



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:17 AM GMT

PDB ID : 2RJC  
Title : Crystal structure of L3MBTL1 protein in complex with MES  
Authors : Allali-Hassani, A.; Liu, Y.; Herzanych, N.; Ouyang, H.; Mackenzie, F.; Crombet, L.; Loppnau, P.; Kozieradzki, I.; Vedadi, M.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Min, J.R.; Structural Genomics Consortium (SGC)  
Deposited on : 2007-10-14  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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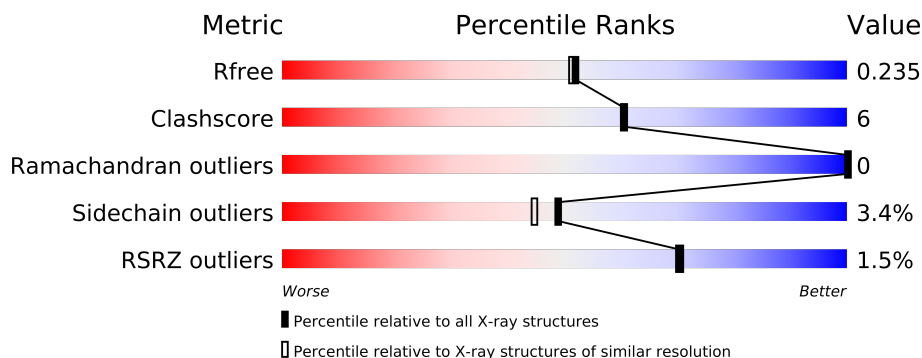
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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  $\geq 3$ , 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	331	
1	B	331	
1	C	331	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	MES	C	603	-	X
3	MES	C	606	-	X

## 2 Entry composition

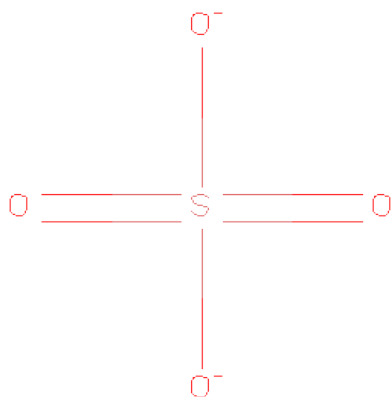
There are 4 unique types of molecules in this entry. The entry contains 8433 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lethal(3)malignant brain tumor-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2545	1638	432	463	12			
1	B	314	Total	C	N	O	S	0	2	0
			2568	1650	443	462	13			
1	C	306	Total	C	N	O	S	0	0	0
			2484	1602	423	447	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



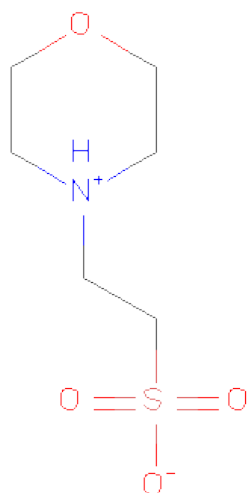
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	263	Total	O	0	0
			263	263		

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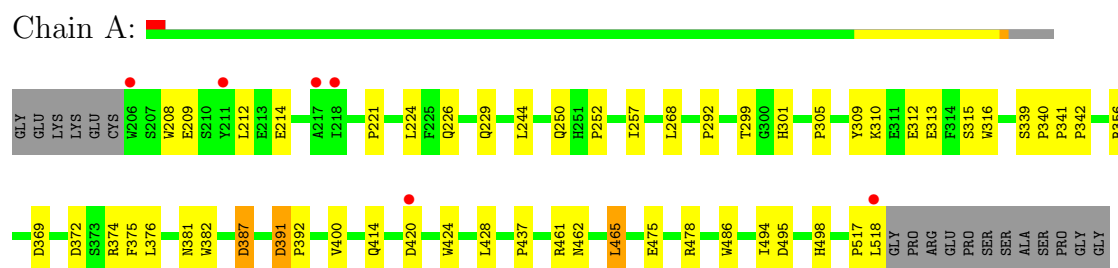
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	262	Total 262	O 262	0	0
4	C	214	Total 214	O 214	0	0

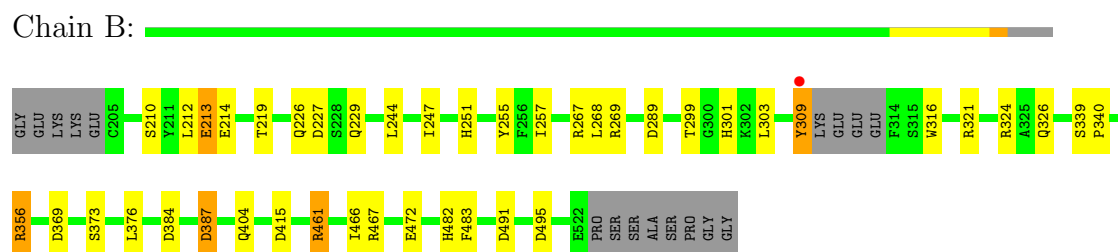
### 3 Residue-property plots

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.

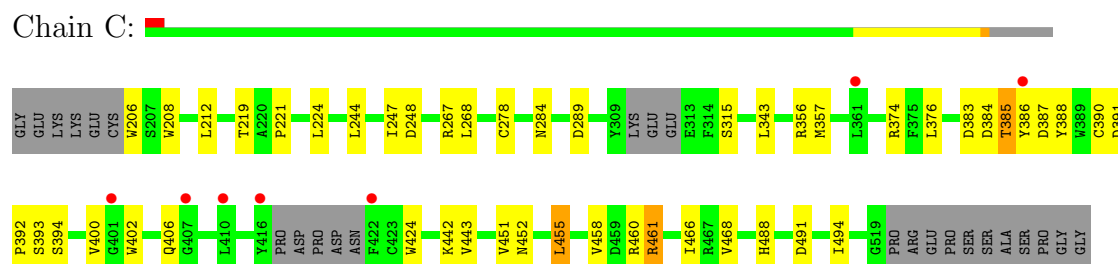
- Molecule 1: Lethal(3)malignant brain tumor-like protein



- Molecule 1: Lethal(3)malignant brain tumor-like protein



- Molecule 1: Lethal(3)malignant brain tumor-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.55Å 108.78Å 90.35Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	90.17 – 2.00 47.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.17-2.00) 99.7 (47.18-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.195 , 0.241 0.191 , 0.235	Depositor DCC
$R_{free}$ test set	4116 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.6	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 82166 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: SO4, MES

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	0.97	0/2644	0.83	2/3614 (0.1%)
1	B	0.94	1/2667 (0.0%)	0.90	5/3643 (0.1%)
1	C	0.92	1/2579 (0.0%)	0.79	4/3521 (0.1%)
All	All	0.94	2/7890 (0.0%)	0.84	11/10778 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	278	CYS	CB-SG	5.67	1.91	1.82
1	B	255	TYR	CD1-CE1	5.15	1.47	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ARG	NE-CZ-NH2	-19.55	110.53	120.30
1	B	269	ARG	NE-CZ-NH1	17.06	128.83	120.30
1	C	455	LEU	CA-CB-CG	7.84	133.33	115.30
1	B	269	ARG	CD-NE-CZ	6.67	132.94	123.60
1	C	455	LEU	CB-CG-CD1	6.34	121.78	111.00
1	B	387	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	387	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	461	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	391	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	374	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	ASP	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	2545	0	2380	29	0
1	B	2568	0	2406	29	0
1	C	2484	0	2328	29	0
2	A	10	0	0	0	0
2	B	10	0	0	2	0
2	C	5	0	0	0	0
3	A	24	0	24	1	0
3	B	12	0	12	0	0
3	C	36	0	36	5	0
4	A	263	0	0	3	1
4	B	262	0	0	3	1
4	C	214	0	0	0	0
All	All	8433	0	7186	87	1

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 6.

All (87) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:257:ILE:HD11	1:B:303:LEU:HD21	1.19	1.10
1:B:301:HIS:HE1	1:B:369:ASP:OD1	1.51	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:257:ILE:CD1	1:B:303:LEU:HD21	2.03	0.86
1:B:482:HIS:HE1	2:B:611:SO4:O3	1.63	0.81
1:A:301:HIS:HE1	1:A:369:ASP:OD1	1.63	0.81
1:C:248:ASP:OD2	3:C:603:MES:H72	1.83	0.76
1:A:299:THR:OG1	1:A:301:HIS:HD2	1.70	0.73
1:C:248:ASP:OD2	3:C:603:MES:C7	2.37	0.71
1:C:212:LEU:HD11	1:C:219:THR:HG23	1.73	0.69
1:B:226:GLN:H	1:B:229:GLN:NE2	1.95	0.65
1:C:451:VAL:O	1:C:452:ASN:HB2	1.98	0.62
1:B:472:GLU:OE2	1:C:461:ARG:HG2	2.00	0.62
1:C:460:ARG:NH1	1:C:494:ILE:HD12	2.16	0.60
1:B:356:ARG:NH1	1:B:495:ASP:OD2	2.31	0.59
1:C:206:TRP:CD1	3:C:606:MES:H51	2.38	0.59
1:B:301:HIS:CE1	1:B:369:ASP:OD1	2.44	0.59
1:C:460:ARG:HH11	1:C:494:ILE:HD12	1.68	0.59
1:A:374:ARG:NH1	4:A:736:HOH:O	2.06	0.59
1:B:212:LEU:HD11	1:B:219:THR:HG23	1.86	0.57
3:C:603:MES:O3S	3:C:603:MES:H32	2.05	0.57
1:C:488:HIS:HD2	1:C:491:ASP:OD2	1.88	0.56
1:C:221:PRO:HD2	1:C:224:LEU:CD1	2.35	0.56
1:A:226:GLN:H	1:A:229:GLN:NE2	2.04	0.56
1:A:209:GLU:HB2	4:A:828:HOH:O	2.05	0.56
1:B:482:HIS:HD2	1:B:491:ASP:OD1	1.89	0.55
1:B:321:ARG:O	1:B:324:ARG:NH1	2.38	0.55
1:B:226:GLN:H	1:B:229:GLN:HE21	1.55	0.55
1:C:383:ASP:OD1	1:C:385:THR:HB	2.06	0.54
1:B:461:ARG:HD3	1:B:461:ARG:N	2.21	0.54
1:B:214:GLU:HG3	4:B:1007:HOH:O	2.07	0.54
1:C:376:LEU:HD11	1:C:387:ASP:HB3	1.89	0.54
1:B:257:ILE:HD12	1:B:316:TRP:CZ2	2.42	0.54
1:A:517:PRO:O	1:A:518:LEU:HG	2.10	0.52
1:B:321:ARG:NH2	4:B:999:HOH:O	2.20	0.51
1:A:226:GLN:H	1:A:229:GLN:HE21	1.58	0.51
1:B:210:SER:O	1:B:213:GLU:HG3	2.11	0.51
1:A:517:PRO:C	1:A:518:LEU:HG	2.31	0.50
1:C:248:ASP:OD2	3:C:603:MES:H71	2.10	0.50
1:C:460:ARG:NH1	1:C:494:ILE:CD1	2.75	0.50
1:A:391:ASP:HB2	1:A:392:PRO:CD	2.42	0.50
1:C:393:SER:HA	1:C:442:LYS:O	2.12	0.50
1:C:212:LEU:HD11	1:C:219:THR:CG2	2.41	0.50
1:C:221:PRO:HD2	1:C:224:LEU:HD11	1.92	0.50
1:B:299:THR:OG1	1:B:301:HIS:HD2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:ARG:NH1	1:A:495:ASP:OD2	2.36	0.49
1:A:257:ILE:HD12	1:A:316:TRP:CZ2	2.48	0.49
1:A:310:LYS:HG2	1:A:313:GLU:OE1	2.13	0.48
1:C:356:ARG:HG2	1:C:388:TYR:CE2	2.48	0.48
1:A:301:HIS:CE1	1:A:369:ASP:OD1	2.54	0.48
1:B:339:SER:HB2	1:B:340:PRO:HD2	1.96	0.48
1:A:341:PRO:HA	1:A:372:ASP:O	2.13	0.48
1:C:391:ASP:HB2	1:C:392:PRO:HD2	1.95	0.47
1:A:376:LEU:HD11	1:A:387:ASP:HB3	1.95	0.47
1:C:390:CYS:HB2	1:C:394:SER:HB2	1.96	0.47
1:C:267:ARG:HG2	1:C:284:ASN:HD22	1.79	0.47
1:C:402:TRP:O	1:C:406:GLN:HG2	2.14	0.47
1:A:462:ASN:ND2	1:A:465:LEU:CD2	2.78	0.47
1:C:247:ILE:HG12	1:C:289:ASP:HB3	1.96	0.47
1:A:339:SER:HB2	1:A:340:PRO:HD2	1.96	0.46
1:B:251:HIS:HD2	1:B:384:ASP:OD1	1.99	0.46
1:B:482:HIS:CE1	2:B:611:SO4:O3	2.54	0.46
1:A:221:PRO:HD2	1:A:224:LEU:HD22	1.97	0.46
1:B:376:LEU:HD11	1:B:387:ASP:HB3	1.99	0.45
1:A:486:TRP:CE3	3:A:602:MES:H51	2.52	0.45
1:A:400:VAL:HG13	1:A:424:TRP:CG	2.52	0.44
1:A:208:TRP:O	1:A:212:LEU:HG	2.18	0.44
1:C:391:ASP:HB2	1:C:392:PRO:CD	2.48	0.43
1:A:342:PRO:HG3	1:A:375:PHE:HD2	1.82	0.43
1:C:357:MET:HG3	1:C:386:TYR:CD1	2.53	0.43
1:B:373:SER:HB3	4:B:1033:HOH:O	2.18	0.43
1:A:305:PRO:HB2	1:A:309:TYR:HB2	2.01	0.43
1:C:400:VAL:HG13	1:C:424:TRP:CG	2.54	0.42
1:C:458:VAL:HG22	1:C:466:ILE:HG12	2.00	0.42
1:B:309:TYR:CD2	1:B:309:TYR:C	2.93	0.42
1:A:382:TRP:CE2	1:A:414:GLN:HB2	2.55	0.42
1:B:247:ILE:HG12	1:B:289:ASP:HB3	2.02	0.42
1:A:461:ARG:NH1	4:A:712:HOH:O	2.52	0.41
1:A:381:ASN:N	1:A:381:ASN:HD22	2.17	0.41
1:B:309:TYR:HD2	1:B:309:TYR:C	2.24	0.41
1:A:391:ASP:HB2	1:A:392:PRO:HD2	2.01	0.41
1:A:475:GLU:OE1	1:A:478:ARG:HD3	2.20	0.41
1:C:208:TRP:CH2	1:C:468:VAL:HG13	2.55	0.41
1:A:494:ILE:HD11	1:A:498:HIS:CG	2.56	0.41
1:B:226:GLN:N	1:B:229:GLN:HE21	2.19	0.41
1:C:400:VAL:HG22	1:C:424:TRP:CZ2	2.56	0.40
1:B:267:ARG:HD2	1:B:466:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:467:ARG:HB2	1:B:483:PHE:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:869:HOH:O	4:B:809:HOH:O[2_756]	1.91	0.29

## 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	311/331 (94%)	304 (98%)	7 (2%)	0	100	100
1	B	312/331 (94%)	308 (99%)	4 (1%)	0	100	100
1	C	300/331 (91%)	292 (97%)	8 (3%)	0	100	100
All	All	923/993 (93%)	904 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	277/290 (96%)	266 (96%)	11 (4%)	42	36
1	B	279/290 (96%)	270 (97%)	9 (3%)	51	47
1	C	269/290 (93%)	261 (97%)	8 (3%)	53	50
All	All	825/870 (95%)	797 (97%)	28 (3%)	49	45

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLU
1	A	244	LEU
1	A	250	GLN
1	A	252	PRO
1	A	268	LEU
1	A	292	PRO
1	A	312	GLU
1	A	315	SER
1	A	428	LEU
1	A	437	PRO
1	A	465	LEU
1	B	213	GLU
1	B	244	LEU
1	B	268	LEU
1	B	309	TYR
1	B	326	GLN
1	B	356	ARG
1	B	404	GLN
1	B	415	ASP
1	B	461	ARG
1	C	244	LEU
1	C	268	LEU
1	C	315	SER
1	C	343	LEU
1	C	384	ASP
1	C	385	THR
1	C	443	VAL
1	C	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	301	HIS
1	A	331	HIS
1	A	381	ASN
1	A	488	HIS
1	B	229	GLN
1	B	251	HIS
1	B	301	HIS
1	B	304	GLN

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Mol	Chain	Res	Type
1	B	482	HIS
1	C	251	HIS
1	C	284	ASN
1	C	326	GLN
1	C	488	HIS
1	C	515	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

11 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	MES	A	601	-	12,12,12	1.39	1 (8%)	16,16,16	2.72	6 (37%)
3	MES	A	602	-	12,12,12	1.89	2 (16%)	16,16,16	2.71	8 (50%)
2	SO4	A	607	-	4,4,4	0.36	0	6,6,6	0.88	0
2	SO4	A	609	-	4,4,4	0.19	0	6,6,6	0.47	0
3	MES	B	604	-	12,12,12	1.97	2 (16%)	16,16,16	2.69	3 (18%)
2	SO4	B	608	-	4,4,4	0.48	0	6,6,6	0.16	0
2	SO4	B	611	-	4,4,4	0.20	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MES	C	603	-	12,12,12	2.12	2 (16%)	16,16,16	3.04	7 (43%)
3	MES	C	605	-	12,12,12	1.87	2 (16%)	16,16,16	2.75	6 (37%)
3	MES	C	606	-	12,12,12	1.92	2 (16%)	16,16,16	2.09	4 (25%)
2	SO4	C	610	-	4,4,4	0.11	0	6,6,6	0.47	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	MES	A	601	-	-	0/6/14/14	0/1/1/1
3	MES	A	602	-	-	0/6/14/14	0/1/1/1
2	SO4	A	607	-	-	0/0/0/0	0/0/0/0
2	SO4	A	609	-	-	0/0/0/0	0/0/0/0
3	MES	B	604	-	-	0/6/14/14	0/1/1/1
2	SO4	B	608	-	-	0/0/0/0	0/0/0/0
2	SO4	B	611	-	-	0/0/0/0	0/0/0/0
3	MES	C	603	-	-	0/6/14/14	1/1/1/1
3	MES	C	605	-	-	0/6/14/14	0/1/1/1
3	MES	C	606	-	-	0/6/14/14	0/1/1/1
2	SO4	C	610	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	MES	C8-S	-6.08	1.67	1.78
3	B	604	MES	C8-S	-5.51	1.68	1.78
3	C	606	MES	C8-S	-5.35	1.68	1.78
3	C	605	MES	C8-S	-5.20	1.69	1.78
3	A	602	MES	C8-S	-4.74	1.69	1.78
3	A	601	MES	C8-S	-4.01	1.71	1.78
3	C	605	MES	O2S-S	2.58	1.51	1.45
3	A	602	MES	O3S-S	2.58	1.51	1.45
3	B	604	MES	O2S-S	2.53	1.51	1.45
3	C	603	MES	O1S-S	2.05	1.50	1.45
3	C	606	MES	O2S-S	2.01	1.50	1.45

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	MES	C5-N4-C3	8.06	125.73	109.75
3	C	605	MES	C5-N4-C3	8.03	125.67	109.75
3	A	601	MES	C5-N4-C3	7.76	125.14	109.75
3	A	602	MES	C5-N4-C3	7.43	124.49	109.75
3	C	603	MES	C6-C5-N4	-6.81	101.23	109.96
3	C	603	MES	C5-N4-C3	6.11	121.87	109.75
3	C	606	MES	C5-N4-C3	5.88	121.42	109.75
3	C	603	MES	O1-C2-C3	-4.86	105.55	111.34
3	B	604	MES	O1-C2-C3	4.81	117.07	111.34
3	A	602	MES	C6-C5-N4	4.10	115.22	109.96
3	A	601	MES	O2S-S-O1S	-3.99	104.73	112.44
3	B	604	MES	C7-N4-C5	3.92	121.90	111.66
3	C	605	MES	O1-C2-C3	-3.66	106.98	111.34
3	C	603	MES	C7-N4-C3	3.56	120.95	111.66
3	C	605	MES	C2-C3-N4	3.39	114.31	109.96
3	C	605	MES	C7-N4-C5	3.17	119.94	111.66
3	A	601	MES	C7-N4-C3	3.09	119.72	111.66
3	C	606	MES	C7-N4-C5	3.01	119.53	111.66
3	C	606	MES	C7-N4-C3	2.83	119.05	111.66
3	C	603	MES	C2-C3-N4	-2.79	106.38	109.96
3	A	601	MES	O3S-S-O1S	2.75	119.56	112.48
3	A	602	MES	O3S-S-C8	2.66	112.85	105.99
3	A	601	MES	O1-C6-C5	-2.66	108.18	111.34
3	C	606	MES	C8-C7-N4	-2.64	107.93	112.44
3	C	605	MES	C8-C7-N4	2.61	116.91	112.44
3	A	602	MES	C2-C3-N4	2.56	113.25	109.96
3	A	602	MES	C7-N4-C3	2.55	118.34	111.66
3	A	601	MES	C8-C7-N4	2.49	116.70	112.44
3	C	605	MES	O1-C6-C5	-2.46	108.41	111.34
3	C	603	MES	C8-C7-N4	-2.11	108.82	112.44
3	C	603	MES	C7-N4-C5	2.11	117.17	111.66
3	A	602	MES	C7-C8-S	2.08	118.16	112.49
3	A	602	MES	C7-N4-C5	2.08	117.09	111.66
3	A	602	MES	C6-O1-C2	2.03	116.84	109.90

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	603	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, 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	313/331 (94%)	0.00	6 (1%) 64 64	13, 23, 38, 46	0
1	B	314/331 (94%)	-0.05	1 (0%) 91 93	16, 22, 35, 44	0
1	C	306/331 (92%)	0.01	7 (2%) 57 57	14, 27, 40, 47	0
All	All	933/993 (93%)	-0.01	14 (1%) 70 70	13, 24, 38, 47	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	416	TYR	3.5
1	A	518	LEU	3.3
1	A	218	ILE	2.9
1	A	206	TRP	2.8
1	C	422	PHE	2.7
1	A	211	TYR	2.6
1	A	217	ALA	2.4
1	A	420	ASP	2.4
1	C	401	GLY	2.3
1	C	361	LEU	2.2
1	C	410	LEU	2.2
1	C	386	TYR	2.1
1	C	407	GLY	2.1
1	B	309	TYR	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MES	C	606	12/12	0.18	4.52	57,59,67,69	0
3	MES	C	603	12/12	0.23	2.57	61,69,86,86	0
3	MES	B	604	12/12	0.14	1.95	26,31,42,42	0
2	SO4	B	611	5/5	0.15	1.53	46,50,51,51	0
3	MES	C	605	12/12	0.13	1.48	32,35,39,40	0
2	SO4	A	609	5/5	0.20	0.55	45,45,49,50	0
3	MES	A	602	12/12	0.14	0.51	40,45,58,61	0
3	MES	A	601	12/12	0.11	0.51	18,21,30,30	0
2	SO4	B	608	5/5	0.10	-0.26	47,48,51,52	0
2	SO4	A	607	5/5	0.09	-0.57	44,51,53,54	0
2	SO4	C	610	5/5	0.09	-1.32	48,49,52,52	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.