



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:28 PM GMT

PDB ID : 3SWS
Title : Crystal Structure of the Quinone Form of Methylamine Dehydrogenase in Complex with the Diferric Form of MauG
Authors : Jensen, L.M.R.; Wilmot, C.M.
Deposited on : 2011-07-14
Resolution : 1.86 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

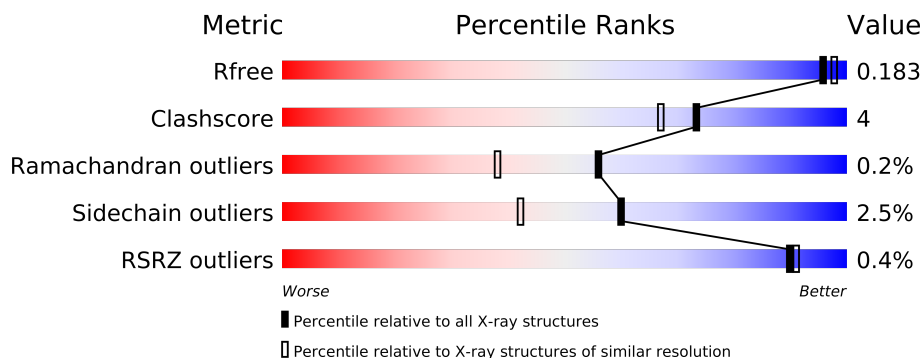
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.86 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}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
2	C	137	
2	E	137	
3	D	386	
3	F	386	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	1PE	D	390	-	X
11	PG4	F	387	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
4	CA	B	400	-	X
7	EDO	D	388	-	X
8	MES	D	387	-	X
9	ACT	D	389	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15667 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	3	0
			2753	1721	494	527	11			
1	B	354	Total	C	N	O	S	0	8	0
			2781	1740	495	534	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	HIS	-	EXPRESSION TAG	UNP Q51658
A	369	HIS	-	EXPRESSION TAG	UNP Q51658
A	370	HIS	-	EXPRESSION TAG	UNP Q51658
A	371	HIS	-	EXPRESSION TAG	UNP Q51658
A	372	HIS	-	EXPRESSION TAG	UNP Q51658
A	373	HIS	-	EXPRESSION TAG	UNP Q51658
B	368	HIS	-	EXPRESSION TAG	UNP Q51658
B	369	HIS	-	EXPRESSION TAG	UNP Q51658
B	370	HIS	-	EXPRESSION TAG	UNP Q51658
B	371	HIS	-	EXPRESSION TAG	UNP Q51658
B	372	HIS	-	EXPRESSION TAG	UNP Q51658
B	373	HIS	-	EXPRESSION TAG	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	126	Total	C	N	O	S	0	2	0
			979	605	167	194	13			
2	E	125	Total	C	N	O	S	0	2	0
			964	596	161	193	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP P22619
C	133	HIS	-	EXPRESSION TAG	UNP P22619
C	134	HIS	-	EXPRESSION TAG	UNP P22619
C	135	HIS	-	EXPRESSION TAG	UNP P22619
C	136	HIS	-	EXPRESSION TAG	UNP P22619
C	137	HIS	-	EXPRESSION TAG	UNP P22619
E	132	HIS	-	EXPRESSION TAG	UNP P22619
E	133	HIS	-	EXPRESSION TAG	UNP P22619
E	134	HIS	-	EXPRESSION TAG	UNP P22619
E	135	HIS	-	EXPRESSION TAG	UNP P22619
E	136	HIS	-	EXPRESSION TAG	UNP P22619
E	137	HIS	-	EXPRESSION TAG	UNP P22619

- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	12	0
			2994	1904	508	574	8			
3	F	376	Total	C	N	O	S	0	5	0
			2952	1874	504	566	8			

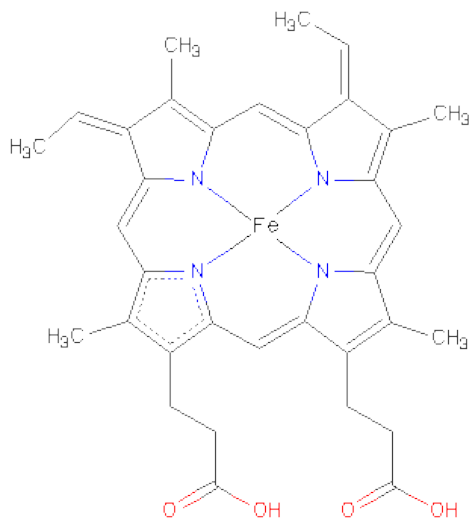
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

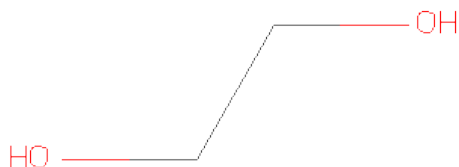
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



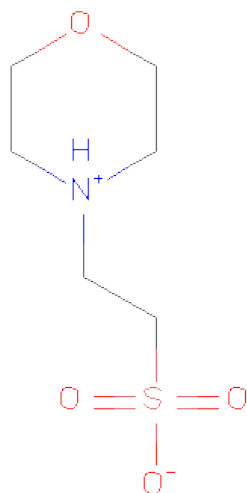
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



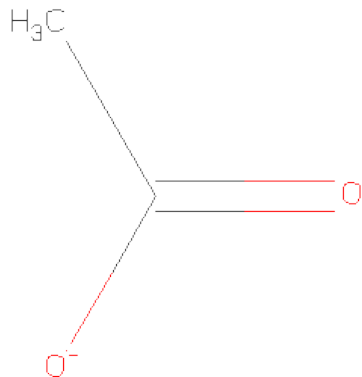
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



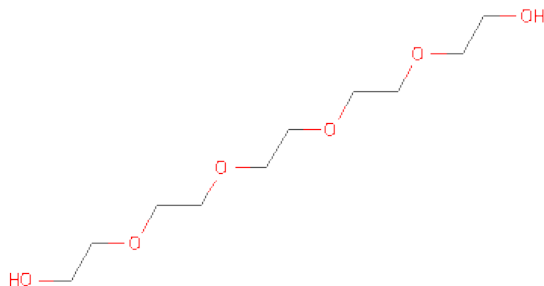
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



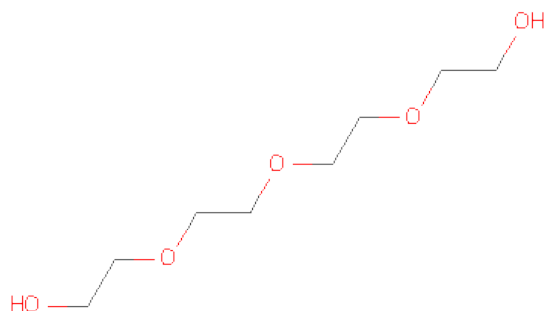
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is water.

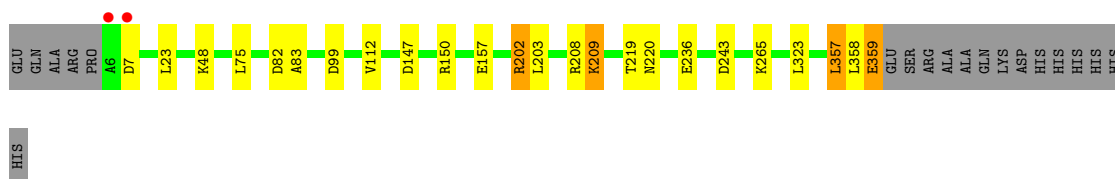
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	359	Total	O	0	0
			359	359		
12	B	415	Total	O	0	0
			415	415		
12	C	151	Total	O	0	0
			151	151		
12	D	475	Total	O	0	0
			475	475		
12	E	131	Total	O	0	0
			131	131		
12	F	478	Total	O	0	0
			478	478		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

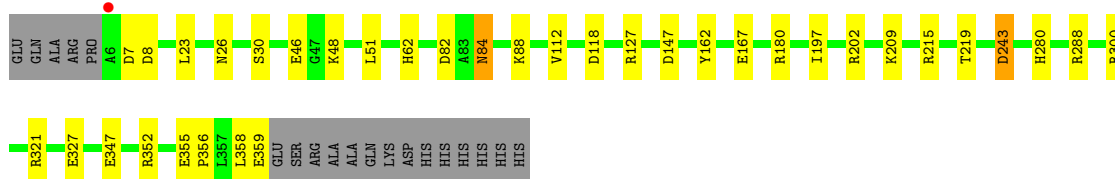
- Molecule 1: Methylamine utilization protein MauG

Chain A: 



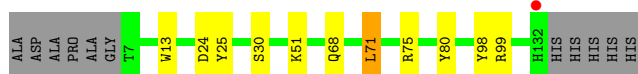
- Molecule 1: Methylamine utilization protein MauG

Chain B: 



- Molecule 2: Methylamine dehydrogenase light chain

Chain C: 



- Molecule 2: Methylamine dehydrogenase light chain

Chain E: 



- Molecule 3: Methylamine dehydrogenase heavy chain

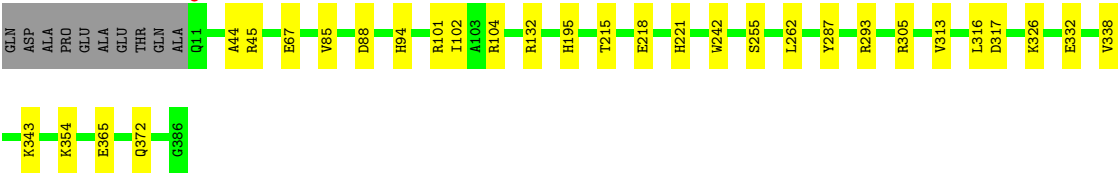
Chain D: 





● Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.22Å 99.42Å 102.83Å 64.77° 74.77° 75.14°	Depositor
Resolution (Å)	49.12 – 1.86 49.11 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.12-1.86) 97.1 (49.11-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.136 , 0.178 0.142 , 0.183	Depositor DCC
R_{free} test set	7734 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.6	EDS
Estimated twinning fraction	0.017 for h,h-k,h-l 0.009 for -h,-l,-k 0.004 for -h,-h+l,-h+k	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 154077 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15667	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, ACT, EDO, 1PE, PG4, MES, HEC, TRQ

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	1.13	1/2826 (0.0%)	1.01	13/3834 (0.3%)
1	B	1.20	3/2869 (0.1%)	1.07	12/3891 (0.3%)
2	C	1.36	5/994 (0.5%)	1.09	3/1357 (0.2%)
2	E	1.21	2/978 (0.2%)	0.97	1/1335 (0.1%)
3	D	1.29	7/3107 (0.2%)	1.06	7/4231 (0.2%)
3	F	1.26	9/3044 (0.3%)	1.02	7/4147 (0.2%)
All	All	1.23	27/13818 (0.2%)	1.04	43/18795 (0.2%)

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	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	62	TYR	CD2-CE2	7.32	1.50	1.39
3	D	48	TYR	CE1-CZ	6.86	1.47	1.38
3	D	342	GLU	C-O	6.15	1.35	1.23
3	F	287	TYR	CD1-CE1	6.03	1.48	1.39
3	F	242	TRP	CE3-CZ3	5.86	1.48	1.38

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	B	180	ARG	NE-CZ-NH2	-9.07	115.77	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ASP	CB-CG-OD1	7.79	125.31	118.30
3	D	224	ASP	CB-CG-OD1	7.58	125.12	118.30
3	F	104	ARG	NE-CZ-NH1	7.54	124.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	358	LEU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2753	0	0	5	0
1	B	2781	0	0	16	0
2	C	979	0	0	3	0
2	E	964	0	0	1	0
3	D	2994	0	0	14	0
3	F	2952	0	0	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	0	0	0
6	B	86	0	0	1	0
7	A	4	0	6	0	0
7	B	4	0	6	1	0
7	D	4	0	6	6	0
8	D	12	0	12	1	0
9	D	4	0	3	0	0
10	D	16	0	22	4	0
11	F	13	0	18	4	0
12	A	359	0	0	4	0
12	B	415	0	0	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	151	0	0	4	0
12	D	475	0	0	9	0
12	E	131	0	0	1	0
12	F	478	0	0	10	0
All	All	15667	0	73	57	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 57 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:372[A]:GLN:OE1	12:F:1498:HOH:O	1.62	1.17
1:B:26[A]:ASN:ND2	12:B:2258:HOH:O	1.82	1.10
3:F:372[B]:GLN:NE2	12:F:1047:HOH:O	2.02	0.93
2:C:99[A]:ARG:NH2	12:C:1827:HOH:O	2.07	0.88
3:D:236[A]:LYS:NZ	12:D:976:HOH:O	2.11	0.83

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	
1	A	355/373 (95%)	346 (98%)	8 (2%)	1 (0%)	50	32
1	B	360/373 (96%)	350 (97%)	9 (2%)	1 (0%)	50	32
2	C	125/137 (91%)	120 (96%)	5 (4%)	0	100	100
2	E	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
3	D	386/386 (100%)	372 (96%)	12 (3%)	2 (0%)	38	19
3	F	379/386 (98%)	365 (96%)	13 (3%)	1 (0%)	50	32
All	All	1729/1792 (96%)	1674 (97%)	50 (3%)	5 (0%)	56	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	ASP
1	A	358	LEU
3	D	102[A]	ILE
3	D	102[B]	ILE
3	F	102	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	279/292 (96%)	267 (96%)	12 (4%)	40	19
1	B	284/292 (97%)	279 (98%)	5 (2%)	71	57
2	C	107/112 (96%)	105 (98%)	2 (2%)	69	55
2	E	106/112 (95%)	103 (97%)	3 (3%)	56	37
3	D	316/311 (102%)	305 (96%)	11 (4%)	48	26
3	F	309/311 (99%)	304 (98%)	5 (2%)	75	62
All	All	1401/1430 (98%)	1363 (97%)	38 (3%)	60	39

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	68	GLN
3	D	94	HIS
3	F	293	ARG
3	D	14[A]	GLN
3	D	174	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
2	TRQ	C	57	2	17,17,18	5.21	8 (47%)	20,24,26	2.49	6 (30%)
2	TRQ	E	57	2	17,17,18	4.72	4 (23%)	20,24,26	3.37	4 (20%)

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
2	TRQ	C	57	2	-	0/4/19/21	0/0/2/2
2	TRQ	E	57	2	-	0/4/19/21	0/0/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	TRQ	O-C	18.70	1.24	1.11
2	E	57	TRQ	O-C	17.14	1.23	1.11
2	E	57	TRQ	CZ3-CE3	7.32	1.46	1.34
2	C	57	TRQ	CZ3-CE3	6.63	1.45	1.34
2	C	57	TRQ	CE2-CZ2	-4.86	1.46	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	TRQ	C-CA-N	-13.48	100.36	113.83
2	C	57	TRQ	C-CA-N	-8.41	105.43	113.83
2	E	57	TRQ	CD1-CG-CD2	3.55	106.67	104.97
2	E	57	TRQ	CB-CG-CD1	-3.44	122.22	128.12
2	C	57	TRQ	CD1-CG-CD2	3.07	106.44	104.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
7	EDO	A	374	-	3,3,3	0.60	0	2,2,2	0.30	0
6	HEC	A	500	1,12	50,50,50	3.05	22 (44%)	56,82,82	3.20	27 (48%)
6	HEC	A	600	1	50,50,50	2.57	22 (44%)	56,82,82	3.24	29 (51%)
7	EDO	B	374	-	3,3,3	0.79	0	2,2,2	0.78	0
6	HEC	B	500	1,12	50,50,50	2.97	20 (40%)	56,82,82	3.13	28 (50%)
6	HEC	B	600	1	50,50,50	2.72	20 (40%)	56,82,82	3.28	27 (48%)
8	MES	D	387	-	12,12,12	1.74	3 (25%)	16,16,16	3.29	8 (50%)
7	EDO	D	388	-	3,3,3	1.70	0	2,2,2	2.33	1 (50%)
9	ACT	D	389	-	1,3,3	3.32	1 (100%)	0,3,3	0.00	-
10	1PE	D	390	-	15,15,15	0.46	0	14,14,14	0.66	0
11	PG4	F	387	-	12,12,12	0.38	0	11,11,11	0.51	0

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
7	EDO	A	374	-	-	0/1/1/1	0/0/0/0
6	HEC	A	500	1,12	-	0/10/54/54	0/0/8/8
6	HEC	A	600	1	-	0/10/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	374	-	-	0/1/1/1	0/0/0/0
6	HEC	B	500	1,12	-	0/10/54/54	0/0/8/8
6	HEC	B	600	1	-	0/10/54/54	0/0/8/8
8	MES	D	387	-	-	0/6/14/14	1/1/1/1
7	EDO	D	388	-	-	0/1/1/1	0/0/0/0
9	ACT	D	389	-	-	0/0/0/0	0/0/0/0
10	1PE	D	390	-	-	0/13/13/13	0/0/0/0
11	PG4	F	387	-	-	0/10/10/10	0/0/0/0

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	500	HEC	C3B-CAB	9.33	1.54	1.35
6	B	500	HEC	C3C-CAC	8.54	1.53	1.35
6	A	600	HEC	C3B-CAB	8.02	1.52	1.35
6	B	500	HEC	C3B-CAB	8.00	1.51	1.35
6	B	600	HEC	C3C-CAC	7.87	1.51	1.35

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	CBD-CAD-C3D	-8.55	97.62	112.69
6	B	600	HEC	CBB-CAB-C3B	-8.37	104.89	128.44
6	A	600	HEC	CBC-CAC-C3C	-8.18	105.42	128.44
6	B	500	HEC	CBB-CAB-C3B	-8.09	105.66	128.44
6	A	600	HEC	CBB-CAB-C3B	-8.01	105.90	128.44

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	387	MES	C2-C3-C5-C6-N4-O1

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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, 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	354/373 (94%)	-0.52	2 (0%) 86 87	14, 23, 38, 58	0
1	B	354/373 (94%)	-0.74	1 (0%) 91 92	15, 21, 34, 56	0
2	C	126/137 (91%)	-0.31	1 (0%) 83 83	13, 15, 24, 55	0
2	E	125/137 (91%)	-0.58	1 (0%) 83 83	14, 18, 28, 56	0
3	D	376/386 (97%)	-0.56	1 (0%) 91 92	12, 17, 28, 53	0
3	F	376/386 (97%)	-0.59	1 (0%) 91 92	13, 19, 30, 55	0
All	All	1711/1792 (95%)	-0.58	7 (0%) 90 91	12, 19, 34, 58	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	132	HIS	6.4
1	A	6	ALA	4.7
3	F	11	GLN	3.0
3	D	11	GLN	2.9
1	A	7	ASP	2.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TRQ	C	57	16/17	0.10	-0.34	14,16,21,26	0
2	TRQ	E	57	16/17	0.06	-1.04	17,18,25,29	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	MES	D	387	12/12	0.15	6.47	32,52,60,62	0
11	PG4	F	387	13/13	0.11	6.33	42,50,62,63	0
10	1PE	D	390	16/16	0.19	4.65	38,51,59,62	0
7	EDO	D	388	4/4	0.18	4.20	29,29,30,33	0
4	CA	B	400	1/1	0.07	2.29	15,15,15,15	0
9	ACT	D	389	4/4	0.11	2.03	25,28,31,32	0
7	EDO	B	374	4/4	0.21	1.19	38,38,40,41	0
6	HEC	B	500	43/43	0.07	1.05	12,15,20,21	0
6	HEC	B	600	43/43	0.06	0.38	10,16,17,18	0
7	EDO	A	374	4/4	0.08	0.14	46,47,49,50	0
5	NA	A	401	1/1	0.07	-0.25	24,24,24,24	0
6	HEC	A	500	43/43	0.06	-0.26	15,19,23,24	0
6	HEC	A	600	43/43	0.06	-0.61	10,14,17,20	0
5	NA	A	402	1/1	0.06	-1.24	31,31,31,31	0
5	NA	B	401	1/1	0.04	-1.64	22,22,22,22	0
5	NA	B	402	1/1	0.04	-2.34	27,27,27,27	0
4	CA	A	400	1/1	0.04	-3.42	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.