



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:44 PM BST

PDB ID : 6WC4  
Title : Crystal structure of the SNARE Use1 bound to Dsl1 complex subunits Sec39 and Dsl1  
Authors : Travis, S.M.; Jeffrey, P.D.; Hughson, F.M.  
Deposited on : 2020-03-29  
Resolution : 5.73 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

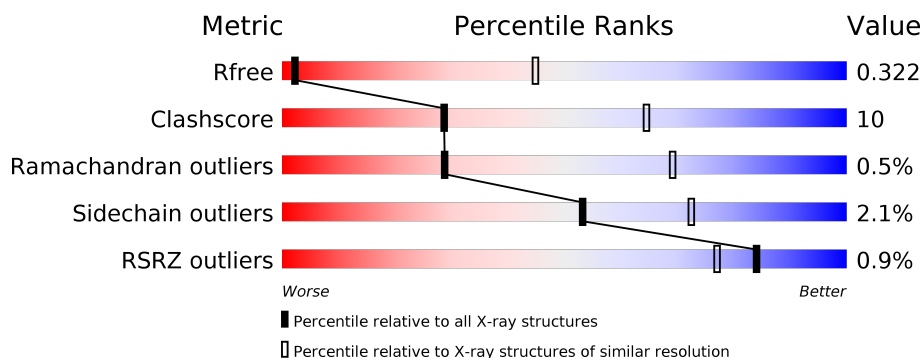
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.73 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	1004 (7.58-3.86)
Clashscore	141614	1030 (7.54-3.90)
Ramachandran outliers	138981	1000 (7.58-3.86)
Sidechain outliers	138945	1004 (7.60-3.82)
RSRZ outliers	127900	1003 (7.66-3.78)

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 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  $\leq 5\%$ . 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	667	
2	B	87	
3	C	306	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6126 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 Protein transport protein SEC39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			3249	2038	587	621	3			

- Molecule 2 is a protein called Vesicle transport protein USE1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	0	0	0
			435	261	87	87			

- Molecule 3 is a protein called Protein transport protein DSL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	295	Total	C	N	O	S	0	0	0
			2442	1578	402	455	7			

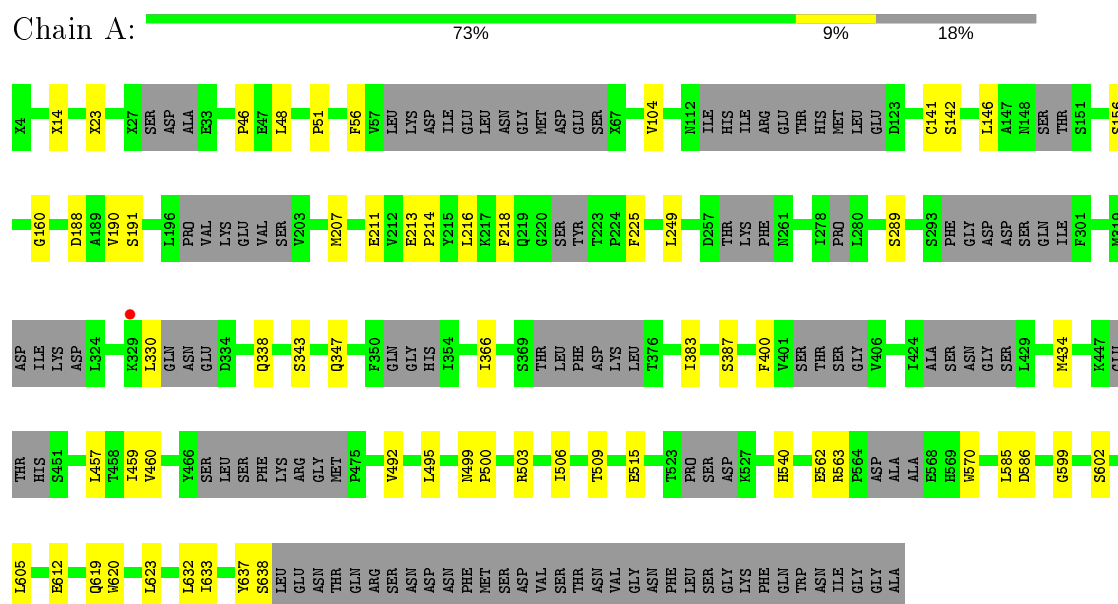
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	329	MET	-	initiating methionine	UNP Q6CUS2
C	330	GLY	-	expression tag	UNP Q6CUS2
C	331	SER	-	expression tag	UNP Q6CUS2
C	419	GLY	-	linker	UNP Q6CUS2
C	420	ASP	-	linker	UNP Q6CUS2
C	421	GLY	-	linker	UNP Q6CUS2
C	422	ASP	-	linker	UNP Q6CUS2
C	423	GLY	-	linker	UNP Q6CUS2

### 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 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: Protein transport protein SEC39

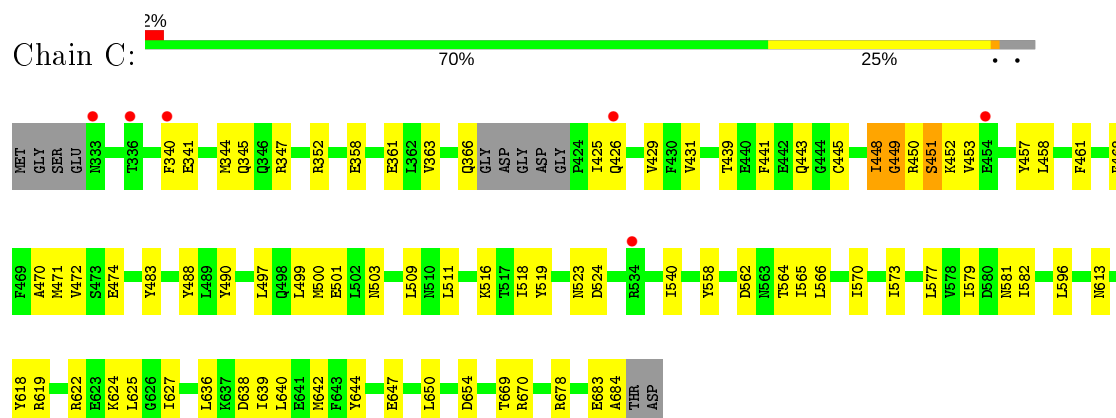


- Molecule 2: Vesicle transport protein USE1



There are no outlier residues recorded for this chain.

- Molecule 3: Protein transport protein DSL1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	240.79Å 87.85Å 161.43Å 90.00° 107.61° 90.00°	Depositor
Resolution (Å)	29.60 – 5.73 29.60 – 5.73	Depositor EDS
% Data completeness (in resolution range)	74.5 (29.60-5.73) 74.5 (29.60-5.73)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 5.67Å)	Xtriage
Refinement program	PHENIX 1.13.2998	Depositor
R, $R_{free}$	0.276 , 0.322 0.276 , 0.322	Depositor DCC
$R_{free}$ test set	703 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	317.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 323.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	6126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	397.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.44	3/3057 (0.1%)	0.55	0/4200
3	C	0.44	0/2486	0.59	0/3367
All	All	0.44	3/5543 (0.1%)	0.57	0/7567

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	PHE	C-N	5.42	1.46	1.34
1	A	190	VAL	C-N	5.34	1.46	1.34
1	A	104	VAL	C-N	-5.27	1.22	1.34

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	3249	0	2079	57	0
2	B	435	0	93	0	0
3	C	2442	0	2476	67	0
All	All	6126	0	4648	104	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 (104) 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)
3:C:340:PHE:O	3:C:344:MET:HG2	1.77	0.85
1:A:509:THR:HG21	1:A:540:HIS:CE1	2.11	0.84
1:A:620:TRP:CE2	3:C:470:ALA:HB2	2.14	0.81
1:A:620:TRP:CE2	3:C:470:ALA:CB	2.64	0.81
1:A:51:PRO:CB	1:A:146:LEU:HD13	2.15	0.76
3:C:639:ILE:HA	3:C:642:MET:HE3	1.69	0.74
1:A:599:GLY:HA2	3:C:474:GLU:OE2	1.88	0.74
1:A:51:PRO:HB3	1:A:146:LEU:HD13	1.68	0.73
1:A:459:ILE:HG21	1:A:515:GLU:CB	2.19	0.73
1:A:503:ARG:O	1:A:540:HIS:HD2	1.72	0.72
3:C:654:ASP:OD1	3:C:678:ARG:NH2	2.25	0.69
1:A:343:SER:HB2	1:A:383:ILE:CB	2.22	0.69
3:C:439:THR:HG22	3:C:443:GLN:HE21	1.60	0.66
1:A:434:MET:HE3	1:A:457:LEU:HD22	1.77	0.65
3:C:636:LEU:HD23	3:C:669:THR:HG22	1.78	0.64
1:A:620:TRP:NE1	3:C:470:ALA:HB1	2.13	0.64
3:C:511:LEU:HD11	3:C:565:ILE:HG23	1.78	0.64
1:A:620:TRP:CD2	3:C:470:ALA:HB2	2.32	0.63
1:A:605:LEU:O	3:C:352:ARG:NE	2.31	0.62
1:A:23:UNK:CB	1:A:56:PHE:CE1	2.81	0.62
3:C:431:VAL:HG11	3:C:488:TYR:CD2	2.34	0.62
1:A:434:MET:CE	1:A:457:LEU:HD22	2.29	0.62
1:A:605:LEU:O	3:C:352:ARG:NH2	2.32	0.62
3:C:618:TYR:CZ	3:C:622:ARG:HD2	2.34	0.62
3:C:639:ILE:HA	3:C:642:MET:CE	2.30	0.61
1:A:599:GLY:HA2	3:C:474:GLU:CD	2.23	0.59
1:A:602:SER:CB	3:C:474:GLU:CG	2.81	0.58
1:A:14:UNK:O	1:A:46:PRO:HD3	2.03	0.58
1:A:156:SER:O	1:A:160:GLY:N	2.38	0.57
1:A:347:GLN:CB	1:A:387:SER:CB	2.82	0.57
1:A:509:THR:HG21	1:A:540:HIS:HE1	1.67	0.56
1:A:23:UNK:CB	1:A:56:PHE:CZ	2.88	0.56
1:A:492:VAL:HA	1:A:495:LEU:HD12	1.89	0.55
1:A:459:ILE:CG2	1:A:515:GLU:CB	2.85	0.55
1:A:602:SER:CB	3:C:474:GLU:HG2	2.37	0.54
1:A:216:LEU:HD11	1:A:225:PHE:CB	2.37	0.54
3:C:425:ILE:HG13	3:C:426:GLN:N	2.22	0.54
1:A:620:TRP:CE2	3:C:470:ALA:HB1	2.43	0.53
1:A:632:LEU:HG	3:C:509:LEU:HD12	1.92	0.52
1:A:51:PRO:HB2	1:A:146:LEU:HD13	1.89	0.52
1:A:570:TRP:CZ2	1:A:612:GLU:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:SER:CB	3:C:470:ALA:O	2.59	0.51
3:C:638:ASP:O	3:C:642:MET:HG3	2.11	0.50
3:C:573:ILE:O	3:C:577:LEU:HB3	2.11	0.50
1:A:620:TRP:CZ2	3:C:470:ALA:HA	2.47	0.50
3:C:431:VAL:CG1	3:C:488:TYR:CD2	2.95	0.50
1:A:602:SER:CB	3:C:474:GLU:HG3	2.42	0.49
1:A:605:LEU:HB2	3:C:471:MET:HG2	1.93	0.49
3:C:511:LEU:HD11	3:C:565:ILE:CG2	2.43	0.49
1:A:585:LEU:O	1:A:586:ASP:HB2	2.13	0.49
1:A:620:TRP:CD1	3:C:470:ALA:HB1	2.48	0.48
3:C:340:PHE:HE1	3:C:344:MET:SD	2.36	0.48
3:C:366:GLN:OE1	3:C:366:GLN:HA	2.13	0.48
3:C:441:PHE:CE2	3:C:461:PHE:CD1	3.02	0.47
1:A:213:GLU:N	1:A:214:PRO:CD	2.77	0.47
1:A:160:GLY:HA3	1:A:218:PHE:CB	2.44	0.47
3:C:523:ASN:OD1	3:C:581:ASN:ND2	2.47	0.47
3:C:483:TYR:CD1	3:C:503:ASN:ND2	2.84	0.46
3:C:579:ILE:HD13	3:C:624:LYS:HD3	1.97	0.46
1:A:619:GLN:HE21	1:A:623:LEU:HD11	1.80	0.46
3:C:582:ILE:HD13	3:C:596:LEU:HD22	1.97	0.46
3:C:358:GLU:HG2	3:C:429:VAL:HG12	1.98	0.46
3:C:497:LEU:O	3:C:500:MET:HG2	2.15	0.46
3:C:450:ARG:C	3:C:452:LYS:H	2.19	0.45
3:C:627:ILE:HD13	3:C:647:GLU:O	2.16	0.45
1:A:459:ILE:HG13	1:A:460:VAL:N	2.31	0.45
3:C:613:ASN:O	3:C:619:ARG:NH1	2.49	0.45
1:A:612:GLU:OE1	1:A:612:GLU:HA	2.14	0.45
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.81	0.45
3:C:562:ASP:OD1	3:C:564:THR:HB	2.16	0.45
1:A:216:LEU:HD11	1:A:225:PHE:HB3	1.99	0.45
3:C:468:PHE:CE1	3:C:472:VAL:HG21	2.52	0.45
1:A:343:SER:CB	1:A:383:ILE:CB	2.94	0.44
1:A:499:ASN:HA	1:A:500:PRO:HD3	1.80	0.44
3:C:558:TYR:HD1	3:C:566:LEU:HD11	1.81	0.44
3:C:453:VAL:HG12	3:C:457:TYR:HB2	2.00	0.44
3:C:558:TYR:CD1	3:C:566:LEU:HD11	2.53	0.44
3:C:361:GLU:O	3:C:429:VAL:HG23	2.17	0.44
3:C:431:VAL:CG1	3:C:488:TYR:HD2	2.30	0.43
3:C:636:LEU:HD21	3:C:670:ARG:HA	2.01	0.43
3:C:524:ASP:HB3	3:C:540:ILE:HD13	2.01	0.43
3:C:640:LEU:HG	3:C:644:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:518:ILE:HD13	3:C:573:ILE:HD11	2.00	0.43
3:C:625:LEU:HD23	3:C:625:LEU:HA	1.83	0.43
3:C:683:GLU:O	3:C:684:ALA:C	2.56	0.43
1:A:188:ASP:HA	1:A:191:SER:CB	2.49	0.42
3:C:347:ARG:HA	3:C:347:ARG:NE	2.34	0.42
3:C:499:LEU:HD23	3:C:499:LEU:HA	1.91	0.42
3:C:490:TYR:CE2	3:C:500:MET:HA	2.54	0.42
1:A:562:GLU:O	1:A:563:ARG:C	2.57	0.42
1:A:605:LEU:O	3:C:352:ARG:CZ	2.68	0.41
3:C:340:PHE:HE2	3:C:453:VAL:HG13	1.85	0.41
3:C:519:TYR:CZ	3:C:523:ASN:ND2	2.88	0.41
1:A:141:CYS:O	1:A:142:SER:C	2.58	0.41
1:A:620:TRP:CZ2	3:C:470:ALA:HB2	2.53	0.41
1:A:207:MET:O	1:A:211:GLU:HB2	2.20	0.41
1:A:330:LEU:CB	1:A:338:GLN:NE2	2.83	0.41
1:A:633:ILE:HA	3:C:516:LYS:HB2	2.02	0.41
1:A:637:TYR:O	1:A:638:SER:CB	2.69	0.41
3:C:445:CYS:O	3:C:449:GLY:N	2.54	0.41
3:C:340:PHE:CE1	3:C:344:MET:SD	3.14	0.40
3:C:341:GLU:O	3:C:345:GLN:HG3	2.21	0.40
1:A:506:ILE:O	1:A:509:THR:HG22	2.22	0.40
1:A:457:LEU:HA	1:A:457:LEU:HD23	1.74	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	464/667 (70%)	439 (95%)	24 (5%)	1 (0%)	47	81
3	C	291/306 (95%)	279 (96%)	9 (3%)	3 (1%)	15	54
All	All	755/973 (78%)	718 (95%)	33 (4%)	4 (0%)	29	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	448	ILE
3	C	451	SER
3	C	449	GLY
1	A	366	ILE

### 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	149/581 (26%)	147 (99%)	2 (1%)	69	82
3	C	276/288 (96%)	269 (98%)	7 (2%)	47	68
All	All	425/869 (49%)	416 (98%)	9 (2%)	53	72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	289	SER
3	C	363	VAL
3	C	448	ILE
3	C	451	SER
3	C	458	LEU
3	C	501	GLU
3	C	570	ILE
3	C	650	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	A	540	HIS
1	A	619	GLN
3	C	443	GLN
3	C	563	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 monosaccharides 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
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	14:UNK	C	15:UNK	N	11.60
1	B	33:UNK	C	39:UNK	N	10.68
1	A	86:UNK	C	89:ASP	N	9.90
1	A	76:UNK	C	78:UNK	N	6.50
1	B	70:UNK	C	74:UNK	N	6.45

## 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, 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	502/667 (75%)	-0.36	1 (0%) 95 93	74, 373, 685, 947	0
2	B	0/87	-	-	-	-
3	C	295/306 (96%)	-0.11	6 (2%) 65 57	140, 362, 659, 966	0
All	All	797/1060 (75%)	-0.27	7 (0%) 84 77	74, 366, 679, 966	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	426	GLN	4.6
3	C	336	THR	3.7
3	C	333	ASN	3.4
3	C	340	PHE	3.4
3	C	534	ARG	2.4
1	A	329	LYS	2.4
3	C	454	GLU	2.1

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.