12%)

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	-	-	2/55/55/55	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	100	P6L	O17-C16	6.53	1.42	1.22
3	B	100	P6L	O15-C14	6.51	1.42	1.22
3	B	100	P6L	C34-C33	4.56	1.56	1.31
3	B	100	P6L	C23-C22	4.25	1.55	1.31
3	B	100	P6L	O8-C16	3.19	1.43	1.33
3	B	100	P6L	P11-O10	3.18	1.63	1.51
3	B	100	P6L	C18-C14	2.64	1.58	1.50
3	B	100	P6L	O4-C14	2.23	1.41	1.34
3	B	100	P6L	C27-C16	2.12	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	-5.42	109.14	123.65
3	B	100	P6L	O8-C16-O17	-4.52	111.08	123.43
3	B	100	P6L	O12-C1-C2	4.12	121.55	108.62
3	B	100	P6L	O15-C14-C18	-3.41	109.70	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	100	P6L	O8-C6-C5	2.29	114.82	108.83
3	B	100	P6L	O4-C14-C18	2.29	116.57	111.56
3	B	100	P6L	O12-P11-O9	2.23	111.05	104.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	100	P6L	C5-O4-C14-O15
3	B	100	P6L	C5-O4-C14-C18

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	504/527 (95%)	0.12	3 (0%) 86 89	43, 64, 104, 130	0
2	B	218/352 (61%)	0.18	6 (2%) 50 54	52, 77, 115, 122	0
All	All	722/879 (82%)	0.14	9 (1%) 75 78	43, 68, 107, 130	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	299	ALA	2.8
2	B	413	TYR	2.6
1	A	645	HIS	2.5
2	B	404	PHE	2.5
2	B	339	LEU	2.4
1	A	647	ARG	2.4
2	B	318	VAL	2.2
1	A	189	MET	2.1
2	B	326	LEU	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	P6L	B	100	51/51	0.37	3.67	57,76,96,103	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.