



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2024 – 12:09 PM EST

PDB ID : 1FZ8  
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II COCRYSTALLIZED WITH DIBROMOMETHANE  
Authors : Whittington, D.A.; Rosenzweig, A.C.; Frederick, C.A.; Lippard, S.J.  
Deposited on : 2000-10-03  
Resolution : 2.10 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

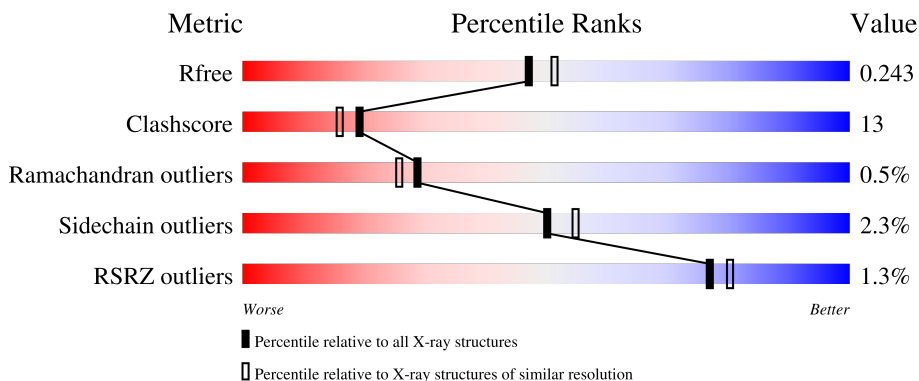
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of 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	527	 71% 25% ..
1	B	527	 71% 24% ..
2	C	389	 79% 19% .
2	D	389	 66% 33% .
3	E	170	 78% 19% ..

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Mol	Chain	Length	Quality of chain
3	F	170	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	2BM	B	9002	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18611 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 METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	4185	2677	721	769	18	0	0	0
1	B	510	4177	2673	719	767	18	0	0	0

- Molecule 2 is a protein called METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	388	3193	2054	551	580	8	0	0	0
2	D	388	3189	2051	550	580	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	370	ARG	ALA	conflict	UNP P18798
D	370	ARG	ALA	conflict	UNP P18798

- Molecule 3 is a protein called METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	167	1375	872	247	251	5	0	0	0
3	F	168	1386	878	250	253	5	0	0	0

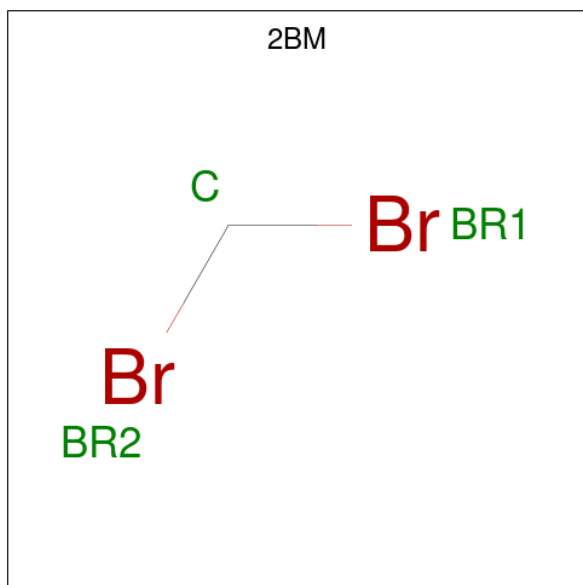
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Fe 2 2	0	0
4	B	2	Total Fe 2 2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	2	Total Ca 2 2	0	0

- Molecule 6 is DIBROMOMETHANE (three-letter code: 2BM) (formula: CH<sub>2</sub>Br<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Br C 3 2 1	0	0
6	A	1	Total Br C 3 2 1	0	0
6	A	1	Total Br C 3 2 1	0	0
6	B	1	Total Br C 3 2 1	0	0
6	B	1	Total Br C 3 2 1	0	0
6	B	1	Total Br C 3 2 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 3	Br 2	C 1	0	0
6	C	1	Total 3	Br 2	C 1	0	0
6	C	1	Total 3	Br 2	C 1	0	0
6	D	1	Total 3	Br 2	C 1	0	0

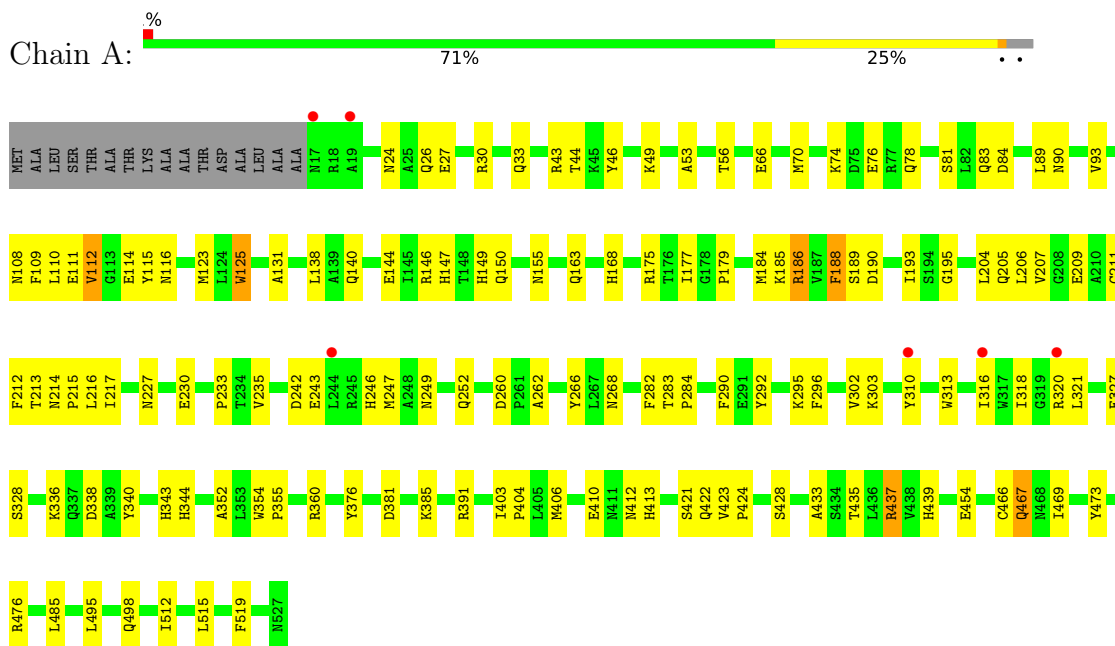
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	245	Total 245	O 245	0	0
7	B	247	Total 247	O 247	0	0
7	C	268	Total 268	O 268	0	0
7	D	140	Total 140	O 140	0	0
7	E	123	Total 123	O 123	0	0
7	F	46	Total 46	O 46	0	0

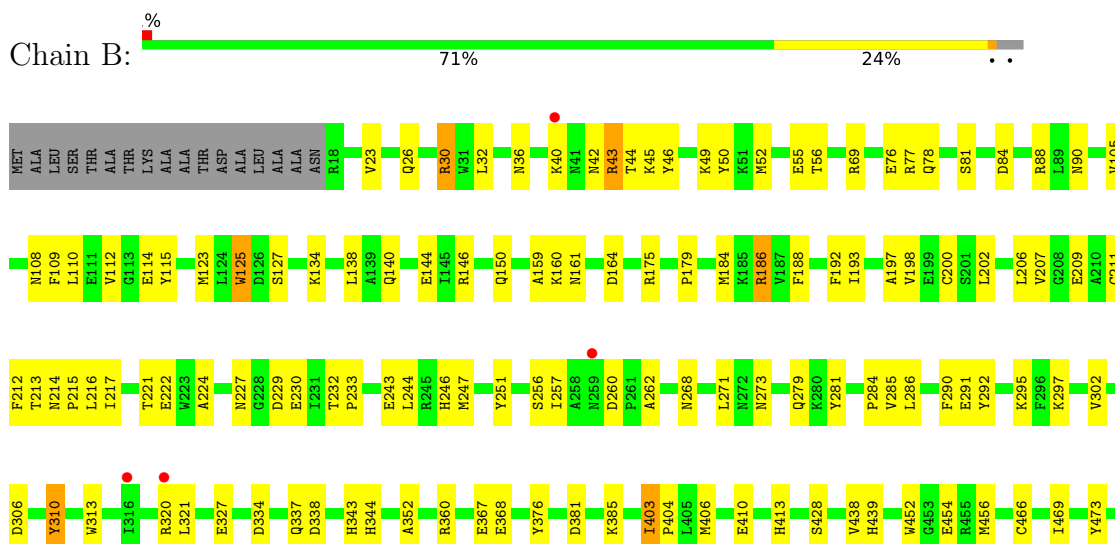
### 3 Residue-property plots [i](#)

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: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

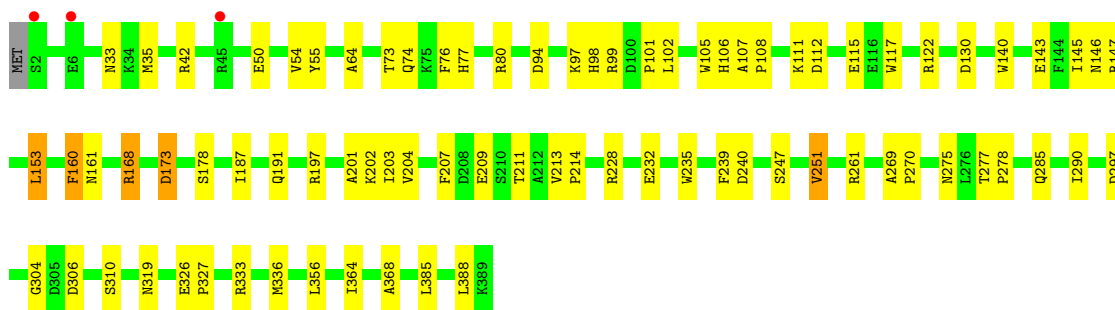
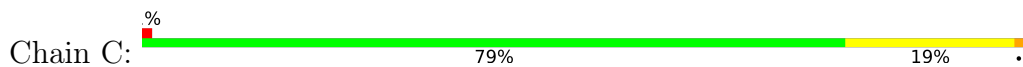


- Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

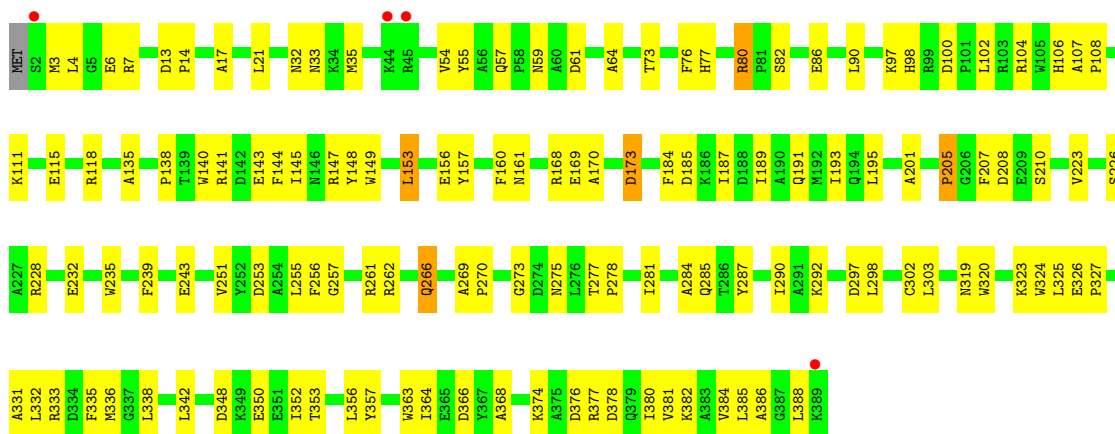




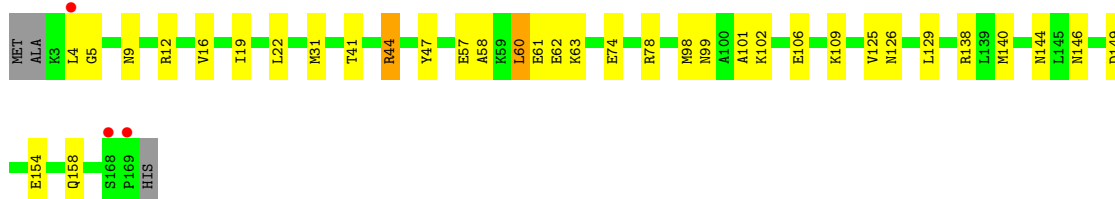
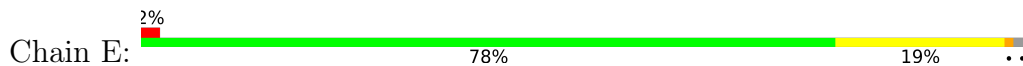
- Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



- Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



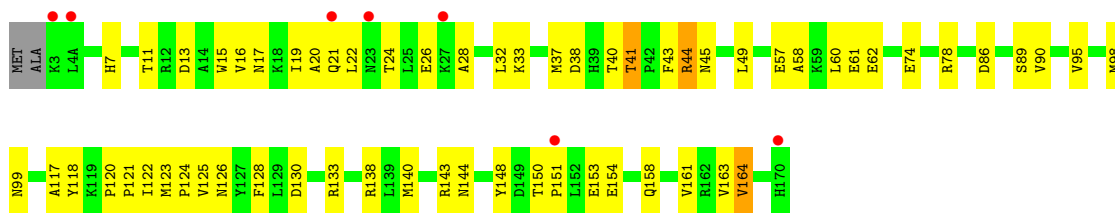
- Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



- Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.17Å 171.99Å 221.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.50 – 2.10 23.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	77.7 (23.50-2.10) 77.8 (23.50-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.10Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.201 , 0.250 0.195 , 0.243	Depositor DCC
$R_{free}$ test set	4359 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18611	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 2BM, CA

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	0.33	0/4310	0.55	0/5853
1	B	0.33	0/4302	0.56	0/5842
2	C	0.36	0/3289	0.57	0/4464
2	D	0.34	0/3285	0.54	0/4460
3	E	0.34	0/1404	0.57	0/1892
3	F	0.30	0/1416	0.50	0/1907
All	All	0.34	0/18006	0.55	0/24418

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

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	4185	0	3981	110	0
1	B	4177	0	3975	128	0
2	C	3193	0	3042	73	0
2	D	3189	0	3031	103	0
3	E	1375	0	1370	30	0
3	F	1386	0	1377	57	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
6	A	9	0	0	2	0
6	B	9	0	0	2	0
6	C	9	0	0	1	0
6	D	3	0	0	0	0
7	A	245	0	0	6	0
7	B	247	0	0	8	0
7	C	268	0	0	8	0
7	D	140	0	0	3	0
7	E	123	0	0	2	0
7	F	46	0	0	1	0
All	All	18611	0	16776	443	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 13.

The worst 5 of 443 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:A:209:GLU:HA	1:A:213:THR:HG22	1.23	1.12
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.05	0.98
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.45	0.97
1:B:44:THR:HG22	1:B:46:TYR:H	1.30	0.94
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.11	0.93

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	509/527 (97%)	487 (96%)	21 (4%)	1 (0%)	47	49
1	B	508/527 (96%)	475 (94%)	31 (6%)	2 (0%)	34	32
2	C	386/389 (99%)	376 (97%)	8 (2%)	2 (0%)	29	26
2	D	386/389 (99%)	364 (94%)	18 (5%)	4 (1%)	15	11
3	E	165/170 (97%)	163 (99%)	2 (1%)	0	100	100
3	F	166/170 (98%)	158 (95%)	7 (4%)	1 (1%)	25	21
All	All	2120/2172 (98%)	2023 (95%)	87 (4%)	10 (0%)	29	26

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	TYR
1	B	40	LYS
2	D	205	PRO
2	D	374	LYS
2	D	64	ALA

### 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	433/442 (98%)	422 (98%)	11 (2%)	47	52
1	B	432/442 (98%)	422 (98%)	10 (2%)	50	55
2	C	322/323 (100%)	314 (98%)	8 (2%)	47	52
2	D	321/323 (99%)	314 (98%)	7 (2%)	52	57
3	E	145/147 (99%)	143 (99%)	2 (1%)	67	73
3	F	146/147 (99%)	142 (97%)	4 (3%)	44	48
All	All	1799/1824 (99%)	1757 (98%)	42 (2%)	50	55

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	173	ASP

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Mol	Chain	Res	Type
2	D	266	GLN
2	D	4	LEU
2	D	153	LEU
3	E	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	144	ASN
3	F	7	HIS
3	F	167	GLN
1	B	78	GLN
1	B	36	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](#)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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
6	2BM	C	9010	-	2,2,2	0.07	0	1,1,1	0.31	0
6	2BM	A	9007	-	2,2,2	0.27	0	1,1,1	0.37	0
6	2BM	A	9006	-	2,2,2	0.10	0	1,1,1	0.95	0
6	2BM	B	9003	-	2,2,2	0.03	0	1,1,1	0.42	0
6	2BM	C	9009	-	2,2,2	0.05	0	1,1,1	0.44	0
6	2BM	B	9002	-	2,2,2	0.14	0	1,1,1	0.22	0
6	2BM	D	9004	-	2,2,2	0.14	0	1,1,1	0.13	0
6	2BM	A	9008	-	2,2,2	0.17	0	1,1,1	0.10	0
6	2BM	B	9001	-	2,2,2	0.32	0	1,1,1	0.36	0
6	2BM	C	9005	-	2,2,2	0.04	0	1,1,1	0.54	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	9010	2BM	1	0
6	A	9007	2BM	1	0
6	B	9002	2BM	2	0
6	A	9008	2BM	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 [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	511/527 (96%)	-0.32	6 (1%) 79 82	11, 27, 47, 64	0
1	B	510/527 (96%)	-0.36	5 (0%) 82 85	15, 27, 44, 60	0
2	C	388/389 (99%)	-0.59	3 (0%) 86 88	12, 19, 33, 53	0
2	D	388/389 (99%)	-0.16	4 (1%) 82 85	15, 30, 51, 68	0
3	E	167/170 (98%)	-0.44	3 (1%) 68 72	14, 23, 38, 68	0
3	F	168/170 (98%)	0.28	7 (4%) 36 42	27, 39, 55, 67	0
All	All	2132/2172 (98%)	-0.31	28 (1%) 77 80	11, 26, 48, 68	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	169	PRO	4.5
1	A	316	ILE	3.8
3	F	4(A)	LEU	3.3
3	E	4	LEU	3.3
2	C	6	GLU	3.0

### 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](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	2BM	C	9010	3/3	0.90	0.16	38,38,40,42	3
5	CA	C	5007	1/1	0.94	0.05	49,49,49,49	0
6	2BM	C	9009	3/3	0.97	0.07	34,34,37,38	3
4	FE	A	5002	1/1	0.98	0.05	36,36,36,36	0
5	CA	A	5005	1/1	0.98	0.04	35,35,35,35	0
5	CA	C	5006	1/1	0.98	0.10	50,50,50,50	0
6	2BM	A	9008	3/3	0.99	0.06	28,28,29,30	3
6	2BM	B	9001	3/3	0.99	0.07	25,25,29,34	3
6	2BM	C	9005	3/3	0.99	0.04	28,28,29,32	3
4	FE	B	5004	1/1	0.99	0.03	33,33,33,33	0
6	2BM	A	9006	3/3	0.99	0.04	29,29,29,30	0
6	2BM	D	9004	3/3	0.99	0.06	28,28,33,34	3
6	2BM	B	9003	3/3	1.00	0.04	27,27,28,33	0
6	2BM	A	9007	3/3	1.00	0.04	30,30,33,35	3
4	FE	B	5003	1/1	1.00	0.05	25,25,25,25	0
4	FE	A	5001	1/1	1.00	0.03	27,27,27,27	0
6	2BM	B	9002	3/3	1.00	0.04	27,27,29,33	3

## 6.5 Other polymers [i](#)

There are no such residues in this entry.