



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:32 am GMT

PDB ID : 1MJQ
Title : METHIONINE REPRESSOR MUTANT (Q44K) PLUS COREPRESSOR (S-ADENOSYL METHIONINE) COMPLEXED TO AN ALTERED MET CONSENSUS OPERATOR SEQUENCE
Authors : Garvie, C.W.; Phillips, S.E.V.
Deposited on : 1998-01-30
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

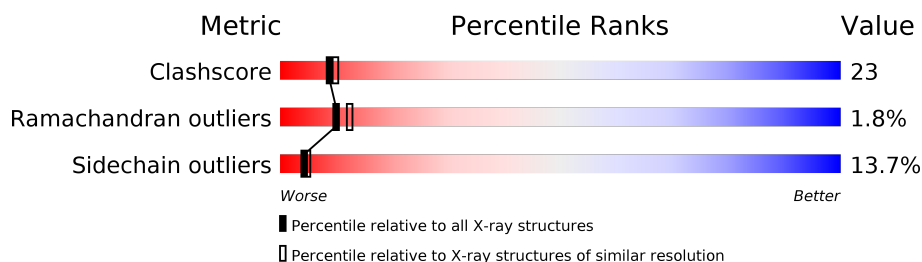
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	19	
1	F	19	
1	K	19	
1	L	19	
2	A	104	
2	B	104	
2	C	104	

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Mol	Chain	Length	Quality of chain
2	D	104	<div><div></div><div>49%</div><div>43%</div><div>8%</div></div>
2	G	104	<div><div></div><div>58%</div><div>36%</div><div>6%</div></div>
2	H	104	<div><div></div><div>58%</div><div>34%</div><div>9%</div></div>
2	I	104	<div><div></div><div>54%</div><div>39%</div><div>7%</div></div>
2	J	104	<div><div></div><div>50%</div><div>39%</div><div>11%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8706 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 DNA chain called MUTATED MET CONSENSUS OPERATOR DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	19	Total	C	N	O	P	0	0	0
			386	188	67	113	18			
1	F	19	Total	C	N	O	P	0	0	0
			386	188	67	113	18			
1	K	19	Total	C	N	O	P	0	0	0
			386	188	67	113	18			
1	L	19	Total	C	N	O	P	0	0	0
			386	188	67	113	18			

- Molecule 2 is a protein called METHIONINE REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			
2	B	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			
2	C	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			
2	D	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			
2	G	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			
2	H	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			
2	I	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			
2	J	104	Total	C	N	O	S	0	0	0
			845	530	148	164	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LYS	GLN	ENGINEERED	UNP P0A8U6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	44	LYS	GLN	ENGINEERED	UNP P0A8U6
C	44	LYS	GLN	ENGINEERED	UNP P0A8U6
D	44	LYS	GLN	ENGINEERED	UNP P0A8U6
G	44	LYS	GLN	ENGINEERED	UNP P0A8U6
H	44	LYS	GLN	ENGINEERED	UNP P0A8U6
I	44	LYS	GLN	ENGINEERED	UNP P0A8U6
J	44	LYS	GLN	ENGINEERED	UNP P0A8U6

- # SAM
-
- A 3D ball-and-stick model of S-adenosylmethionine (SAM). The molecule consists of an adenine base, a ribose sugar, and a methionine side chain. The adenine base is shown with atoms labeled H16 (NH2), H11, C6, C5, H17, C8, C2, C4, H13, and N19. The ribose sugar is shown with atoms labeled O4', C1'(R), C2'(R), C3'(S), C4'(S), and C5'. The methionine side chain is shown with atoms labeled CE, SD(S), C6', CG, CB, CA(S), C, OXT, and H. The model uses color coding: carbon (grey), hydrogen (white), nitrogen (blue), oxygen (red), sulfur (yellow), and phosphorus (orange). Stereochemistry is indicated with wedges and dashes.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	B	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	C	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	D	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	G	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	H	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	I	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	J	1	Total 27	C 15	N 6	O 5	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	24	Total O 24 24	0	0
4	C	20	Total O 20 20	0	0
4	D	21	Total O 21 21	0	0
4	E	18	Total O 18 18	0	0
4	F	14	Total O 14 14	0	0
4	G	19	Total O 19 19	0	0
4	H	25	Total O 25 25	0	0
4	I	8	Total O 8 8	0	0
4	J	11	Total O 11 11	0	0
4	K	4	Total O 4 4	0	0
4	L	5	Total O 5 5	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.


Note EDS was not executed.

• Molecule 1: MUTATED MET CONSENSUS OPERATOR DUPLEX

Chain E: 



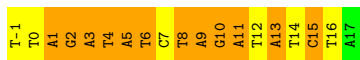
• Molecule 1: MUTATED MET CONSENSUS OPERATOR DUPLEX

Chain F: 



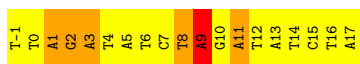
• Molecule 1: MUTATED MET CONSENSUS OPERATOR DUPLEX

Chain K: 



• Molecule 1: MUTATED MET CONSENSUS OPERATOR DUPLEX

Chain L: 

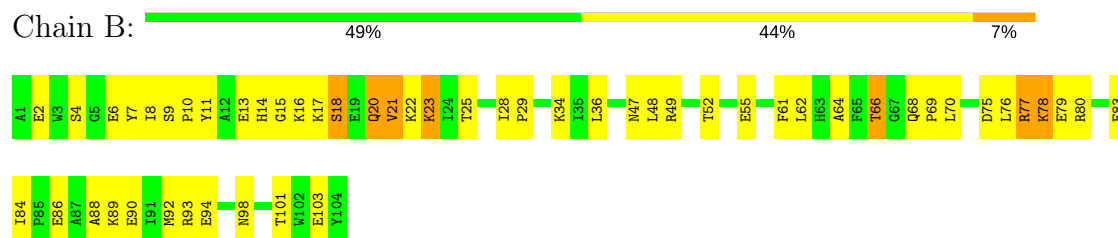


• Molecule 2: METHIONINE REPRESSOR

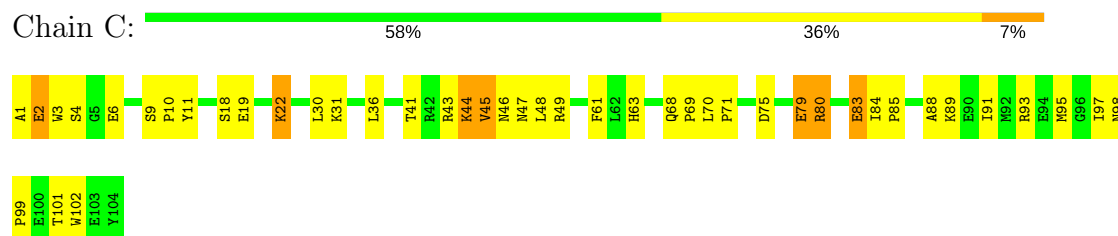
Chain A: 



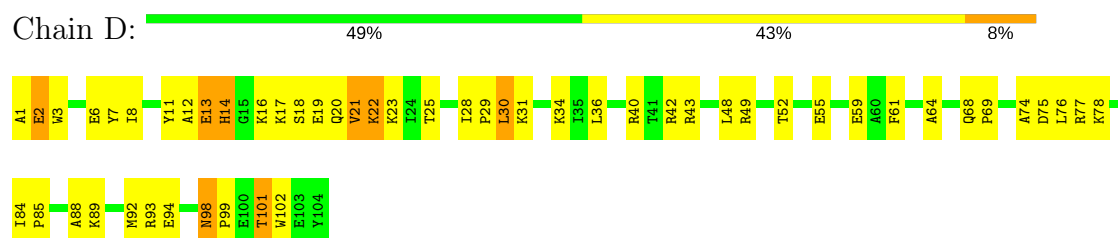
• Molecule 2: METHIONINE REPRESSOR



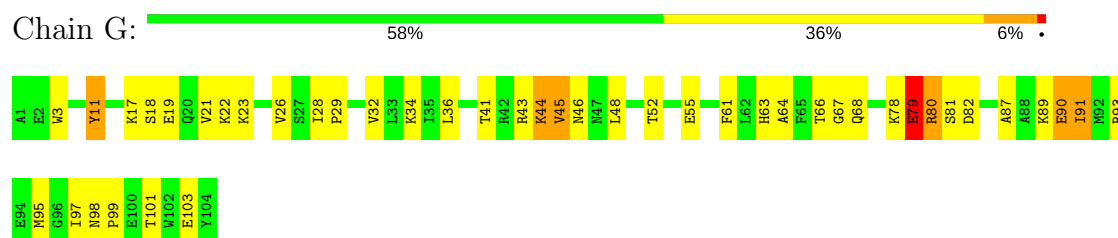
- Molecule 2: METHIONINE REPRESSOR



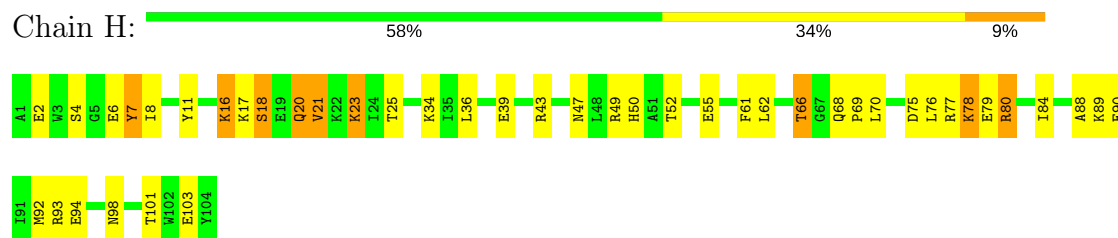
- Molecule 2: METHIONINE REPRESSOR



- Molecule 2: METHIONINE REPRESSOR

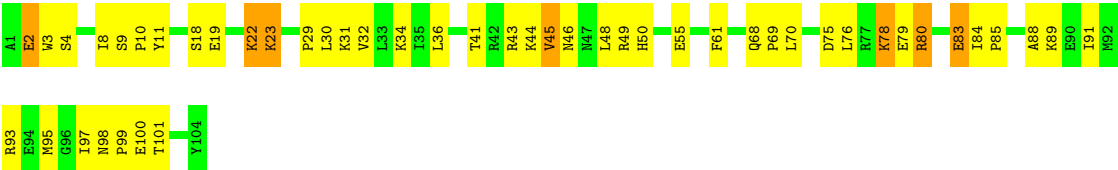


- Molecule 2: METHIONINE REPRESSOR

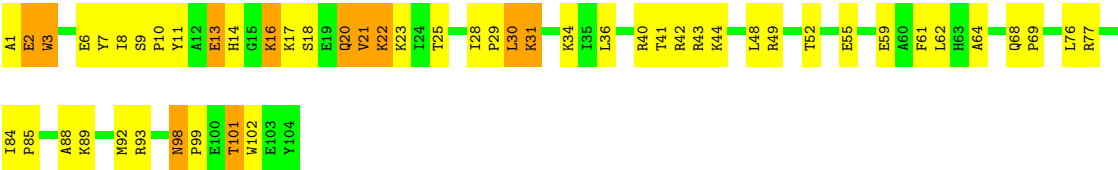


- Molecule 2: METHIONINE REPRESSOR





● Molecule 2: METHIONINE REPRESSOR



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	119.42Å 119.42Å 84.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.30 – 2.40	Depositor
% Data completeness (in resolution range)	85.3 (27.30-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.860	Depositor
R, R_{free}	0.223 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	E	0.56	0/432	0.85	0/665
1	F	0.56	0/432	0.88	0/665
1	K	0.69	0/432	1.31	4/665 (0.6%)
1	L	0.72	0/432	1.32	3/665 (0.5%)
2	A	0.39	0/862	0.63	0/1162
2	B	0.35	0/862	0.56	0/1162
2	C	0.34	0/862	0.53	0/1162
2	D	0.40	0/862	0.62	0/1162
2	G	0.35	0/862	0.55	0/1162
2	H	0.36	0/862	0.55	0/1162
2	I	0.35	0/862	0.54	0/1162
2	J	0.36	0/862	0.55	0/1162
All	All	0.43	0/8624	0.73	7/11956 (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	K	0	10
1	L	0	9
All	All	0	19

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	2	DG	O4'-C1'-N9	5.97	112.18	108.00
1	L	16	DT	N1-C1'-C2'	5.46	122.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	4	DT	O4'-C4'-C3'	-5.37	102.35	104.50
1	K	10	DG	O4'-C4'-C3'	-5.18	102.43	104.50
1	L	9	DA	O4'-C1'-C2'	5.10	109.98	105.90

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	-1	DT	Sidechain
1	K	1	DA	Sidechain
1	K	3	DA	Sidechain
1	K	5	DA	Sidechain
1	K	6	DT	Sidechain

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	E	386	0	219	5	0
1	F	386	0	219	5	0
1	K	386	0	219	31	0
1	L	386	0	219	31	0
2	A	845	0	841	60	0
2	B	845	0	841	38	0
2	C	845	0	841	44	0
2	D	845	0	841	46	0
2	G	845	0	841	41	0
2	H	845	0	841	32	0
2	I	845	0	841	41	0
2	J	845	0	841	44	0
3	A	27	0	22	5	0
3	B	27	0	22	2	0
3	C	27	0	22	4	0
3	D	27	0	22	1	0
3	G	27	0	22	0	0
3	H	27	0	22	2	0
3	I	27	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	27	0	22	1	0
4	A	17	0	0	0	0
4	B	24	0	0	0	0
4	C	20	0	0	2	0
4	D	21	0	0	1	0
4	E	18	0	0	0	0
4	F	14	0	0	0	0
4	G	19	0	0	1	0
4	H	25	0	0	0	0
4	I	8	0	0	0	0
4	J	11	0	0	0	0
4	K	4	0	0	0	0
4	L	5	0	0	0	0
All	All	8706	0	7780	363	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 23.

The worst 5 of 363 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)
2:B:16:LYS:O	2:B:20:GLN:HG3	1.57	1.05
2:A:44:LYS:HE3	2:D:22:LYS:HD3	1.40	1.03
2:A:98:ASN:HB3	2:A:101:THR:HB	1.47	0.95
2:I:80:ARG:HH11	2:I:83:GLU:HB2	1.35	0.91
2:A:98:ASN:CB	2:A:101:THR:HB	2.02	0.88

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	
2	A	102/104 (98%)	93 (91%)	6 (6%)	3 (3%)	5	5
2	B	102/104 (98%)	98 (96%)	3 (3%)	1 (1%)	18	26
2	C	102/104 (98%)	91 (89%)	10 (10%)	1 (1%)	18	26
2	D	102/104 (98%)	88 (86%)	11 (11%)	3 (3%)	5	5
2	G	102/104 (98%)	94 (92%)	6 (6%)	2 (2%)	9	10
2	H	102/104 (98%)	97 (95%)	3 (3%)	2 (2%)	9	10
2	I	102/104 (98%)	90 (88%)	11 (11%)	1 (1%)	18	26
2	J	102/104 (98%)	89 (87%)	11 (11%)	2 (2%)	9	10
All	All	816/832 (98%)	740 (91%)	61 (8%)	15 (2%)	10	12

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	79	GLU
2	G	79	GLU
2	J	3	TRP
2	B	77	ARG
2	C	45	VAL

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	
2	A	92/92 (100%)	81 (88%)	11 (12%)	6	7
2	B	92/92 (100%)	78 (85%)	14 (15%)	3	4
2	C	92/92 (100%)	81 (88%)	11 (12%)	6	7
2	D	92/92 (100%)	81 (88%)	11 (12%)	6	7
2	G	92/92 (100%)	80 (87%)	12 (13%)	5	5
2	H	92/92 (100%)	77 (84%)	15 (16%)	3	3
2	I	92/92 (100%)	79 (86%)	13 (14%)	4	4
2	J	92/92 (100%)	78 (85%)	14 (15%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	736/736 (100%)	635 (86%)	101 (14%)	4 5

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	98	ASN
2	G	90	GLU
2	J	22	LYS
2	G	11	TYR
2	G	44	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	68	GLN
2	D	98	ASN
2	I	98	ASN
2	C	98	ASN
2	H	68	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are 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	SAM	A	200	-	21,29,29	1.84	5 (23%)	17,42,42	2.80	2 (11%)
3	SAM	B	200	-	21,29,29	1.74	6 (28%)	17,42,42	2.63	2 (11%)
3	SAM	C	199	-	21,29,29	2.31	8 (38%)	17,42,42	2.70	3 (17%)
3	SAM	D	200	-	21,29,29	1.82	8 (38%)	17,42,42	2.62	2 (11%)
3	SAM	G	199	-	21,29,29	1.98	7 (33%)	17,42,42	2.65	3 (17%)
3	SAM	H	200	-	21,29,29	1.73	5 (23%)	17,42,42	2.62	2 (11%)
3	SAM	I	199	-	21,29,29	1.81	5 (23%)	17,42,42	2.68	3 (17%)
3	SAM	J	200	-	21,29,29	1.77	5 (23%)	17,42,42	2.63	2 (11%)

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	SAM	A	200	-	-	0/8/33/33	0/3/3/3
3	SAM	B	200	-	-	0/8/33/33	0/3/3/3
3	SAM	C	199	-	-	0/8/33/33	0/3/3/3
3	SAM	D	200	-	-	0/8/33/33	0/3/3/3
3	SAM	G	199	-	-	0/8/33/33	0/3/3/3
3	SAM	H	200	-	-	0/8/33/33	0/3/3/3
3	SAM	I	199	-	-	0/8/33/33	0/3/3/3
3	SAM	J	200	-	-	0/8/33/33	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	200	SAM	C5-C4	-2.20	1.35	1.40
3	C	199	SAM	O3'-C3'	-2.17	1.38	1.43
3	H	200	SAM	C5-C4	-2.15	1.35	1.40
3	D	200	SAM	O2'-C2'	-2.15	1.38	1.43
3	A	200	SAM	C5-C4	-2.12	1.35	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	200	SAM	N3-C2-N1	-10.42	119.79	128.86
3	C	199	SAM	N3-C2-N1	-9.78	120.34	128.86
3	I	199	SAM	N3-C2-N1	-9.68	120.43	128.86
3	D	200	SAM	N3-C2-N1	-9.64	120.46	128.86
3	H	200	SAM	N3-C2-N1	-9.64	120.46	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	200	SAM	5	0
3	B	200	SAM	2	0
3	C	199	SAM	4	0
3	D	200	SAM	1	0
3	H	200	SAM	2	0
3	I	199	SAM	1	0
3	J	200	SAM	1	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.