



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:06 AM UTC

PDB ID : 2RJC / pdb_00002rjc
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	:	4-5-2 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

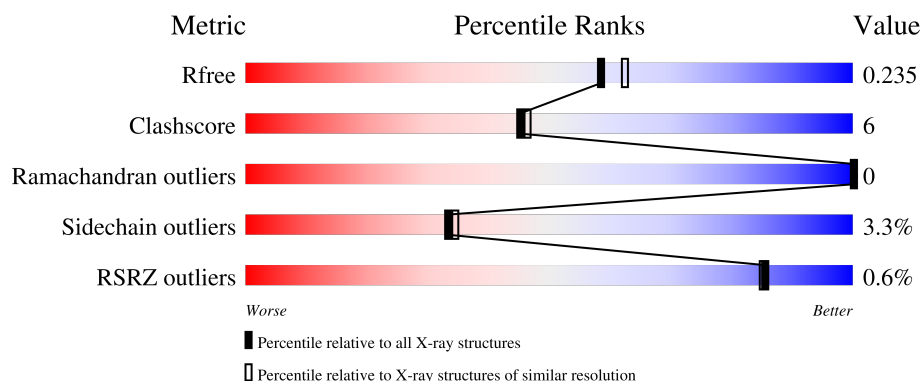
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	
1	B	331	
1	C	331	

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
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 (CCD ID: SO4) (formula: O₄S).



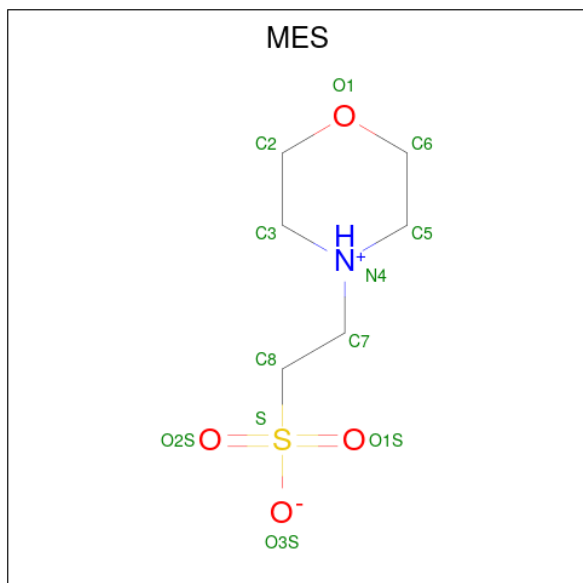
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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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)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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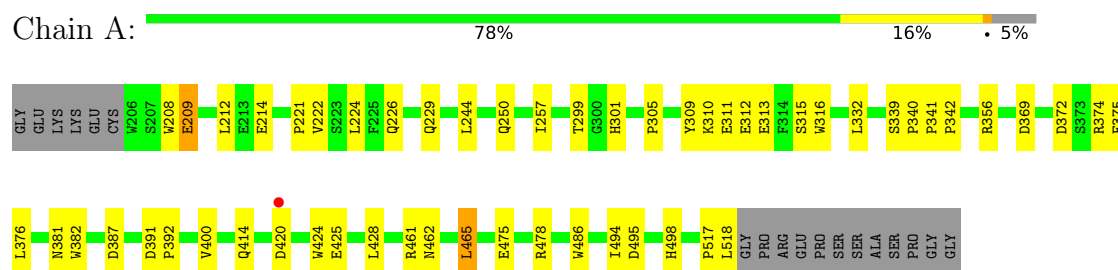
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	262	Total 262	O 262	0	0
4	C	214	Total 214	O 214	0	0

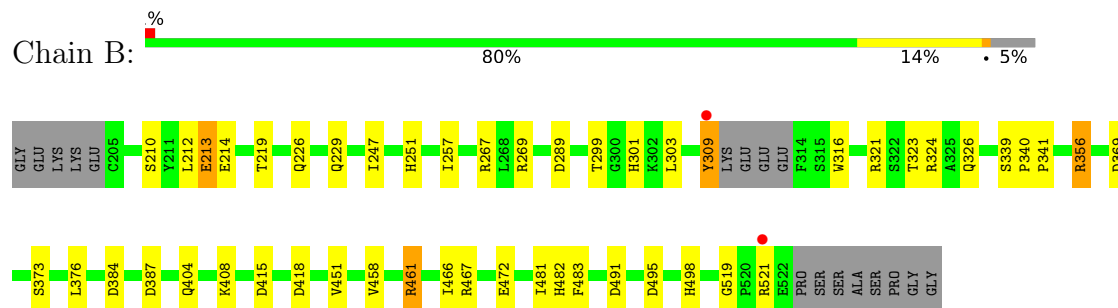
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

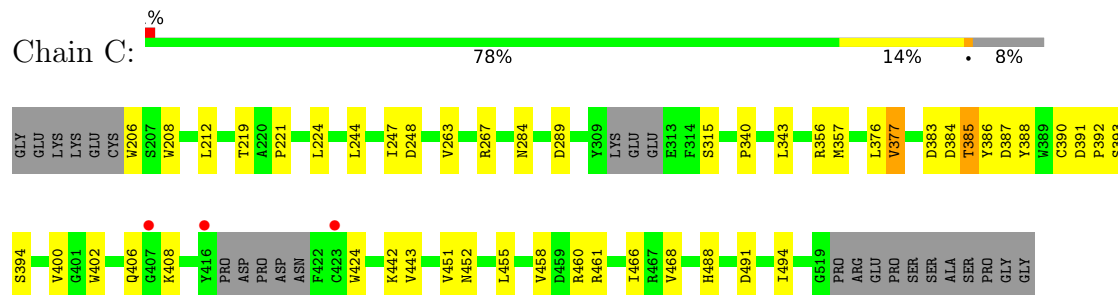
- Molecule 1: Lethal(3)malignant brain tumor-like protein



- 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 90.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.17-2.00) 99.6 (90.17-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.00Å)	Xtriage
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 (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
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

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.*

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, SO4

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	1.13	1/2644 (0.0%)	1.07	2/3614 (0.1%)
1	B	1.14	5/2667 (0.2%)	1.05	9/3643 (0.2%)
1	C	1.08	2/2579 (0.1%)	1.01	1/3521 (0.0%)
All	All	1.12	8/7890 (0.1%)	1.04	12/10778 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	377	VAL	CA-CB	6.60	1.61	1.54
1	B	341	PRO	CA-C	5.74	1.57	1.52
1	B	481	ILE	CA-CB	5.73	1.61	1.54
1	B	458	VAL	CA-CB	5.62	1.60	1.54
1	A	222	VAL	CA-CB	5.55	1.61	1.54
1	B	323	THR	CA-CB	5.42	1.62	1.53
1	B	451	VAL	CA-CB	5.14	1.59	1.54
1	C	263	VAL	CA-CB	5.06	1.61	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ARG	NE-CZ-NH2	-9.64	110.53	119.20
1	B	418	ASP	CA-C-N	7.79	127.97	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	ASP	C-N-CA	7.79	127.97	119.87
1	B	269	ARG	NE-CZ-NH1	7.33	128.83	121.50
1	B	519	GLY	CA-C-N	6.91	127.49	119.47
1	B	519	GLY	C-N-CA	6.91	127.49	119.47
1	B	269	ARG	CD-NE-CZ	6.10	132.94	124.40
1	C	340	PRO	N-CA-C	5.64	117.58	110.70
1	A	311	GLU	N-CA-C	5.53	118.02	111.33
1	B	498	HIS	CA-C-N	5.51	125.22	119.82
1	B	498	HIS	C-N-CA	5.51	125.22	119.82
1	A	332	LEU	N-CA-C	5.32	117.82	111.71

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

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
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:A:517:PRO:C	1:A:518:LEU:HG	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:309:TYR:C	1:B:309:TYR:CD2	2.93	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:309:TYR:C	1:B:309:TYR:HD2	2.24	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	268 (97%)	9 (3%)	34	35
1	B	279/290 (96%)	269 (96%)	10 (4%)	31	31
1	C	269/290 (93%)	260 (97%)	9 (3%)	33	34
All	All	825/870 (95%)	797 (97%)	28 (3%)	33	33

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

Mol	Chain	Res	Type
1	A	209	GLU
1	A	214	GLU
1	A	244	LEU
1	A	250	GLN
1	A	312	GLU
1	A	315	SER
1	A	425	GLU
1	A	428	LEU
1	A	465	LEU
1	B	213	GLU
1	B	309	TYR
1	B	326	GLN
1	B	356	ARG
1	B	404	GLN
1	B	408	LYS
1	B	415	ASP
1	B	461	ARG
1	B	521[A]	ARG
1	B	521[B]	ARG
1	C	244	LEU
1	C	315	SER
1	C	343	LEU
1	C	377	VAL
1	C	384	ASP
1	C	385	THR
1	C	408	LYS
1	C	443	VAL
1	C	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	301	HIS
1	A	381	ASN
1	A	477	HIS
1	A	488	HIS
1	B	229	GLN
1	B	251	HIS
1	B	301	HIS
1	B	304	GLN
1	B	326	GLN
1	B	331	HIS
1	B	482	HIS
1	C	251	HIS
1	C	284	ASN
1	C	326	GLN
1	C	488	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](#)

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
2	SO4	B	608	-	4,4,4	0.12	0	6,6,6	0.24	0
3	MES	A	601	-	12,12,12	1.49	1 (8%)	15,16,16	2.58	4 (26%)
3	MES	A	602	-	12,12,12	1.86	1 (8%)	15,16,16	2.71	8 (53%)
2	SO4	C	610	-	4,4,4	0.29	0	6,6,6	0.33	0
2	SO4	A	609	-	4,4,4	0.36	0	6,6,6	0.80	0
3	MES	B	604	-	12,12,12	2.04	2 (16%)	15,16,16	2.56	4 (26%)
3	MES	C	603	-	12,12,12	2.24	1 (8%)	15,16,16	2.80	7 (46%)
3	MES	C	606	-	12,12,12	1.99	1 (8%)	15,16,16	2.16	4 (26%)
2	SO4	B	611	-	4,4,4	0.26	0	6,6,6	0.54	0
3	MES	C	605	-	12,12,12	1.96	2 (16%)	15,16,16	2.57	4 (26%)
2	SO4	A	607	-	4,4,4	0.34	0	6,6,6	0.83	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	606	-	-	4/6/14/14	0/1/1/1
3	MES	A	602	-	-	5/6/14/14	0/1/1/1
3	MES	C	603	-	-	2/6/14/14	0/1/1/1
3	MES	B	604	-	-	1/6/14/14	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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	MES	C8-S	-7.22	1.67	1.77
3	B	604	MES	C8-S	-6.51	1.68	1.77
3	C	606	MES	C8-S	-6.29	1.68	1.77
3	C	605	MES	C8-S	-6.10	1.69	1.77
3	A	602	MES	C8-S	-5.53	1.69	1.77
3	A	601	MES	C8-S	-4.60	1.71	1.77
3	C	605	MES	O2S-S	2.28	1.51	1.45
3	B	604	MES	O2S-S	2.24	1.51	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	MES	C5-N4-C3	7.84	125.73	108.84
3	C	605	MES	C5-N4-C3	7.82	125.67	108.84
3	A	601	MES	C5-N4-C3	7.57	125.14	108.84
3	A	602	MES	C5-N4-C3	7.26	124.49	108.84
3	C	603	MES	C5-N4-C3	6.05	121.87	108.84
3	C	603	MES	C6-C5-N4	-5.85	101.23	110.12
3	C	606	MES	C5-N4-C3	5.84	121.42	108.84
3	B	604	MES	C7-N4-C5	4.00	121.90	111.24
3	C	603	MES	C7-N4-C3	3.65	120.95	111.24
3	A	602	MES	O3S-S-C8	3.50	112.85	106.00
3	A	602	MES	C6-C5-N4	3.36	115.22	110.12
3	C	605	MES	C7-N4-C5	3.26	119.94	111.24
3	A	601	MES	O3S-S-O1S	3.26	119.56	111.40
3	A	601	MES	C7-N4-C3	3.18	119.72	111.24
3	C	606	MES	C7-N4-C5	3.11	119.53	111.24
3	C	606	MES	O2S-S-C8	3.05	111.34	106.73
3	C	606	MES	C7-N4-C3	2.93	119.05	111.24
3	C	603	MES	O1-C2-C3	-2.89	105.55	111.77
3	A	601	MES	O2S-S-O1S	-2.79	104.73	113.82
3	B	604	MES	O1S-S-C8	2.77	110.92	106.73
3	C	605	MES	C2-C3-N4	2.76	114.31	110.12
3	A	602	MES	C7-N4-C3	2.66	118.34	111.24
3	B	604	MES	O1-C2-C3	2.46	117.07	111.77
3	C	603	MES	C2-C3-N4	-2.46	106.38	110.12
3	C	603	MES	O2S-S-C8	2.43	110.40	106.73
3	C	605	MES	O1-C2-C3	-2.23	106.98	111.77
3	C	603	MES	C7-N4-C5	2.22	117.17	111.24
3	A	602	MES	C7-N4-C5	2.19	117.09	111.24
3	A	602	MES	O2S-S-C8	2.19	110.04	106.73
3	A	602	MES	C6-O1-C2	2.15	116.84	109.88
3	A	602	MES	C2-C3-N4	2.06	113.25	110.12

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
3	C	605	MES	C8-C7-N4-C5
3	C	606	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
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
3	C	603	MES	4	0
3	C	606	MES	1	0
2	B	611	SO4	2	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%)	-0.25	1 (0%) 90 89	13, 23, 38, 46	0
1	B	314/331 (94%)	-0.23	2 (0%) 85 85	9, 22, 35, 44	2 (0%)
1	C	306/331 (92%)	0.01	3 (0%) 79 79	14, 27, 40, 47	0
All	All	933/993 (93%)	-0.16	6 (0%) 85 85	9, 24, 38, 47	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	ASP	3.1
1	B	521[A]	ARG	3.0
1	C	423	CYS	3.0
1	B	309	TYR	3.0
1	C	407	GLY	2.5
1	C	416	TYR	2.4

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 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
3	MES	C	603	12/12	0.79	0.21	61,69,86,86	0
3	MES	C	606	12/12	0.83	0.14	57,59,67,69	0
3	MES	A	602	12/12	0.86	0.13	40,45,58,61	0
2	SO4	A	607	5/5	0.90	0.13	44,51,53,54	0
2	SO4	B	611	5/5	0.92	0.15	46,50,51,51	0
2	SO4	C	610	5/5	0.93	0.12	48,49,52,52	0
2	SO4	A	609	5/5	0.94	0.16	45,45,49,50	0
3	MES	B	604	12/12	0.94	0.08	26,31,42,42	0
3	MES	C	605	12/12	0.95	0.09	32,35,39,40	0
2	SO4	B	608	5/5	0.95	0.08	47,48,51,52	0
3	MES	A	601	12/12	0.97	0.06	18,21,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.