



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:03 AM UTC

PDB ID : 1F0N / pdb_00001f0n
Title : MYCOBACTERIUM TUBERCULOSIS ANTIGEN 85B
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Deposited on : 2000-05-16
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

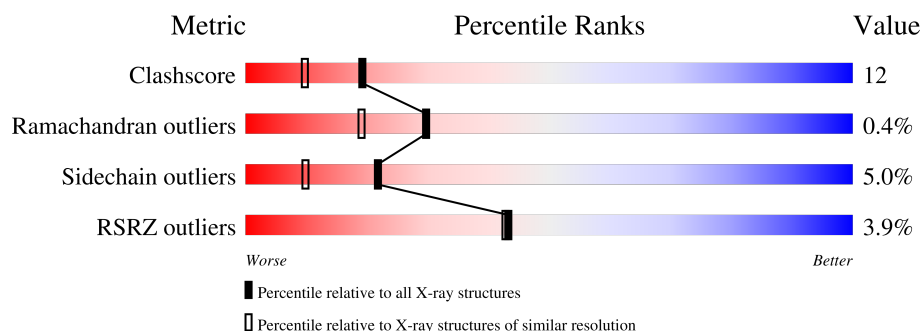
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 ≥ 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	285	

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
2	MES	A	1101	-	-	X	-
3	MPD	A	1003	X	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4414 atoms, of which 2019 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 ANTIGEN 85B.

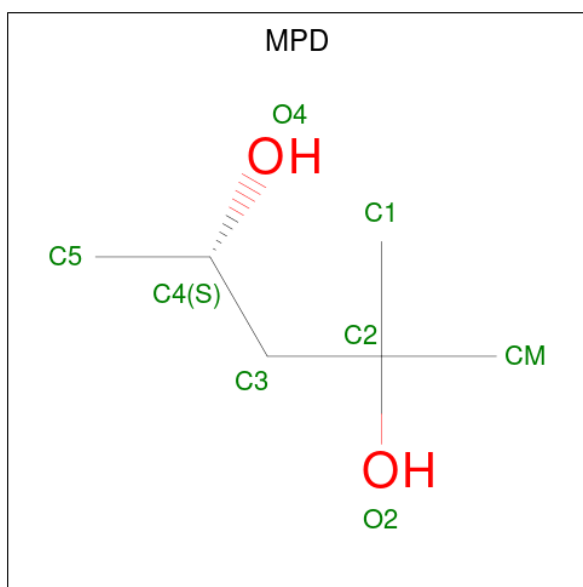
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	H	N	O	S	2019	0	0
			4173	1366	2019	363	414	11			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 6	O 2	0	0
3	A	1	Total 8	C 6	O 2	0	0
3	A	1	Total 8	C 6	O 2	0	0

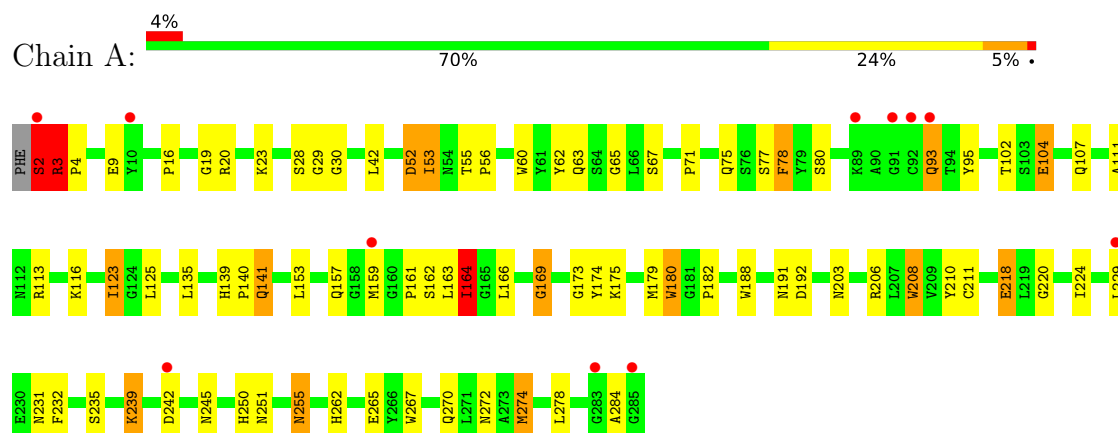
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	205	Total O 205 205	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: ANTIGEN 85B



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.21Å 73.21Å 92.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (20.00-1.80) 96.6 (20.00-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.194 , 0.276 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4414	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 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	0.84	0/2221	2.06	73/3029 (2.4%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	SER	CA-C-N	24.53	151.25	120.34
1	A	28	SER	C-N-CA	24.53	151.25	120.34
1	A	135	LEU	CA-C-O	10.88	132.08	120.55
1	A	78	PHE	CA-C-N	10.64	137.46	122.46
1	A	78	PHE	C-N-CA	10.64	137.46	122.46
1	A	232	PHE	CA-CB-CG	-9.75	104.05	113.80
1	A	211	CYS	O-C-N	8.49	133.16	123.48
1	A	56	PRO	CA-C-O	8.37	127.83	121.38
1	A	29	GLY	CA-C-N	8.05	134.68	122.85
1	A	29	GLY	C-N-CA	8.05	134.68	122.85
1	A	55	THR	O-C-N	7.85	126.73	121.71
1	A	255	ASN	CA-CB-CG	7.64	120.24	112.60
1	A	56	PRO	CA-C-N	7.63	130.84	120.54
1	A	56	PRO	C-N-CA	7.63	130.84	120.54
1	A	164	ILE	CA-C-N	-7.35	110.95	120.14
1	A	164	ILE	C-N-CA	-7.35	110.95	120.14
1	A	65	GLY	CA-C-O	7.33	127.27	119.06
1	A	278	LEU	CA-C-O	7.27	128.26	120.55
1	A	3	ARG	N-CA-CB	7.10	123.01	110.37
1	A	135	LEU	O-C-N	-7.02	114.67	122.12
1	A	245	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	A	71	PRO	O-C-N	-6.86	114.50	123.01
1	A	30	GLY	O-C-N	-6.74	116.94	123.35
1	A	2	SER	CA-C-N	-6.68	105.51	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	SER	C-N-CA	-6.68	105.51	121.80
1	A	169	GLY	O-C-N	6.59	128.52	122.19
1	A	80	SER	CA-CB-OG	-6.39	98.31	111.10
1	A	67	SER	N-CA-CB	6.36	119.81	109.95
1	A	232	PHE	CA-C-O	-6.36	114.14	120.82
1	A	174	TYR	CA-C-N	6.31	131.90	123.00
1	A	174	TYR	C-N-CA	6.31	131.90	123.00
1	A	242	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	210	TYR	CA-C-O	6.26	127.46	120.70
1	A	56	PRO	O-C-N	-6.15	113.93	122.11
1	A	192	ASP	CB-CA-C	6.14	116.25	110.17
1	A	153	LEU	O-C-N	6.13	130.01	122.34
1	A	78	PHE	O-C-N	-6.11	112.40	122.23
1	A	93	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	A	28	SER	O-C-N	-6.01	116.17	122.96
1	A	192	ASP	CA-C-O	5.97	124.37	119.36
1	A	104	GLU	CA-C-O	5.86	126.97	120.82
1	A	123	ILE	CA-C-N	-5.83	115.35	121.35
1	A	123	ILE	C-N-CA	-5.83	115.35	121.35
1	A	19	GLY	CA-C-O	5.79	126.19	119.13
1	A	28	SER	N-CA-CB	-5.75	101.55	110.29
1	A	211	CYS	CA-C-O	-5.69	113.72	120.43
1	A	232	PHE	O-C-N	5.69	127.93	122.07
1	A	224	ILE	N-CA-CB	-5.67	106.93	110.50
1	A	174	TYR	CA-C-O	-5.66	115.27	121.89
1	A	75	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	A	255	ASN	OD1-CG-ND2	5.60	128.20	122.60
1	A	265	GLU	CB-CG-CD	5.58	122.08	112.60
1	A	231	ASN	O-C-N	5.57	128.50	122.15
1	A	180	TRP	O-C-N	5.57	128.93	122.19
1	A	208	TRP	CA-C-O	5.51	126.19	120.40
1	A	113	ARG	CD-NE-CZ	5.42	131.99	124.40
1	A	52	ASP	N-CA-C	-5.42	105.46	111.36
1	A	224	ILE	O-C-N	5.41	123.91	120.07
1	A	191	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	159	MET	CA-C-N	-5.38	113.42	121.87
1	A	159	MET	C-N-CA	-5.38	113.42	121.87
1	A	182	PRO	O-C-N	-5.38	116.40	122.91
1	A	203	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	A	67	SER	O-C-N	5.32	129.27	123.04
1	A	9	GLU	O-C-N	5.32	129.96	123.10
1	A	20	ARG	CA-C-N	-5.27	114.75	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ARG	C-N-CA	-5.27	114.75	122.19
1	A	278	LEU	O-C-N	-5.20	116.61	122.12
1	A	111	ALA	CA-C-O	-5.15	115.09	120.55
1	A	53	ILE	N-CA-C	5.14	115.35	110.42
1	A	262	HIS	CA-CB-CG	5.05	118.85	113.80
1	A	42	LEU	N-CA-C	5.03	117.42	111.33
1	A	220	GLY	O-C-N	5.01	127.61	122.85

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	2154	2019	2018	44	0
2	A	12	0	13	8	0
3	A	24	0	42	18	0
4	A	205	0	0	8	0
All	All	2395	2019	2073	50	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 12.

All (50) 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:141:GLN:H	3:A:1003:MPD:H13	1.36	0.91
1:A:206:ARG:HH12	2:A:1101:MES:H82	1.41	0.85
1:A:270:GLN:O	1:A:274:MET:HG3	1.85	0.76
1:A:141:GLN:HB2	3:A:1003:MPD:HM3	1.68	0.75
1:A:162:SER:O	1:A:166:LEU:HD23	1.88	0.72
3:A:1003:MPD:H11	4:A:565:HOH:O	1.90	0.72
1:A:2:SER:HB2	1:A:4:PRO:O	1.92	0.70
1:A:157:GLN:HG3	4:A:527:HOH:O	1.95	0.65
1:A:251:ASN:HA	2:A:1101:MES:H72	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:NH1	2:A:1101:MES:H82	2.13	0.60
2:A:1101:MES:O3S	2:A:1101:MES:H32	2.01	0.59
2:A:1101:MES:H22	4:A:556:HOH:O	2.04	0.57
1:A:141:GLN:H	3:A:1003:MPD:C1	2.13	0.56
1:A:123:ILE:HD13	1:A:274:MET:HE1	1.85	0.56
3:A:1003:MPD:H53	4:A:504:HOH:O	2.06	0.56
1:A:102:THR:HG21	1:A:139:HIS:CD2	2.42	0.55
1:A:208:TRP:CE2	1:A:274:MET:HG2	2.41	0.54
1:A:139:HIS:HA	3:A:1003:MPD:H12	1.89	0.54
1:A:116:LYS:HE3	4:A:503:HOH:O	2.08	0.53
1:A:235:SER:O	1:A:239:LYS:HG3	2.09	0.52
1:A:16:PRO:HD2	1:A:104:GLU:CD	2.35	0.51
1:A:53:ILE:HG12	3:A:1002:MPD:HM1	1.92	0.51
1:A:3:ARG:HD2	4:A:462:HOH:O	2.09	0.51
1:A:218:GLU:H	1:A:218:GLU:CD	2.18	0.50
1:A:141:GLN:N	3:A:1003:MPD:H13	2.17	0.49
1:A:60:TRP:CH2	1:A:272:ASN:HB2	2.48	0.48
1:A:53:ILE:HA	3:A:1002:MPD:O2	2.13	0.48
1:A:179:MET:HE3	1:A:180:TRP:CD2	2.49	0.48
1:A:78:PHE:CZ	1:A:164:ILE:HD13	2.48	0.48
1:A:141:GLN:CB	3:A:1003:MPD:HM3	2.43	0.47
1:A:179:MET:HG2	1:A:180:TRP:CD1	2.49	0.47
3:A:1003:MPD:HM1	3:A:1003:MPD:H52	1.97	0.47
1:A:140:PRO:HD2	3:A:1003:MPD:H12	1.97	0.47
1:A:3:ARG:HH21	3:A:1002:MPD:C4	2.27	0.47
1:A:141:GLN:CB	3:A:1003:MPD:H13	2.45	0.46
1:A:52:ASP:O	3:A:1002:MPD:O4	2.30	0.46
1:A:163:LEU:HB3	3:A:1001:MPD:H51	1.97	0.46
1:A:206:ARG:HH12	2:A:1101:MES:C8	2.19	0.45
1:A:77:SER:HB3	1:A:95:TYR:CE2	2.52	0.45
1:A:93:GLN:NE2	4:A:586:HOH:O	2.50	0.44
1:A:125:LEU:HD13	1:A:267:TRP:CE3	2.53	0.44
1:A:169:GLY:O	1:A:173:GLY:HA2	2.17	0.44
1:A:62:TYR:O	1:A:63:GLN:HB2	2.18	0.43
1:A:23:LYS:HD3	4:A:550:HOH:O	2.18	0.43
1:A:141:GLN:HG2	3:A:1003:MPD:HM3	2.01	0.43
2:A:1101:MES:H82	2:A:1101:MES:H31	1.88	0.42
1:A:78:PHE:CE2	1:A:164:ILE:HD13	2.54	0.42
1:A:250:HIS:O	2:A:1101:MES:H72	2.20	0.42
1:A:141:GLN:HG2	3:A:1003:MPD:CM	2.51	0.41
1:A:161:PRO:HA	1:A:188:TRP:CZ3	2.56	0.40

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	282/285 (99%)	270 (96%)	11 (4%)	1 (0%)	30 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	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	221/222 (100%)	210 (95%)	11 (5%)	22 10

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	ARG
1	A	107	GLN
1	A	141	GLN
1	A	164	ILE
1	A	175	LYS
1	A	218	GLU

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Mol	Chain	Res	Type
1	A	229	LEU
1	A	239	LYS
1	A	255	ASN
1	A	274	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	141	GLN
1	A	237	ASN
1	A	241	GLN
1	A	250	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	MPD	A	1003	-	7,7,7	0.37	0	9,10,10	0.55	0
3	MPD	A	1001	-	7,7,7	0.28	0	9,10,10	0.32	0
2	MES	A	1101	-	12,12,12	1.06	1 (8%)	15,16,16	0.77	0
3	MPD	A	1002	-	7,7,7	0.26	0	9,10,10	0.33	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	A	1002	-	-	1/5/5/5	-
3	MPD	A	1001	-	-	0/5/5/5	-
2	MES	A	1101	-	-	2/6/14/14	0/1/1/1
3	MPD	A	1003	-	1/1/2/2	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	MES	C5-N4	2.02	1.52	1.46

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1003	MPD	C4

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MES	C8-C7-N4-C3
2	A	1101	MES	C8-C7-N4-C5
3	A	1003	MPD	CM-C2-C3-C4
3	A	1002	MPD	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	MPD	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	MPD	1	0
2	A	1101	MES	8	0
3	A	1002	MPD	4	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, 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	284/285 (99%)	0.51	11 (3%) 43 43	8, 14, 23, 57	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	4.1
1	A	159	MET	3.4
1	A	93	GLN	2.6
1	A	91	GLY	2.4
1	A	2	SER	2.4
1	A	10	TYR	2.2
1	A	283	GLY	2.1
1	A	92	CYS	2.1
1	A	229	LEU	2.1
1	A	89	LYS	2.0
1	A	242	ASP	2.0

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 oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	A	1101	12/12	0.57	0.20	61,86,121,129	0
3	MPD	A	1002	8/8	0.74	0.25	30,56,70,83	0
3	MPD	A	1001	8/8	0.86	0.11	35,40,46,49	0
3	MPD	A	1003	8/8	0.88	0.16	25,40,79,90	0

6.5 Other polymers ⓘ

There are no such residues in this entry.