



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2024 – 06:05 AM EST

PDB ID : 1P3H  
Title : Crystal Structure of the Mycobacterium tuberculosis chaperonin 10 tetradecamer  
Authors : Roberts, M.M.; Coker, A.R.; Fossati, G.; Mascagni, P.; Coates, A.R.M.; Wood, S.P.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2003-04-17  
Resolution : 2.80 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

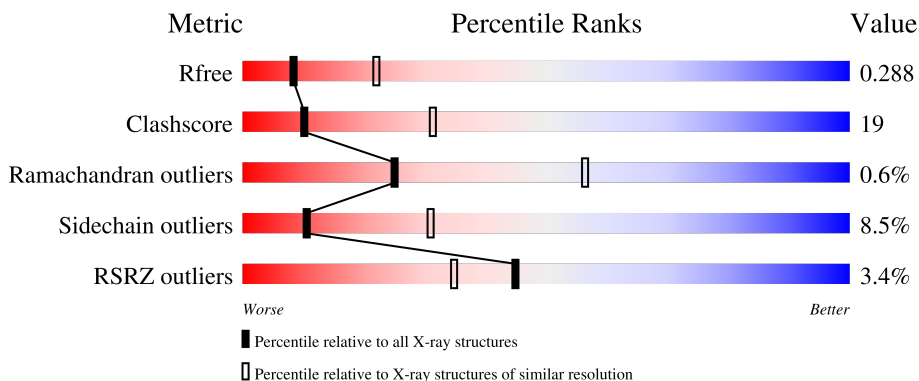
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	99	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange;"></div> </div> <p style="margin-left: 40px;">66%      27%      7%</p>
1	B	99	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">64%      34%      ..</p>
1	C	99	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">62%      33%      . .</p>
1	D	99	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange;"></div> </div> <p style="margin-left: 40px;">68%      28%      .</p>
1	E	99	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">67%      30%      ..</p>

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Mol	Chain	Length	Quality of chain
1	F	99	
1	G	99	
1	H	99	
1	I	99	
1	J	99	
1	K	99	
1	L	99	
1	M	99	
1	N	99	

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
3	MPD	F	106	-	-	X	-
3	MPD	H	117	-	-	-	X
3	MPD	J	110	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10690 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 10 kDa chaperonin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	99	752	473	123	156	8	0	0
1	B	98	747	470	122	155	4	0	0
1	C	98	747	470	122	155	5	0	0
1	D	99	752	473	123	156	18	0	0
1	E	98	747	470	122	155	19	0	0
1	F	99	748	470	122	156	6	0	0
1	G	99	752	473	123	156	24	0	0
1	H	99	752	473	123	156	4	0	0
1	I	98	743	467	121	155	12	0	0
1	J	98	747	470	122	155	10	0	0
1	K	98	747	470	122	155	22	0	0
1	L	98	743	467	121	155	6	0	0
1	M	99	752	473	123	156	0	0	0
1	N	99	752	473	123	156	4	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 8 6 2	0	0
3	H	1	Total C O 8 6 2	0	0
3	I	1	Total C O 8 6 2	0	0
3	J	1	Total C O 8 6 2	0	0
3	K	1	Total C O 8 6 2	0	0
3	L	1	Total C O 8 6 2	0	0
3	M	1	Total C O 8 6 2	0	0
3	N	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	2	Total O 2 2	0	0
4	C	5	Total O 5 5	0	0
4	D	7	Total O 7 7	0	0
4	E	9	Total O 9 9	0	0
4	F	6	Total O 6 6	0	0
4	G	8	Total O 8 8	0	0
4	H	9	Total O 9 9	0	0
4	I	2	Total O 2 2	0	0
4	J	2	Total O 2 2	0	0
4	K	3	Total O 3 3	0	0

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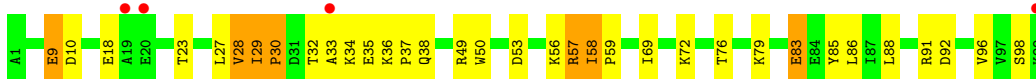
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	N	4	Total	O	0	0
			4	4		

### 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.

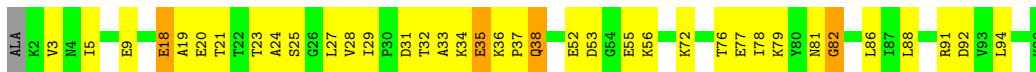
- Molecule 1: 10 kDa chaperonin



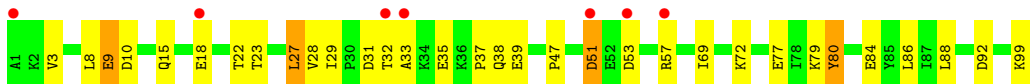
- Molecule 1: 10 kDa chaperonin



- Molecule 1: 10 kDa chaperonin



- Molecule 1: 10 kDa chaperonin



- Molecule 1: 10 kDa chaperonin

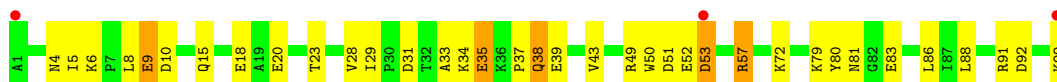


- Molecule 1: 10 kDa chaperonin





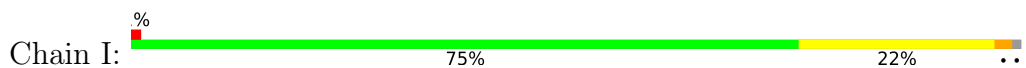
• Molecule 1: 10 kDa chaperonin



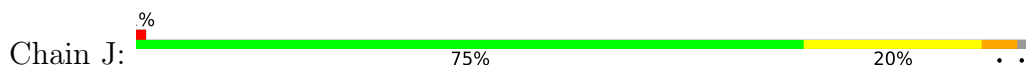
• Molecule 1: 10 kDa chaperonin



• Molecule 1: 10 kDa chaperonin



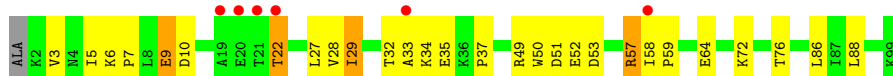
• Molecule 1: 10 kDa chaperonin



• Molecule 1: 10 kDa chaperonin

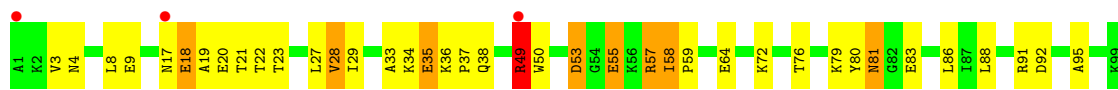


• Molecule 1: 10 kDa chaperonin



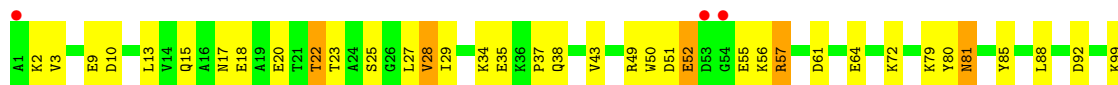
## ● Molecule 1: 10 kDa chaperonin

Chain M:  3% 61% 30% 8%



## ● Molecule 1: 10 kDa chaperonin

Chain N:  3% 63% 32% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.46Å 87.93Å 124.39Å 90.00° 106.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.80) 94.4 (29.98-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.80Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.259 , 0.280 0.250 , 0.288	Depositor DCC
$R_{free}$ test set	1900 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.1	Xtrriage
Anisotropy	0.101	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.51	0/762	0.66	0/1033
1	B	0.55	0/757	0.74	2/1026 (0.2%)
1	C	0.58	0/757	0.72	1/1026 (0.1%)
1	D	0.58	0/762	0.69	0/1033
1	E	0.54	0/757	0.70	0/1026
1	F	0.55	0/758	0.69	0/1029
1	G	0.58	0/762	0.71	0/1033
1	H	0.56	0/762	0.69	0/1033
1	I	0.58	0/753	0.67	0/1022
1	J	0.56	0/757	0.71	0/1026
1	K	0.54	0/757	0.68	0/1026
1	L	0.50	0/753	0.69	0/1022
1	M	0.58	0/762	0.73	1/1033 (0.1%)
1	N	0.57	0/762	0.69	1/1033 (0.1%)
All	All	0.56	0/10621	0.70	5/14401 (0.0%)

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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	49	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	91	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ARG	CG-CD-NE	-6.18	98.82	111.80
1	B	91	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	N	20	GLU	N-CA-C	-5.90	95.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	80	TYR	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	A	752	0	761	42	0
1	B	747	0	753	37	0
1	C	747	0	753	38	0
1	D	752	0	761	34	0
1	E	747	0	753	36	0
1	F	748	0	750	46	0
1	G	752	0	761	38	0
1	H	752	0	761	32	0
1	I	743	0	742	26	0
1	J	747	0	753	32	0
1	K	747	0	753	43	0
1	L	743	0	742	40	0
1	M	752	0	761	37	0
1	N	752	0	761	41	0
2	A	1	0	0	0	0
3	A	16	0	28	0	0
3	B	8	0	14	2	0
3	C	8	0	14	3	0
3	D	8	0	14	0	0
3	E	8	0	14	0	0
3	F	8	0	14	7	0
3	G	8	0	14	1	0
3	H	32	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	8	0	14	0	0
3	J	8	0	14	0	0
3	K	8	0	14	1	0
3	L	8	0	14	0	0
3	M	8	0	14	1	0
3	N	8	0	14	2	0
4	A	7	0	0	2	0
4	B	2	0	0	0	0
4	C	5	0	0	0	0
4	D	7	0	0	1	0
4	E	9	0	0	0	0
4	F	6	0	0	0	0
4	G	8	0	0	0	0
4	H	9	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	3	0	0	0	0
4	N	4	0	0	0	0
All	All	10690	0	10817	399	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 19.

The worst 5 of 399 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:D:33:ALA:HB3	1:N:35:GLU:CD	1.92	0.88
1:A:38:GLN:HG2	4:A:206:HOH:O	1.76	0.85
1:J:4:ASN:HD21	1:J:6:LYS:HD2	1.43	0.83
1:E:83:GLU:HA	1:E:83:GLU:OE1	1.80	0.81
1:K:81:ASN:N	1:K:81:ASN:HD22	1.78	0.81

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	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	15	44
1	B	96/99 (97%)	89 (93%)	7 (7%)	0	100	100
1	C	96/99 (97%)	91 (95%)	4 (4%)	1 (1%)	15	44
1	D	97/99 (98%)	89 (92%)	6 (6%)	2 (2%)	7	23
1	E	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
1	F	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
1	G	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	15	44
1	H	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	44
1	I	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
1	J	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
1	K	96/99 (97%)	89 (93%)	5 (5%)	2 (2%)	7	23
1	L	96/99 (97%)	90 (94%)	6 (6%)	0	100	100
1	M	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
1	N	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
All	All	1351/1386 (98%)	1281 (95%)	62 (5%)	8 (1%)	25	56

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	51	ASP
1	G	51	ASP
1	H	52	GLU
1	K	18	GLU
1	D	32	THR

### 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	81/81 (100%)	71 (88%)	10 (12%)	4	15
1	B	81/81 (100%)	78 (96%)	3 (4%)	34	68
1	C	81/81 (100%)	75 (93%)	6 (7%)	13	37
1	D	81/81 (100%)	75 (93%)	6 (7%)	13	37
1	E	81/81 (100%)	77 (95%)	4 (5%)	25	57
1	F	80/81 (99%)	72 (90%)	8 (10%)	7	22
1	G	81/81 (100%)	74 (91%)	7 (9%)	10	30
1	H	81/81 (100%)	73 (90%)	8 (10%)	8	23
1	I	80/81 (99%)	77 (96%)	3 (4%)	33	67
1	J	81/81 (100%)	76 (94%)	5 (6%)	18	47
1	K	81/81 (100%)	72 (89%)	9 (11%)	6	19
1	L	80/81 (99%)	75 (94%)	5 (6%)	18	46
1	M	81/81 (100%)	67 (83%)	14 (17%)	2	6
1	N	81/81 (100%)	73 (90%)	8 (10%)	8	23
All	All	1131/1134 (100%)	1035 (92%)	96 (8%)	10	31

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	38	GLN
1	L	29	ILE
1	J	73	TYR
1	K	79	LYS
1	M	17	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	81	ASN
1	L	4	ASN
1	K	81	ASN
1	L	15	GLN
1	E	81	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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
3	MPD	H	118	-	7,7,7	0.79	0	9,10,10	0.68	0
3	MPD	H	108	-	7,7,7	0.76	0	9,10,10	0.51	0
3	MPD	E	105	-	7,7,7	0.60	0	9,10,10	0.50	0
3	MPD	D	104	-	7,7,7	0.47	0	9,10,10	0.50	0
3	MPD	L	112	-	7,7,7	0.71	0	9,10,10	0.54	0
3	MPD	F	106	-	7,7,7	0.62	0	9,10,10	0.48	0
3	MPD	G	107	-	7,7,7	0.60	0	9,10,10	0.51	0
3	MPD	A	101	-	7,7,7	0.76	0	9,10,10	0.53	0
3	MPD	H	116	-	7,7,7	1.03	1 (14%)	9,10,10	0.69	0
3	MPD	A	115	-	7,7,7	0.74	0	9,10,10	0.51	0
3	MPD	J	110	-	7,7,7	0.76	0	9,10,10	0.60	0
3	MPD	I	109	-	7,7,7	0.78	0	9,10,10	0.48	0
3	MPD	M	113	-	7,7,7	0.85	0	9,10,10	0.56	0
3	MPD	N	114	-	7,7,7	0.91	0	9,10,10	0.52	0
3	MPD	C	103	-	7,7,7	0.59	0	9,10,10	0.48	0
3	MPD	H	117	-	7,7,7	0.69	0	9,10,10	0.74	0
3	MPD	B	102	-	7,7,7	0.74	0	9,10,10	0.52	0
3	MPD	K	111	-	7,7,7	0.45	0	9,10,10	0.49	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
3	MPD	H	118	-	-	1/5/5/5	-
3	MPD	H	108	-	-	0/5/5/5	-
3	MPD	E	105	-	-	0/5/5/5	-
3	MPD	D	104	-	-	0/5/5/5	-
3	MPD	L	112	-	-	0/5/5/5	-
3	MPD	F	106	-	-	0/5/5/5	-
3	MPD	G	107	-	-	1/5/5/5	-
3	MPD	A	101	-	-	0/5/5/5	-
3	MPD	H	116	-	-	1/5/5/5	-
3	MPD	A	115	-	-	0/5/5/5	-
3	MPD	J	110	-	-	0/5/5/5	-
3	MPD	I	109	-	-	0/5/5/5	-
3	MPD	M	113	-	-	0/5/5/5	-
3	MPD	N	114	-	-	0/5/5/5	-
3	MPD	C	103	-	-	0/5/5/5	-
3	MPD	H	117	-	-	2/5/5/5	-
3	MPD	B	102	-	-	0/5/5/5	-
3	MPD	K	111	-	-	0/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	116	MPD	CM-C2	-2.00	1.46	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	118	MPD	O2-C2-C3-C4
3	G	107	MPD	CM-C2-C3-C4
3	H	116	MPD	CM-C2-C3-C4
3	H	117	MPD	C1-C2-C3-C4
3	H	117	MPD	O2-C2-C3-C4

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	118	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	108	MPD	2	0
3	F	106	MPD	7	0
3	G	107	MPD	1	0
3	M	113	MPD	1	0
3	N	114	MPD	2	0
3	C	103	MPD	3	0
3	H	117	MPD	1	0
3	B	102	MPD	2	0
3	K	111	MPD	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	99/99 (100%)	-0.04	4 (4%) 38 28	50, 74, 103, 110	17 (17%)
1	B	98/99 (98%)	-0.17	1 (1%) 82 77	44, 68, 96, 103	5 (5%)
1	C	98/99 (98%)	-0.16	0 100 100	46, 63, 89, 96	13 (13%)
1	D	99/99 (100%)	0.00	7 (7%) 16 9	45, 77, 100, 111	16 (16%)
1	E	98/99 (98%)	0.11	3 (3%) 49 39	54, 85, 107, 119	16 (16%)
1	F	99/99 (100%)	0.06	5 (5%) 28 19	61, 86, 105, 115	14 (14%)
1	G	99/99 (100%)	-0.18	3 (3%) 50 40	49, 77, 105, 110	16 (16%)
1	H	99/99 (100%)	0.08	4 (4%) 38 28	49, 73, 95, 106	13 (13%)
1	I	98/99 (98%)	-0.17	1 (1%) 82 77	44, 66, 89, 100	10 (10%)
1	J	98/99 (98%)	-0.14	1 (1%) 82 77	46, 63, 93, 98	6 (6%)
1	K	98/99 (98%)	0.14	6 (6%) 21 13	50, 80, 105, 116	12 (12%)
1	L	98/99 (98%)	0.03	6 (6%) 21 13	56, 79, 106, 109	10 (10%)
1	M	99/99 (100%)	-0.21	3 (3%) 50 40	49, 71, 103, 107	9 (9%)
1	N	99/99 (100%)	-0.17	3 (3%) 50 40	44, 70, 97, 118	8 (8%)
All	All	1379/1386 (99%)	-0.06	47 (3%) 45 35	44, 74, 103, 119	165 (11%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1	ALA	7.2
1	G	1	ALA	4.8
1	D	33	ALA	4.5
1	D	53	ASP	4.4
1	L	20	GLU	4.4

## 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
3	MPD	H	116	8/8	0.65	0.33	97,97,98,99	8
3	MPD	J	110	8/8	0.67	0.55	86,87,89,90	8
3	MPD	H	118	8/8	0.68	0.40	83,84,85,85	8
3	MPD	H	117	8/8	0.71	0.43	88,90,91,93	8
3	MPD	N	114	8/8	0.79	0.31	84,87,88,88	0
3	MPD	A	115	8/8	0.80	0.34	90,92,92,93	0
3	MPD	M	113	8/8	0.83	0.32	89,90,91,91	0
3	MPD	F	106	8/8	0.83	0.46	95,96,96,96	0
3	MPD	G	107	8/8	0.84	0.24	84,87,88,88	0
3	MPD	E	105	8/8	0.85	0.23	88,88,89,90	0
3	MPD	A	101	8/8	0.87	0.32	90,91,91,91	0
3	MPD	C	103	8/8	0.87	0.42	85,86,87,88	8
3	MPD	D	104	8/8	0.87	0.30	87,87,88,89	0
3	MPD	H	108	8/8	0.88	0.28	83,84,84,84	8
3	MPD	K	111	8/8	0.89	0.35	88,88,90,90	0
3	MPD	L	112	8/8	0.90	0.19	87,88,90,90	0
3	MPD	I	109	8/8	0.93	0.25	84,86,88,88	0
3	MPD	B	102	8/8	0.93	0.29	87,88,90,90	0
2	CA	A	200	1/1	0.95	0.07	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.