



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 02:21 PM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

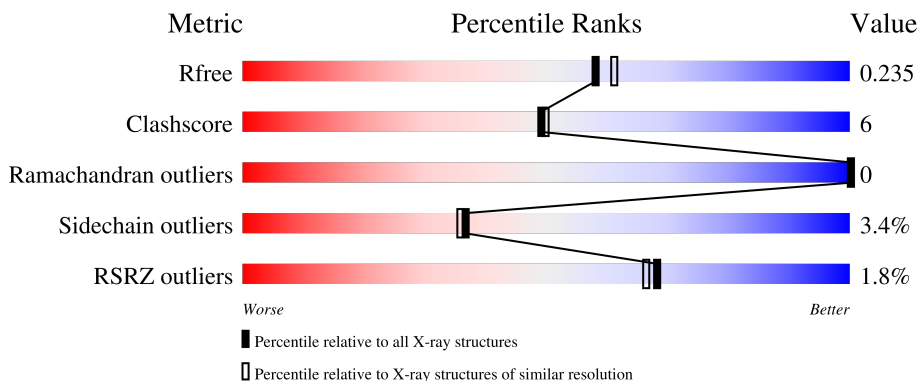
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	331	 3% 78% 16% • 5%
1	B	331	 82% 11% • 5%
1	C	331	 2% 78% 14% • 8%

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	SO4	B	611	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8433 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 Lethal(3)malignant brain tumor-like protein.

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

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



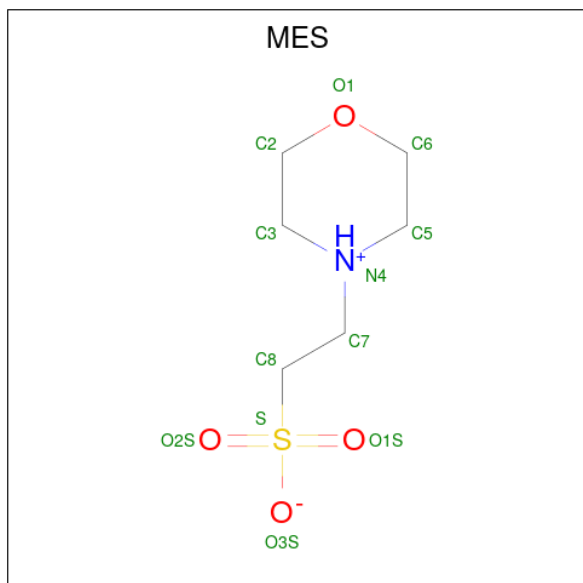
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

Continued on next page...

Continued from previous page...

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)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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		

Continued on next page...

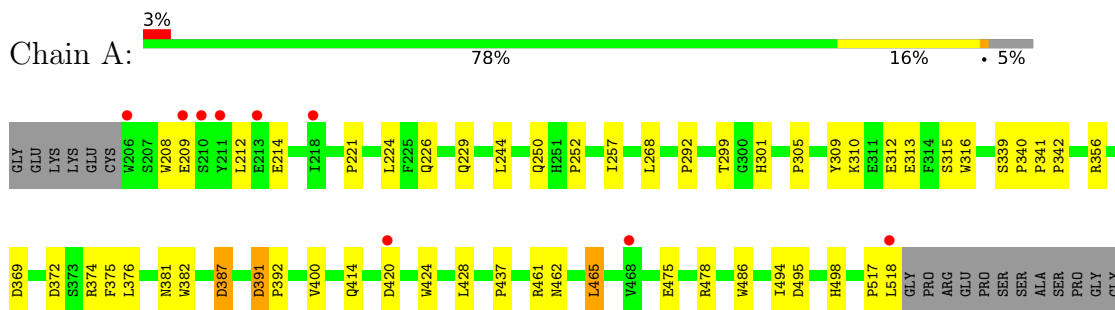
Continued from previous page...

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

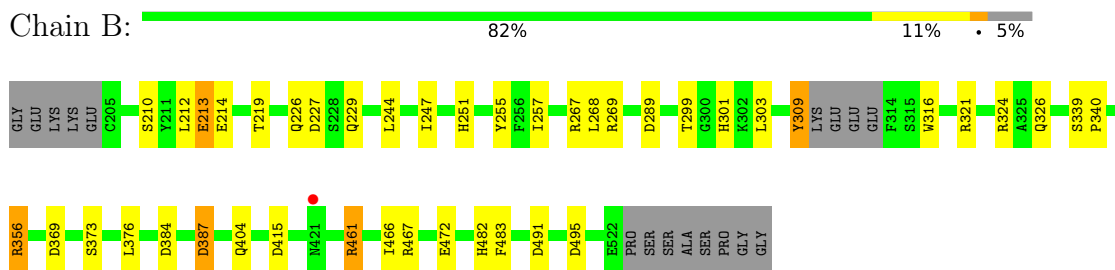
3 Residue-property plots [i](#)

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.

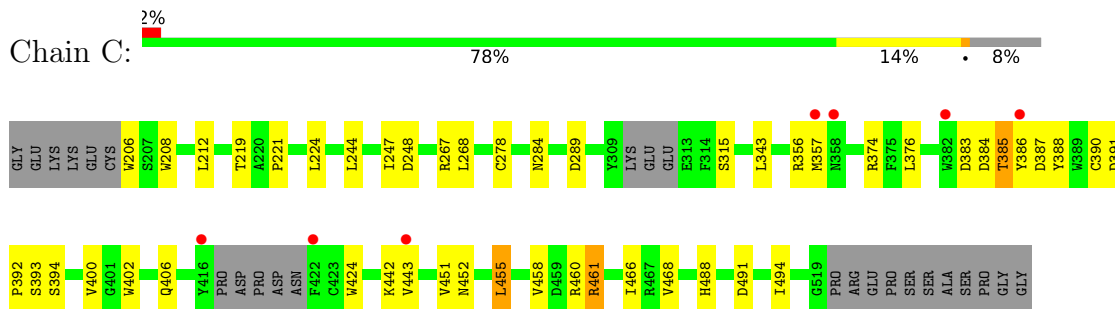
- Molecule 1: Lethal(3)malignant brain tumor-like protein



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.241 0.190 , 0.235	Depositor DCC
R_{free} test set	4116 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtrriage
Anisotropy	0.029	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8433	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage'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.*

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 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

Continued on next page...

Continued from previous page...

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 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	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

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 6.

All (87) 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:B:257:ILE:HD11	1:B:303:LEU:HD21	1.19	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:HIS:HE1	1:B:369:ASP:OD1	1.51	0.92
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:221:PRO:HD2	1:C:224:LEU:CD1	2.35	0.56
1:C:488:HIS:HD2	1:C:491:ASP:OD2	1.88	0.56
1:A:209:GLU:HB2	4:A:828:HOH:O	2.05	0.56
1:A:226:GLN:H	1:A:229:GLN:NE2	2.04	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:N	1:B:461:ARG:HD3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:376:LEU:HD11	1:A:387:ASP:HB3	1.95	0.47
1:C:391:ASP:HB2	1:C:392:PRO:HD2	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:A:462:ASN:ND2	1:A:465:LEU:CD2	2.78	0.47
1:C:402:TRP:O	1:C:406:GLN:HG2	2.14	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:C	1:B:309:TYR:CD2	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:381:ASN:HD22	1:A:381:ASN:N	2.17	0.41
1:A:461:ARG:NH1	4:A:712:HOH:O	2.52	0.41
1:B:309:TYR:C	1:B:309:TYR:HD2	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:A:494:ILE:HD11	1:A:498:HIS:CG	2.56	0.41
1:C:208:TRP:CH2	1:C:468:VAL:HG13	2.55	0.41

Continued on next page...

Continued from previous page...

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

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	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 [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	277/290 (96%)	266 (96%)	11 (4%)	31	29
1	B	279/290 (96%)	270 (97%)	9 (3%)	39	38
1	C	269/290 (93%)	261 (97%)	8 (3%)	41	41
All	All	825/870 (95%)	797 (97%)	28 (3%)	37	36

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

Sometimes 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 [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](#)

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	602	-	12,12,12	1.81	1 (8%)	14,16,16	2.90	9 (64%)
2	SO4	B	611	-	4,4,4	0.16	0	6,6,6	0.57	0
3	MES	C	603	-	12,12,12	2.19	1 (8%)	14,16,16	2.92	8 (57%)
3	MES	B	604	-	12,12,12	1.99	2 (16%)	14,16,16	2.65	4 (28%)
3	MES	C	605	-	12,12,12	1.91	2 (16%)	14,16,16	2.60	4 (28%)
3	MES	A	601	-	12,12,12	1.46	1 (8%)	14,16,16	2.61	4 (28%)
2	SO4	A	609	-	4,4,4	0.25	0	6,6,6	0.80	0
3	MES	C	606	-	12,12,12	1.94	1 (8%)	14,16,16	2.27	4 (28%)
2	SO4	B	608	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	A	607	-	4,4,4	0.25	0	6,6,6	0.87	0
2	SO4	C	610	-	4,4,4	0.18	0	6,6,6	0.35	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	C	603	-	-	2/6/14/14	0/1/1/1
3	MES	C	605	-	-	2/6/14/14	0/1/1/1
3	MES	A	601	-	-	1/6/14/14	0/1/1/1
3	MES	C	606	-	-	4/6/14/14	0/1/1/1
3	MES	A	602	-	-	5/6/14/14	0/1/1/1
3	MES	B	604	-	-	1/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	MES	C8-S	-7.07	1.67	1.77
3	B	604	MES	C8-S	-6.36	1.68	1.77
3	C	606	MES	C8-S	-6.15	1.68	1.77
3	C	605	MES	C8-S	-5.96	1.69	1.77
3	A	602	MES	C8-S	-5.40	1.69	1.77
3	A	601	MES	C8-S	-4.48	1.71	1.77
3	C	605	MES	O2S-S	2.21	1.51	1.45
3	B	604	MES	O2S-S	2.17	1.51	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	MES	C5-N4-C3	7.51	125.73	108.83
3	C	605	MES	C5-N4-C3	7.48	125.67	108.83
3	A	601	MES	C5-N4-C3	7.25	125.14	108.83
3	A	602	MES	C5-N4-C3	6.96	124.49	108.83
3	C	603	MES	C6-C5-N4	-5.85	101.23	110.10
3	C	603	MES	C5-N4-C3	5.79	121.87	108.83
3	C	606	MES	C5-N4-C3	5.59	121.42	108.83
3	A	602	MES	O3S-S-C8	4.38	112.85	105.77
3	B	604	MES	C7-N4-C5	4.17	121.90	111.23
3	C	603	MES	C7-N4-C3	3.80	120.95	111.23
3	C	606	MES	O2S-S-C8	3.68	111.34	106.92
3	C	605	MES	C7-N4-C5	3.40	119.94	111.23
3	A	601	MES	O3S-S-O1S	3.39	119.56	111.27
3	A	602	MES	C6-C5-N4	3.38	115.22	110.10
3	B	604	MES	O1S-S-C8	3.32	110.92	106.92
3	A	601	MES	C7-N4-C3	3.32	119.72	111.23
3	C	606	MES	C7-N4-C5	3.24	119.53	111.23
3	C	606	MES	C7-N4-C3	3.06	119.05	111.23
3	C	603	MES	O2S-S-C8	2.90	110.40	106.92
3	C	603	MES	O1-C2-C3	-2.84	105.55	111.80
3	A	602	MES	C7-N4-C3	2.78	118.34	111.23
3	C	605	MES	C2-C3-N4	2.77	114.31	110.10
3	A	601	MES	O2S-S-O1S	-2.66	104.73	113.95
3	A	602	MES	O2S-S-C8	2.60	110.04	106.92
3	A	602	MES	O1S-S-C8	-2.59	103.80	106.92
3	C	603	MES	C2-C3-N4	-2.45	106.38	110.10
3	B	604	MES	O1-C2-C3	2.40	117.07	111.80
3	C	603	MES	C7-N4-C5	2.32	117.17	111.23
3	C	603	MES	O3S-S-C8	2.30	109.48	105.77
3	A	602	MES	C7-N4-C5	2.29	117.09	111.23
3	C	605	MES	O1-C2-C3	-2.19	106.98	111.80
3	A	602	MES	C6-O1-C2	2.08	116.84	109.89
3	A	602	MES	C2-C3-N4	2.07	113.25	110.10

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	MES	C8-C7-N4-C3
3	A	602	MES	C7-C8-S-O2S
3	A	602	MES	C7-C8-S-O3S
3	B	604	MES	C8-C7-N4-C5
3	C	603	MES	N4-C7-C8-S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	605	MES	C8-C7-N4-C5
3	C	606	MES	C8-C7-N4-C3
3	C	606	MES	C7-C8-S-O3S
3	A	602	MES	C8-C7-N4-C3
3	A	602	MES	C8-C7-N4-C5
3	C	603	MES	C8-C7-N4-C5
3	A	602	MES	C7-C8-S-O1S
3	C	606	MES	C7-C8-S-O1S
3	C	606	MES	C7-C8-S-O2S
3	C	605	MES	C8-C7-N4-C3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	MES	1	0
2	B	611	SO4	2	0
3	C	603	MES	4	0
3	C	606	MES	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, 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	313/331 (94%)	0.16	9 (2%) 51 50	13, 23, 38, 46	0
1	B	314/331 (94%)	-0.03	1 (0%) 94 93	16, 22, 35, 44	0
1	C	306/331 (92%)	0.16	7 (2%) 60 59	14, 27, 40, 47	0
All	All	933/993 (93%)	0.10	17 (1%) 68 66	13, 24, 38, 47	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	416	TYR	3.0
1	A	206	TRP	2.9
1	C	357	MET	2.8
1	A	518	LEU	2.7
1	A	218	ILE	2.6
1	A	468	VAL	2.5
1	C	422	PHE	2.5
1	A	420	ASP	2.5
1	A	211	TYR	2.5
1	B	421	ASN	2.4
1	C	386	TYR	2.4
1	C	382	TRP	2.4
1	C	443	VAL	2.2
1	A	209	GLU	2.2
1	C	358	ASN	2.1
1	A	213	GLU	2.1
1	A	210	SER	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 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, 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(Å ²)	Q<0.9
3	MES	C	603	12/12	0.58	0.28	61,69,86,86	0
3	MES	C	606	12/12	0.84	0.17	57,59,67,69	0
3	MES	A	602	12/12	0.91	0.16	40,45,58,61	0
2	SO4	C	610	5/5	0.95	0.10	48,49,52,52	0
2	SO4	B	611	5/5	0.96	0.17	46,50,51,51	0
3	MES	B	604	12/12	0.97	0.14	26,31,42,42	0
2	SO4	A	609	5/5	0.97	0.23	45,45,49,50	0
3	MES	C	605	12/12	0.97	0.14	32,35,39,40	0
2	SO4	A	607	5/5	0.97	0.13	44,51,53,54	0
3	MES	A	601	12/12	0.98	0.10	18,21,30,30	0
2	SO4	B	608	5/5	0.98	0.10	47,48,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.