



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 06:57 pm GMT

PDB ID : 3DD9
Title : Structure of DocH66Y dimer
Authors : Garcia-Pino, A.; Loris, R.
Deposited on : 2008-06-05
Resolution : 2.45 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
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

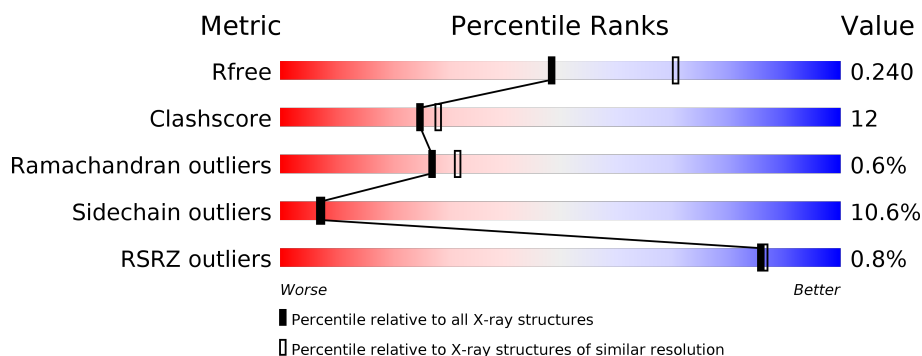
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	111664	1259 (2.48-2.44)
Clashscore	122126	1323 (2.48-2.44)
Ramachandran outliers	120053	1314 (2.48-2.44)
Sidechain outliers	120020	1314 (2.48-2.44)
RSRZ outliers	108989	1238 (2.48-2.44)

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. 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	135	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	135	<div> <div>69%</div> <div>15%</div> <div>•</div> <div>13%</div> </div>
1	C	135	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div></div> <div>15%</div> </div> </div>
1	D	135	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>••</div> <div>10%</div> </div> </div>
1	E	135	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>16%</div> <div>•</div> <div>16%</div> </div> </div>
1	F	135	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>18%</div> <div>•</div> <div>19%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	135	<div><div>%</div><div><div></div><div>62%</div><div>19%</div><div>•</div><div>16%</div></div></div>
1	H	135	<div><div></div><div>80%</div><div>7%</div><div>• •</div><div>10%</div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6855 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 Death on curing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			861	545	150	165	1			
1	B	118	Total	C	N	O	S	0	0	0
			871	550	150	170	1			
1	C	115	Total	C	N	O	S	0	0	0
			836	524	148	163	1			
1	D	122	Total	C	N	O	S	0	0	0
			906	567	164	174	1			
1	E	113	Total	C	N	O	S	0	0	0
			824	518	146	159	1			
1	F	110	Total	C	N	O	S	0	0	0
			801	508	136	156	1			
1	G	114	Total	C	N	O	S	0	0	0
			816	519	139	157	1			
1	H	122	Total	C	N	O	S	0	0	0
			903	569	155	178	1			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
A	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259
A	127	PRO	-	EXPRESSION TAG	UNP Q06259
A	128	LEU	-	EXPRESSION TAG	UNP Q06259
A	129	GLU	-	EXPRESSION TAG	UNP Q06259
A	130	HIS	-	EXPRESSION TAG	UNP Q06259
A	131	HIS	-	EXPRESSION TAG	UNP Q06259
A	132	HIS	-	EXPRESSION TAG	UNP Q06259
A	133	HIS	-	EXPRESSION TAG	UNP Q06259
A	134	HIS	-	EXPRESSION TAG	UNP Q06259
A	135	HIS	-	EXPRESSION TAG	UNP Q06259
B	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
B	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259

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Chain	Residue	Modelled	Actual	Comment	Reference
B	127	PRO	-	EXPRESSION TAG	UNP Q06259
B	128	LEU	-	EXPRESSION TAG	UNP Q06259
B	129	GLU	-	EXPRESSION TAG	UNP Q06259
B	130	HIS	-	EXPRESSION TAG	UNP Q06259
B	131	HIS	-	EXPRESSION TAG	UNP Q06259
B	132	HIS	-	EXPRESSION TAG	UNP Q06259
B	133	HIS	-	EXPRESSION TAG	UNP Q06259
B	134	HIS	-	EXPRESSION TAG	UNP Q06259
B	135	HIS	-	EXPRESSION TAG	UNP Q06259
C	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
C	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259
C	127	PRO	-	EXPRESSION TAG	UNP Q06259
C	128	LEU	-	EXPRESSION TAG	UNP Q06259
C	129	GLU	-	EXPRESSION TAG	UNP Q06259
C	130	HIS	-	EXPRESSION TAG	UNP Q06259
C	131	HIS	-	EXPRESSION TAG	UNP Q06259
C	132	HIS	-	EXPRESSION TAG	UNP Q06259
C	133	HIS	-	EXPRESSION TAG	UNP Q06259
C	134	HIS	-	EXPRESSION TAG	UNP Q06259
C	135	HIS	-	EXPRESSION TAG	UNP Q06259
D	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
D	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259
D	127	PRO	-	EXPRESSION TAG	UNP Q06259
D	128	LEU	-	EXPRESSION TAG	UNP Q06259
D	129	GLU	-	EXPRESSION TAG	UNP Q06259
D	130	HIS	-	EXPRESSION TAG	UNP Q06259
D	131	HIS	-	EXPRESSION TAG	UNP Q06259
D	132	HIS	-	EXPRESSION TAG	UNP Q06259
D	133	HIS	-	EXPRESSION TAG	UNP Q06259
D	134	HIS	-	EXPRESSION TAG	UNP Q06259
D	135	HIS	-	EXPRESSION TAG	UNP Q06259
E	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
E	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259
E	127	PRO	-	EXPRESSION TAG	UNP Q06259
E	128	LEU	-	EXPRESSION TAG	UNP Q06259
E	129	GLU	-	EXPRESSION TAG	UNP Q06259
E	130	HIS	-	EXPRESSION TAG	UNP Q06259
E	131	HIS	-	EXPRESSION TAG	UNP Q06259
E	132	HIS	-	EXPRESSION TAG	UNP Q06259
E	133	HIS	-	EXPRESSION TAG	UNP Q06259
E	134	HIS	-	EXPRESSION TAG	UNP Q06259
E	135	HIS	-	EXPRESSION TAG	UNP Q06259

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Chain	Residue	Modelled	Actual	Comment	Reference
F	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
F	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259
F	127	PRO	-	EXPRESSION TAG	UNP Q06259
F	128	LEU	-	EXPRESSION TAG	UNP Q06259
F	129	GLU	-	EXPRESSION TAG	UNP Q06259
F	130	HIS	-	EXPRESSION TAG	UNP Q06259
F	131	HIS	-	EXPRESSION TAG	UNP Q06259
F	132	HIS	-	EXPRESSION TAG	UNP Q06259
F	133	HIS	-	EXPRESSION TAG	UNP Q06259
F	134	HIS	-	EXPRESSION TAG	UNP Q06259
F	135	HIS	-	EXPRESSION TAG	UNP Q06259
G	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
G	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259
G	127	PRO	-	EXPRESSION TAG	UNP Q06259
G	128	LEU	-	EXPRESSION TAG	UNP Q06259
G	129	GLU	-	EXPRESSION TAG	UNP Q06259
G	130	HIS	-	EXPRESSION TAG	UNP Q06259
G	131	HIS	-	EXPRESSION TAG	UNP Q06259
G	132	HIS	-	EXPRESSION TAG	UNP Q06259
G	133	HIS	-	EXPRESSION TAG	UNP Q06259
G	134	HIS	-	EXPRESSION TAG	UNP Q06259
G	135	HIS	-	EXPRESSION TAG	UNP Q06259
H	66	TYR	HIS	ENGINEERED MUTATION	UNP Q06259
H	126	ASP	GLU	ENGINEERED MUTATION	UNP Q06259
H	127	PRO	-	EXPRESSION TAG	UNP Q06259
H	128	LEU	-	EXPRESSION TAG	UNP Q06259
H	129	GLU	-	EXPRESSION TAG	UNP Q06259
H	130	HIS	-	EXPRESSION TAG	UNP Q06259
H	131	HIS	-	EXPRESSION TAG	UNP Q06259
H	132	HIS	-	EXPRESSION TAG	UNP Q06259
H	133	HIS	-	EXPRESSION TAG	UNP Q06259
H	134	HIS	-	EXPRESSION TAG	UNP Q06259
H	135	HIS	-	EXPRESSION TAG	UNP Q06259

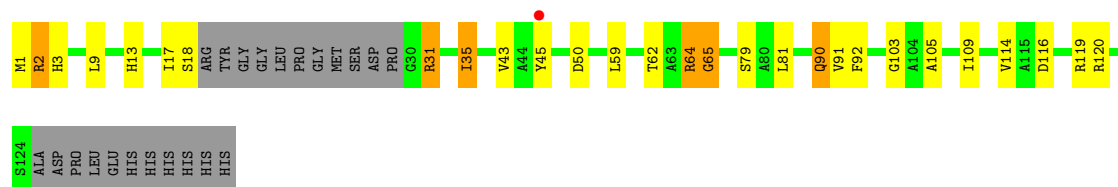
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	12	Total O 12 12	0	0
2	C	2	Total O 2 2	0	0

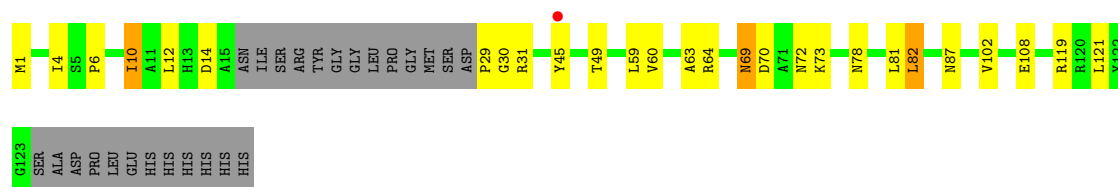
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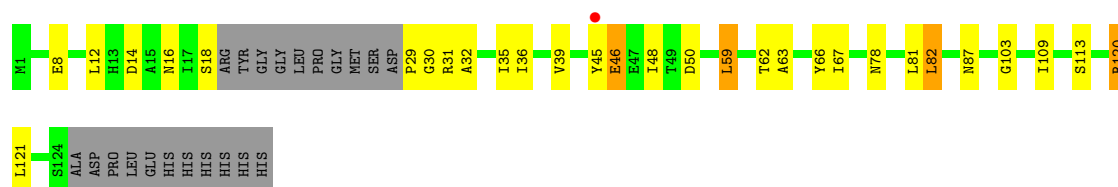
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	6	Total 6	O 6	0	0
2	G	2	Total 2	O 2	0	0
2	H	8	Total 8	O 8	0	0



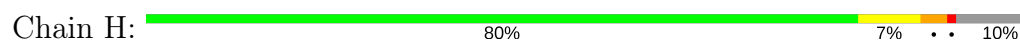
- Molecule 1: Death on curing protein



- Molecule 1: Death on curing protein



- Molecule 1: Death on curing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.08Å 197.99Å 54.11Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	14.99 – 2.45 14.99 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (14.99-2.45) 99.7 (14.99-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.245 0.208 , 0.240	Depositor DCC
R_{free} test set	2026 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.159 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6855	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.53 % 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 9.5283e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.71	0/872	0.78	1/1186 (0.1%)
1	B	0.71	0/883	0.81	2/1199 (0.2%)
1	C	0.70	0/847	0.73	0/1148
1	D	0.70	0/918	0.85	3/1244 (0.2%)
1	E	0.60	0/833	0.74	2/1132 (0.2%)
1	F	0.57	0/812	0.71	0/1105
1	G	0.90	3/827 (0.4%)	0.78	2/1127 (0.2%)
1	H	0.63	0/916	0.75	1/1247 (0.1%)
All	All	0.70	3/6908 (0.0%)	0.77	11/9388 (0.1%)

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	B	0	2
1	D	0	2
1	E	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	45	TYR	CE2-CZ	11.65	1.53	1.38
1	G	45	TYR	CG-CD1	10.13	1.52	1.39
1	G	45	TYR	CG-CD2	6.19	1.47	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	SER	N-CA-C	8.38	133.63	111.00
1	G	45	TYR	CB-CG-CD2	-8.21	116.07	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	N-CA-C	7.96	132.49	111.00
1	A	64	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	27	SER	CB-CA-C	-6.22	98.29	110.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19	ARG	Peptide
1	B	64	ARG	Peptide
1	D	26	MET	Peptide
1	D	64	ARG	Peptide
1	E	31	ARG	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	861	0	845	33	0
1	B	871	0	845	20	0
1	C	836	0	805	19	0
1	D	906	0	883	28	0
1	E	824	0	807	25	0
1	F	801	0	781	14	0
1	G	816	0	785	25	0
1	H	903	0	874	15	1
2	A	7	0	0	1	0
2	B	12	0	0	1	0
2	C	2	0	0	0	0
2	D	6	0	0	0	1
2	G	2	0	0	0	0
2	H	8	0	0	0	0
All	All	6855	0	6625	156	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 12.

The worst 5 of 156 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:C:44:ALA:HA	1:C:46:GLU:H	1.10	1.16
1:D:19:ARG:HH11	1:D:19:ARG:CG	1.64	1.08
1:H:86:ARG:HG3	1:H:86:ARG:HH11	1.17	1.06
1:D:19:ARG:NH1	1:D:19:ARG:HG3	1.71	1.03
1:A:28:ASP:CB	1:A:29:PRO:HA	1.85	1.02

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)
1:H:86:ARG:NH1	2:D:204:HOH:O[1_655]	1.71	0.49

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	113/135 (84%)	111 (98%)	0	2 (2%)	9	7
1	B	114/135 (84%)	108 (95%)	5 (4%)	1 (1%)	19	22
1	C	111/135 (82%)	103 (93%)	6 (5%)	2 (2%)	9	7
1	D	118/135 (87%)	111 (94%)	7 (6%)	0	100	100
1	E	109/135 (81%)	105 (96%)	4 (4%)	0	100	100
1	F	106/135 (78%)	103 (97%)	3 (3%)	0	100	100
1	G	110/135 (82%)	108 (98%)	2 (2%)	0	100	100
1	H	118/135 (87%)	113 (96%)	5 (4%)	0	100	100
All	All	899/1080 (83%)	862 (96%)	32 (4%)	5 (1%)	27	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	PRO
1	C	41	ALA
1	A	18	SER
1	A	29	PRO
1	C	17	ILE

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	84/108 (78%)	74 (88%)	10 (12%)	6	5
1	B	86/108 (80%)	78 (91%)	8 (9%)	10	10
1	C	82/108 (76%)	77 (94%)	5 (6%)	20	26
1	D	90/108 (83%)	82 (91%)	8 (9%)	11	12
1	E	81/108 (75%)	74 (91%)	7 (9%)	11	13
1	F	79/108 (73%)	64 (81%)	15 (19%)	1	1
1	G	78/108 (72%)	67 (86%)	11 (14%)	4	3
1	H	91/108 (84%)	84 (92%)	7 (8%)	14	17
All	All	671/864 (78%)	600 (89%)	71 (11%)	7	7

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	35	ILE
1	F	10	ILE
1	H	28	ASP
1	E	43	VAL
1	E	90	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	ASN

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Mol	Chain	Res	Type
1	D	13	HIS
1	G	87	ASN
1	C	16	ASN
1	F	87	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](#)

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	117/135 (86%)	-0.45	1 (0%) 84 84	32, 47, 67, 81	0
1	B	118/135 (87%)	-0.37	0 100 100	34, 47, 73, 84	0
1	C	115/135 (85%)	-0.34	1 (0%) 84 84	30, 49, 80, 93	0
1	D	122/135 (90%)	-0.32	2 (1%) 72 69	31, 48, 70, 85	0
1	E	113/135 (83%)	-0.37	1 (0%) 84 84	39, 54, 78, 92	0
1	F	110/135 (81%)	-0.43	1 (0%) 84 84	36, 51, 66, 88	0
1	G	114/135 (84%)	-0.33	1 (0%) 84 84	30, 51, 79, 92	0
1	H	122/135 (90%)	-0.37	0 100 100	35, 50, 73, 89	0
All	All	931/1080 (86%)	-0.37	7 (0%) 86 86	30, 49, 76, 93	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	MET	5.7
1	F	45	TYR	3.0
1	G	45	TYR	2.7
1	C	43	VAL	2.6
1	E	45	TYR	2.5

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 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.