



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2016 – 04:07 PM EDT

PDB ID : 5F0N  
Title : Cohesin subunit Pds5  
Authors : Lee, B.-G.; Jansma, M.; Nasmyth, K.; Lowe, J.  
Deposited on : 2015-11-27  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

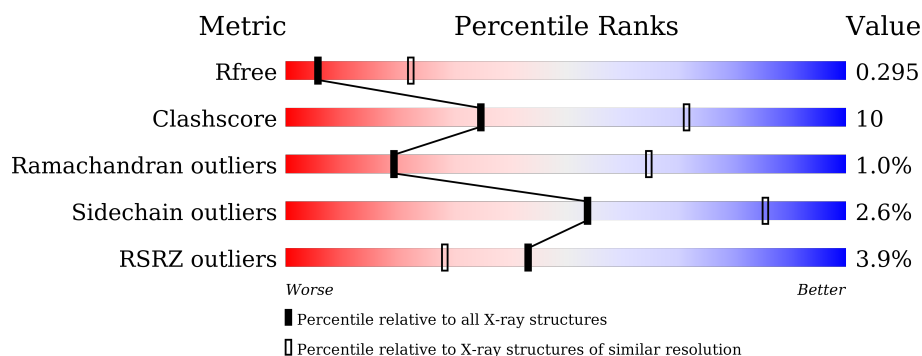
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1175	<div> <div>3%</div> <div>64%</div> <div>23%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition

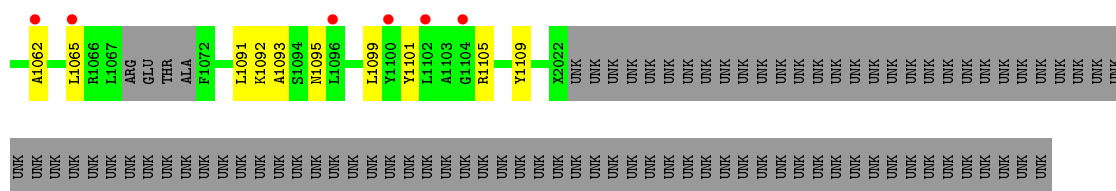
There is only 1 type of molecule in this entry. The entry contains 8213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cohesin subunit Pds5,cohesin subunit Pds5, cohesin subunit Pds5,KLTH0D07062p,cohesin subunit Pds5,cohesin subunit Pds5, cohesin subunit Pds5,KLTH0D07062p,cohesin subunit Pds5,cohesin subunit Pds5, cohesin subunit Pds5,KLTH0D07062p,cohesin subunit Pds5,cohesin subunit Pds5, cohesin subunit Pds5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0	0
			8213	5280	1374	1532	27			





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	238.21 Å   238.21 Å   80.66 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	46.67 – 3.20 46.67 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.8 (46.67-3.20) 92.8 (46.67-3.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 3.19 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.236 , 0.295 0.233 , 0.295	Depositor DCC
$R_{free}$ test set	1384 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.7	EDS
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 26119 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/8169	0.46	0/11047

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	763	THR	Peptide
1	A	764	PHE	Peptide
1	A	931	ASN	Peptide

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8213	0	8172	162	0
All	All	8213	0	8172	162	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 10.

All (162) 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:1095:ASN:HB3	1:A:1099:LEU:HD13	1.60	0.83
1:A:323:LEU:HD23	1:A:360:ILE:HG23	1.64	0.79
1:A:170:LEU:HD12	1:A:171:PRO:HD2	1.66	0.77
1:A:1036:GLU:HA	1:A:1039:ARG:HB3	1.65	0.76
1:A:165:VAL:HG13	1:A:210:GLU:HG2	1.70	0.74
1:A:223:PHE:HB3	1:A:300:LEU:HD21	1.67	0.74
1:A:764:PHE:O	1:A:768:LYS:N	2.20	0.72
1:A:1091:LEU:HG	1:A:1092:LYS:H	1.55	0.71
1:A:127:THR:HA	1:A:170:LEU:HD21	1.71	0.71
1:A:696:LYS:HB3	1:A:700:ARG:HH12	1.59	0.68
1:A:986:ARG:NH1	1:A:1016:GLU:OE2	2.27	0.67
1:A:113:ARG:HG3	1:A:161:TYR:CG	2.29	0.67
1:A:126:LEU:HA	1:A:129:ILE:HG12	1.76	0.66
1:A:1019:GLN:HA	1:A:1022:ARG:HB3	1.77	0.66
1:A:982:SER:HB3	1:A:985:VAL:HG22	1.77	0.66
1:A:765:PHE:O	1:A:769:LEU:HB2	1.97	0.64
1:A:362:LEU:HD21	1:A:393:ASP:HB3	1.79	0.64
1:A:808:LEU:HD23	1:A:815:PHE:HE1	1.63	0.64
1:A:681:LEU:HD22	1:A:713:ILE:HG22	1.79	0.63
1:A:111:ILE:HA	1:A:114:LEU:HB2	1.82	0.61
1:A:946:ARG:NH1	1:A:980:ASP:OD2	2.33	0.61
1:A:130:PHE:HA	1:A:133:PHE:HB2	1.84	0.60
1:A:942:GLN:O	1:A:946:ARG:HG3	2.02	0.60
1:A:122:THR:HG22	1:A:123:ASP:H	1.67	0.59
1:A:143:PRO:HA	1:A:148:LEU:HD13	1.83	0.59
1:A:783:TYR:HA	1:A:786:LYS:HB2	1.84	0.59
1:A:170:LEU:HD12	1:A:171:PRO:CD	2.34	0.58
1:A:745:THR:O	1:A:749:ILE:HG13	2.04	0.58
1:A:830:PRO:HG3	1:A:894:VAL:HG11	1.85	0.58
1:A:947:CYS:HB2	1:A:985:VAL:HG12	1.86	0.58
1:A:643:LEU:HB3	1:A:657:ARG:HH22	1.69	0.57
1:A:1105:ARG:NH2	1:A:1109:TYR:OH	2.37	0.57
1:A:937:THR:O	1:A:942:GLN:NE2	2.35	0.57
1:A:113:ARG:HG3	1:A:161:TYR:CD1	2.40	0.56
1:A:370:PRO:HA	1:A:373:ARG:HD2	1.86	0.56
1:A:430:PRO:HA	1:A:477:ILE:HD11	1.88	0.55
1:A:627:VAL:O	1:A:631:VAL:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:VAL:HB	1:A:484:ILE:HD12	1.88	0.55
1:A:565:ASN:HB2	1:A:606:ASN:HD21	1.71	0.55
1:A:693:GLU:HA	1:A:696:LYS:HD2	1.88	0.54
1:A:829:GLN:HB3	1:A:832:LEU:HD13	1.90	0.54
1:A:416:THR:O	1:A:420:VAL:HG12	2.08	0.54
1:A:83:TYR:HA	1:A:86:ASP:HB2	1.89	0.53
1:A:219:LEU:HD23	1:A:267:PHE:HB2	1.91	0.53
1:A:305:TRP:HA	1:A:312:VAL:HG21	1.91	0.52
1:A:328:GLU:OE1	1:A:331:ARG:NH2	2.25	0.52
1:A:441:LEU:O	1:A:444:GLU:HB2	2.10	0.52
1:A:810:LEU:HD21	1:A:847:ASP:HB3	1.91	0.52
1:A:95:ASN:HB2	1:A:101:ARG:HB3	1.90	0.52
1:A:1058:HIS:O	1:A:1062:ALA:N	2.42	0.52
1:A:306:LYS:HG3	1:A:307:TYR:CE2	2.44	0.52
1:A:98:HIS:ND1	1:A:147:TYR:HE2	2.07	0.52
1:A:406:ASP:OD2	1:A:408:THR:HG22	2.10	0.52
1:A:461:TYR:CZ	1:A:465:ILE:HD11	2.45	0.51
1:A:380:ILE:N	1:A:381:PRO:HD2	2.26	0.51
1:A:575:ASP:O	1:A:579:ILE:HG12	2.10	0.51
1:A:235:LEU:HB3	1:A:240:TYR:CE1	2.46	0.51
1:A:235:LEU:HD23	1:A:235:LEU:H	1.76	0.51
1:A:308:ALA:HB1	1:A:311:LEU:HB3	1.91	0.51
1:A:450:ARG:O	1:A:454:ILE:HG13	2.11	0.51
1:A:958:LYS:HD3	1:A:1001:SER:HB3	1.92	0.50
1:A:231:ARG:NH2	1:A:307:TYR:CZ	2.78	0.50
1:A:701:GLN:O	1:A:705:ASN:ND2	2.42	0.50
1:A:195:ASN:N	1:A:195:ASN:OD1	2.45	0.50
1:A:951:LEU:HD22	1:A:992:ARG:HG3	1.94	0.50
1:A:624:HIS:N	1:A:679:SER:OG	2.44	0.50
1:A:744:ARG:O	1:A:748:LYS:HG2	2.12	0.50
1:A:121:TYR:HB2	1:A:126:LEU:HD13	1.94	0.49
1:A:316:THR:HG21	1:A:354:HIS:CE1	2.47	0.49
1:A:76:ASP:O	1:A:79:SER:OG	2.25	0.49
1:A:517:SER:OG	1:A:518:ASN:N	2.45	0.49
1:A:306:LYS:HB3	1:A:344:THR:HG21	1.95	0.49
1:A:380:ILE:HD11	1:A:398:LEU:HD13	1.95	0.49
1:A:609:ARG:HD3	1:A:637:ARG:HD3	1.95	0.49
1:A:565:ASN:HD21	1:A:603:ARG:HG2	1.78	0.48
1:A:421:PRO:HB2	1:A:423:LYS:HD2	1.95	0.47
1:A:850:LEU:HD23	1:A:926:LEU:HB3	1.97	0.47
1:A:494:ILE:O	1:A:496:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:PHE:C	1:A:764:PHE:CD2	2.88	0.47
1:A:801:VAL:O	1:A:805:ILE:HG23	2.15	0.47
1:A:879:SER:HB2	1:A:883:PHE:CE2	2.50	0.47
1:A:987:SER:HB3	1:A:1021:LEU:HD22	1.97	0.47
1:A:821:VAL:O	1:A:825:ILE:HG13	2.15	0.47
1:A:179:GLU:HA	1:A:182:ASN:HB2	1.96	0.46
1:A:121:TYR:HB2	1:A:126:LEU:CD1	2.46	0.46
1:A:155:ILE:HG13	1:A:203:ILE:HG13	1.97	0.46
1:A:84:ARG:HE	1:A:120:PRO:HB2	1.81	0.46
1:A:766:PHE:HE2	1:A:791:ALA:HB2	1.81	0.46
1:A:163:SER:HA	1:A:166:ILE:HD13	1.97	0.45
1:A:220:LYS:O	1:A:224:ASN:HB2	2.16	0.45
1:A:598:ILE:HG23	1:A:660:PHE:CD1	2.51	0.45
1:A:633:GLU:HG2	1:A:637:ARG:HE	1.81	0.45
1:A:917:PHE:CE1	1:A:970:ASP:HB3	2.51	0.45
1:A:431:ASN:HB3	1:A:434:VAL:HG23	1.98	0.45
1:A:596:GLU:O	1:A:600:LEU:HB2	2.15	0.45
1:A:637:ARG:O	1:A:643:LEU:HD13	2.16	0.45
1:A:642:GLU:HG2	1:A:646:LYS:HB2	1.98	0.45
1:A:322:LEU:HA	1:A:325:SER:OG	2.16	0.45
1:A:168:THR:O	1:A:173:SER:OG	2.34	0.45
1:A:810:LEU:HD11	1:A:843:LEU:HD21	1.99	0.45
1:A:125:GLU:O	1:A:129:ILE:HG23	2.17	0.44
1:A:275:VAL:HG12	1:A:290:ALA:HB1	1.98	0.44
1:A:932:THR:O	1:A:934:ASN:N	2.49	0.44
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.77	0.44
1:A:984:GLU:OE2	1:A:984:GLU:N	2.50	0.44
1:A:696:LYS:HB3	1:A:700:ARG:NH1	2.29	0.44
1:A:954:LEU:HA	1:A:954:LEU:HD12	1.78	0.44
1:A:384:LEU:O	1:A:424:ARG:NH2	2.51	0.44
1:A:260:LEU:HD23	1:A:311:LEU:HD11	1.98	0.43
1:A:91:LYS:HE3	1:A:96:LYS:HE3	2.00	0.43
1:A:423:LYS:CD	1:A:423:LYS:H	2.31	0.43
1:A:272:MET:HG3	1:A:276:LEU:HD13	2.00	0.43
1:A:896:ALA:HB3	1:A:897:PRO:HD3	2.00	0.43
1:A:979:GLU:OE2	1:A:1012:PHE:HB3	2.19	0.43
1:A:598:ILE:HD13	1:A:663:VAL:HG21	2.01	0.43
1:A:547:GLN:OE1	1:A:710:LYS:NZ	2.51	0.43
1:A:180:LEU:O	1:A:183:ILE:HG12	2.19	0.43
1:A:375:ALA:O	1:A:379:GLU:HG2	2.19	0.43
1:A:638:LEU:HD22	1:A:660:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:THR:CG2	1:A:765:PHE:H	2.32	0.43
1:A:1004:ILE:HA	1:A:1004:ILE:HD13	1.91	0.42
1:A:1052:ILE:HA	1:A:1055:ILE:HG22	2.00	0.42
1:A:186:SER:O	1:A:189:ASN:ND2	2.41	0.42
1:A:308:ALA:O	1:A:312:VAL:HG23	2.19	0.42
1:A:132:LEU:HD12	1:A:135:ALA:HB3	2.01	0.42
1:A:865:PHE:HB3	1:A:869:ASP:HB2	2.01	0.42
1:A:153:TYR:O	1:A:157:ASN:HB2	2.19	0.42
1:A:167:LEU:HD11	1:A:176:LEU:HG	2.01	0.42
1:A:356:ASP:O	1:A:360:ILE:HG22	2.19	0.42
1:A:817:SER:O	1:A:821:VAL:HG23	2.20	0.42
1:A:565:ASN:ND2	1:A:606:ASN:OD1	2.53	0.42
1:A:718:VAL:O	1:A:722:VAL:HG13	2.19	0.42
1:A:996:PHE:HB3	1:A:1002:ILE:HG12	2.01	0.42
1:A:677:ASN:HD22	1:A:678:ILE:H	1.67	0.42
1:A:700:ARG:NH2	1:A:736:THR:O	2.53	0.42
1:A:990:ILE:HG22	1:A:994:LYS:HE3	2.02	0.42
1:A:423:LYS:HD2	1:A:423:LYS:H	1.85	0.42
1:A:216:MET:O	1:A:220:LYS:N	2.40	0.41
1:A:919:LEU:HG	1:A:926:LEU:HD21	2.01	0.41
1:A:994:LYS:HD2	1:A:1028:TRP:CG	2.55	0.41
1:A:223:PHE:O	1:A:226:PHE:HB2	2.20	0.41
1:A:651:ILE:HD13	1:A:655:PHE:CZ	2.54	0.41
1:A:947:CYS:O	1:A:951:LEU:HG	2.20	0.41
1:A:589:PHE:CD2	1:A:595:VAL:HG11	2.54	0.41
1:A:661:SER:O	1:A:665:ARG:HG3	2.20	0.41
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.87	0.41
1:A:277:GLY:O	1:A:278:GLU:HG3	2.20	0.41
1:A:841:VAL:O	1:A:845:ILE:HG13	2.20	0.41
1:A:147:TYR:O	1:A:151:GLN:NE2	2.54	0.41
1:A:208:ILE:HA	1:A:214:LEU:HD21	2.02	0.41
1:A:710:LYS:HE3	1:A:713:ILE:HD11	2.01	0.41
1:A:980:ASP:HB3	1:A:985:VAL:HG23	2.03	0.41
1:A:224:ASN:O	1:A:227:LEU:HD12	2.21	0.41
1:A:291:TYR:CE1	1:A:329:LEU:HD13	2.56	0.41
1:A:560:PHE:CE1	1:A:577:LYS:HD2	2.56	0.41
1:A:693:GLU:HA	1:A:696:LYS:HB2	2.03	0.41
1:A:957:THR:HG21	1:A:1006:PHE:CE1	2.56	0.41
1:A:810:LEU:HD21	1:A:847:ASP:CB	2.51	0.40
1:A:799:SER:OG	1:A:832:LEU:HG	2.20	0.40
1:A:841:VAL:HG11	1:A:908:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:HG3	1:A:243:ASP:HB2	2.03	0.40
1:A:1062:ALA:HA	1:A:1065:LEU:CD2	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	986/1175 (84%)	909 (92%)	67 (7%)	10 (1%)	19 65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	PHE
1	A	932	THR
1	A	1093	ALA
1	A	95	ASN
1	A	115	TYR
1	A	120	PRO
1	A	495	ASN
1	A	929	GLU
1	A	902	ASP
1	A	936	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	890/920 (97%)	867 (97%)	23 (3%)	54 85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	82	ARG
1	A	93	LEU
1	A	103	PHE
1	A	113	ARG
1	A	259	ARG
1	A	278	GLU
1	A	302	SER
1	A	423	LYS
1	A	459	ARG
1	A	516	LEU
1	A	537	PHE
1	A	550	MET
1	A	643	LEU
1	A	677	ASN
1	A	764	PHE
1	A	797	TYR
1	A	831	GLN
1	A	835	LYS
1	A	866	SER
1	A	900	HIS
1	A	1054	PHE
1	A	1101	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	HIS
1	A	565	ASN
1	A	606	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2008:UNK	C	2009:UNK	N	31.06
1	A	1109:TYR	C	2000:UNK	N	25.72
1	A	17:UNK	C	76:ASP	N	13.12

## 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	998/1175 (84%)	0.24	39 (3%)	43 28	28, 60, 105, 142	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	THR	5.6
1	A	929	GLU	4.9
1	A	94	ARG	4.0
1	A	114	LEU	3.8
1	A	96	LYS	3.6
1	A	95	ASN	3.4
1	A	1065	LEU	3.3
1	A	92	ILE	3.1
1	A	857	ASP	3.1
1	A	78	ARG	3.0
1	A	1096	LEU	3.0
1	A	111	ILE	2.9
1	A	236	ASP	2.7
1	A	472	ASN	2.7
1	A	178	GLU	2.6
1	A	82	ARG	2.6
1	A	97	ASP	2.6
1	A	1102	LEU	2.5
1	A	81	GLU	2.5
1	A	93	LEU	2.5
1	A	1062	ALA	2.5
1	A	772	TYR	2.4
1	A	80	LEU	2.4
1	A	856	GLY	2.4
1	A	1104	GLY	2.3
1	A	764	PHE	2.3
1	A	100	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	89	ASP	2.3
1	A	763	THR	2.3
1	A	91	LYS	2.2
1	A	109	SER	2.1
1	A	90	ARG	2.1
1	A	87	LEU	2.1
1	A	1100	TYR	2.1
1	A	650	LYS	2.1
1	A	126	LEU	2.1
1	A	860	ASP	2.1
1	A	123	ASP	2.0
1	A	681	LEU	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.