



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 07:54 AM BST

PDB ID : 6SYF
Title : Human Ubc9 with covalent isopeptide ligand
Authors : Hofmann, R.; Akimoto, G.; Wucherpennig, T.G.; Zeymer, C.; Bode, J.W.
Deposited on : 2019-09-27
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.14.4.dev1
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) : 2.14.4.dev1

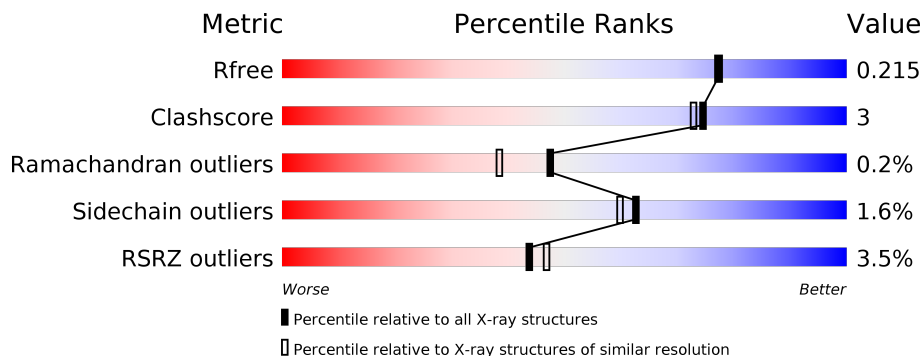
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	158	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">3% 88% 8% ••</p>
1	B	158	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">% 91% 8% •</p>
1	C	158	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">2% 92% 6% •</p>
1	D	158	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">% 89% 8% •</p>
2	E	7	<div style="display: flex; align-items: center;"> <div style="width: 43%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">43% 86% 14%</p>
2	G	7	<div style="display: flex; align-items: center;"> <div style="width: 29%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">29% 86% 14%</p>

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Mol	Chain	Length	Quality of chain
2	I	7	
2	K	7	
3	F	5	
3	H	5	
3	J	5	
3	L	5	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5858 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 SUMO-conjugating enzyme UBC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1230	793	212	218	7	0	1	0
1	B	156	1265	813	220	225	7	0	3	0
1	C	156	1259	810	219	223	7	0	2	0
1	D	153	1230	793	212	218	7	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P63279
A	48	ALA	LYS	engineered mutation	UNP P63279
A	49	ALA	LYS	engineered mutation	UNP P63279
A	54	ALA	GLU	engineered mutation	UNP P63279
A	138	ALA	CYS	engineered mutation	UNP P63279
B	1	GLY	-	expression tag	UNP P63279
B	48	ALA	LYS	engineered mutation	UNP P63279
B	49	ALA	LYS	engineered mutation	UNP P63279
B	54	ALA	GLU	engineered mutation	UNP P63279
B	138	ALA	CYS	engineered mutation	UNP P63279
C	1	GLY	-	expression tag	UNP P63279
C	48	ALA	LYS	engineered mutation	UNP P63279
C	49	ALA	LYS	engineered mutation	UNP P63279
C	54	ALA	GLU	engineered mutation	UNP P63279
C	138	ALA	CYS	engineered mutation	UNP P63279
D	1	GLY	-	expression tag	UNP P63279
D	48	ALA	LYS	engineered mutation	UNP P63279
D	49	ALA	LYS	engineered mutation	UNP P63279
D	54	ALA	GLU	engineered mutation	UNP P63279
D	138	ALA	CYS	engineered mutation	UNP P63279

- Molecule 2 is a protein called ACE-LEU-ARG-LEU-ARG-GLY-CYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	7	Total 51	C 31	N 12	O 7	S 1	0	0	0
2	G	7	Total 51	C 31	N 12	O 7	S 1	0	0	0
2	I	7	Total 51	C 31	N 12	O 7	S 1	0	0	0
2	K	7	Total 51	C 31	N 12	O 7	S 1	0	0	0

- Molecule 3 is a protein called ACE-ILE-LYS-GLN-GLU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	5	Total 38	C 24	N 6	O 8	0	0	0
3	H	5	Total 38	C 24	N 6	O 8	0	0	0
3	J	5	Total 38	C 24	N 6	O 8	0	0	0
3	L	5	Total 38	C 24	N 6	O 8	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total 102	O 102	0	0
4	B	147	Total 147	O 147	0	0
4	C	113	Total 113	O 113	0	0
4	D	117	Total 117	O 117	0	0
4	E	5	Total 5	O 5	0	0
4	F	3	Total 3	O 3	0	0
4	G	10	Total 10	O 10	0	0
4	H	5	Total 5	O 5	0	0
4	J	4	Total 4	O 4	0	0

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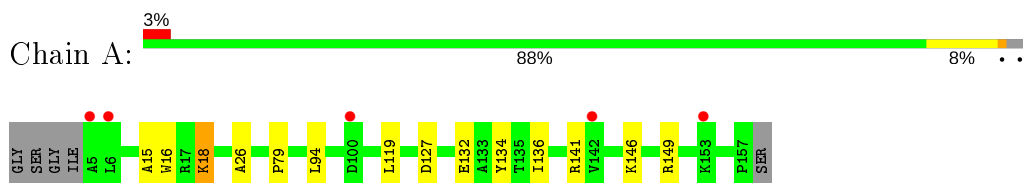
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	5	Total O 5 5	0	0
4	L	7	Total O 7 7	0	0

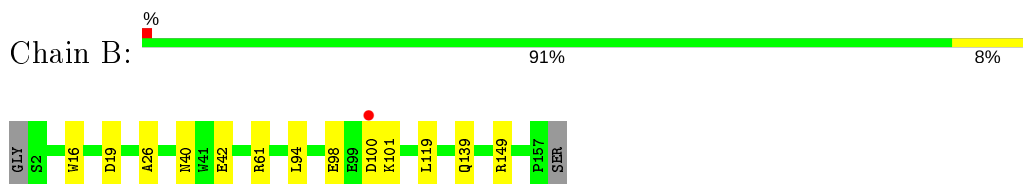
3 Residue-property plots [i](#)

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.

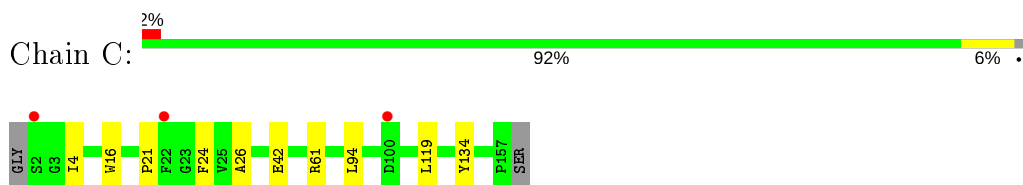
- Molecule 1: SUMO-conjugating enzyme UBC9



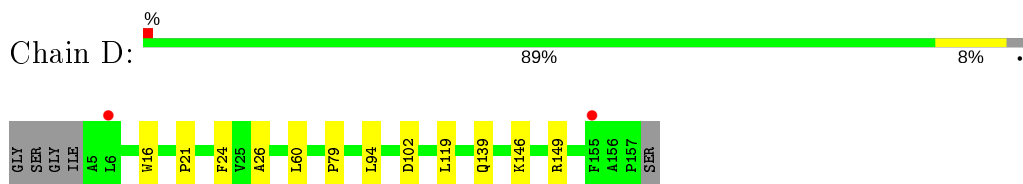
- Molecule 1: SUMO-conjugating enzyme UBC9



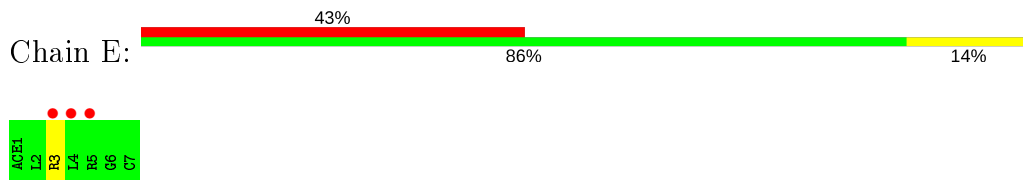
- Molecule 1: SUMO-conjugating enzyme UBC9



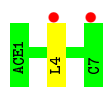
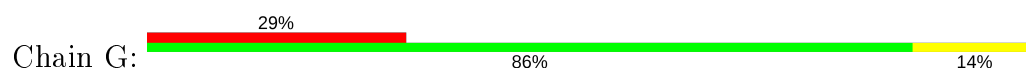
- Molecule 1: SUMO-conjugating enzyme UBC9



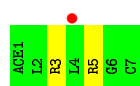
- Molecule 2: ACE-LEU-ARG-LEU-ARG-GLY-CYS



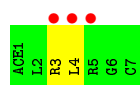
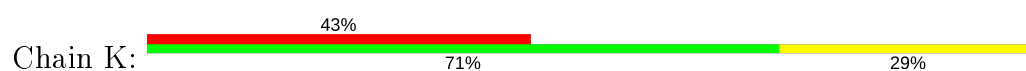
- Molecule 2: ACE-LEU-ARG-LEU-ARG-GLY-CYS



- Molecule 2: ACE-LEU-ARG-LEU-ARG-GLY-CYS



- Molecule 2: ACE-LEU-ARG-LEU-ARG-GLY-CYS



- Molecule 3: ACE-ILE-LYS-GLN-GLU



- Molecule 3: ACE-ILE-LYS-GLN-GLU



- Molecule 3: ACE-ILE-LYS-GLN-GLU



- Molecule 3: ACE-ILE-LYS-GLN-GLU



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.70 Å 38.70 Å 97.80 Å 90.00° 118.90° 90.00°	Depositor
Resolution (Å)	47.00 – 1.90 48.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.00-1.90) 99.0 (48.91-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.90 Å)	Xtrriage
Refinement program	BUSTER 2.10.3 (23-SEP-2019)	Depositor
R, R_{free}	0.213 , 0.263 0.192 , 0.215	Depositor DCC
R_{free} test set	2466 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtrriage
Anisotropy	0.780	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.409 for h,-k,-h-l 0.000 for -h-l,-k,l 0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5858	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6274e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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](#)

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

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	0.41	0/1267	0.58	0/1722
1	B	0.40	0/1302	0.57	0/1768
1	C	0.42	0/1296	0.56	0/1760
1	D	0.43	0/1267	0.59	0/1722
2	E	0.47	0/48	0.63	0/62
2	G	0.55	0/48	0.69	0/62
2	I	0.46	0/48	0.81	0/62
2	K	0.61	0/48	0.95	0/62
3	F	0.28	0/35	0.42	0/45
3	H	0.32	0/35	0.48	0/45
3	J	0.31	0/35	0.41	0/45
3	L	0.41	0/35	0.59	0/45
All	All	0.42	0/5464	0.58	0/7400

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	1230	0	1224	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1265	0	1259	11	0
1	C	1259	0	1255	8	0
1	D	1230	0	1224	12	0
2	E	51	0	58	0	0
2	G	51	0	58	0	0
2	I	51	0	58	1	0
2	K	51	0	58	1	0
3	F	38	0	39	0	0
3	H	38	0	40	0	0
3	J	38	0	39	0	0
3	L	38	0	39	0	0
4	A	102	0	0	0	0
4	B	147	0	0	1	0
4	C	113	0	0	0	1
4	D	117	0	0	0	1
4	E	5	0	0	0	0
4	F	3	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	J	4	0	0	0	0
4	K	5	0	0	0	0
4	L	7	0	0	0	0
All	All	5858	0	5351	34	1

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 3.

The worst 5 of 34 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:B:40:ASN:ND2	1:D:139:GLN:HE22	1.59	1.00
1:B:40:ASN:HD21	1:D:139:GLN:HE22	0.98	0.89
1:D:146:LYS:NZ	1:D:149:ARG:HE	1.71	0.88
1:B:42:GLU:HG2	1:B:61[B]:ARG:NE	2.09	0.68
1:D:146:LYS:NZ	1:D:149:ARG:NE	2.44	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:270:HOH:O	4:D:241:HOH:O[2_654]	2.19	0.01

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	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
1	B	157/158 (99%)	154 (98%)	3 (2%)	0	100	100
1	C	156/158 (99%)	152 (97%)	4 (3%)	0	100	100
1	D	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
2	E	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
2	G	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	I	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	K	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
3	F	3/5 (60%)	3 (100%)	0	0	100	100
3	H	3/5 (60%)	3 (100%)	0	0	100	100
3	J	3/5 (60%)	3 (100%)	0	0	100	100
3	L	3/5 (60%)	3 (100%)	0	0	100	100
All	All	649/680 (95%)	631 (97%)	17 (3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	3	ARG

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	130/132 (98%)	127 (98%)	3 (2%)	50	45
1	B	134/132 (102%)	131 (98%)	3 (2%)	52	47
1	C	133/132 (101%)	133 (100%)	0	100	100
1	D	130/132 (98%)	129 (99%)	1 (1%)	81	82
2	E	5/5 (100%)	5 (100%)	0	100	100
2	G	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	I	5/5 (100%)	5 (100%)	0	100	100
2	K	5/5 (100%)	4 (80%)	1 (20%)	1	0
3	F	4/4 (100%)	4 (100%)	0	100	100
3	H	4/4 (100%)	4 (100%)	0	100	100
3	J	4/4 (100%)	4 (100%)	0	100	100
3	L	4/4 (100%)	4 (100%)	0	100	100
All	All	563/564 (100%)	554 (98%)	9 (2%)	62	60

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	100	ASP
2	K	4	LEU
1	D	60	LEU
1	A	141	ARG
1	B	139	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	126	GLN
1	D	139	GLN

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](#)

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	153/158 (96%)	0.08	5 (3%) 46 49	14, 27, 49, 55	0
1	B	156/158 (98%)	0.10	1 (0%) 89 90	15, 28, 44, 47	0
1	C	156/158 (98%)	0.05	3 (1%) 66 69	17, 30, 49, 58	0
1	D	153/158 (96%)	-0.12	2 (1%) 77 79	13, 24, 41, 47	0
2	E	6/7 (85%)	1.79	3 (50%) 0 0	35, 43, 47, 51	0
2	G	6/7 (85%)	1.50	2 (33%) 0 0	39, 41, 45, 47	0
2	I	6/7 (85%)	1.21	1 (16%) 1 1	35, 37, 42, 44	0
2	K	6/7 (85%)	2.05	3 (50%) 0 0	36, 47, 50, 55	0
3	F	4/5 (80%)	0.73	1 (25%) 0 0	37, 40, 42, 43	0
3	H	4/5 (80%)	0.60	1 (25%) 0 0	38, 40, 41, 44	0
3	J	4/5 (80%)	0.62	1 (25%) 0 0	39, 41, 46, 46	0
3	L	4/5 (80%)	0.24	0 100 100	37, 39, 42, 42	0
All	All	658/680 (96%)	0.10	23 (3%) 44 47	13, 28, 47, 58	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	4	LEU	4.2
3	F	2	ILE	3.9
1	A	100	ASP	3.9
1	C	2	SER	3.7
1	A	6	LEU	3.5

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 [i](#)

There are no such residues in this entry.