



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:01 AM UTC

PDB ID : 1OYX / pdb_00001oyx
Title : CRYSTAL STRUCTURE OF 3-MBT REPEATS OF LETHAL (3) MALIGNANT BRAIN TUMOR (SELENO-MET) AT 1.85 ANGSTROM
Authors : Wang, W.K.; Tereshko, V.; Boccuni, P.; MacGrogan, D.; Nimer, S.D.; Patel, D.J.
Deposited on : 2003-04-07
Resolution : 1.85 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

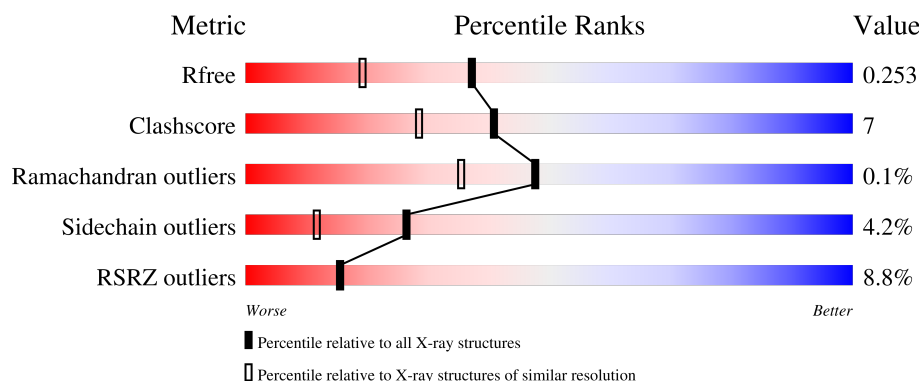
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	12% 78% 15% • 5%
1	B	331	5% 82% 11% • 5%
1	C	331	8% 83% 11% • 5%

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	C	2003	-	-	-	X
3	MES	A	1011	-	-	X	-
3	MES	B	1021	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8296 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.

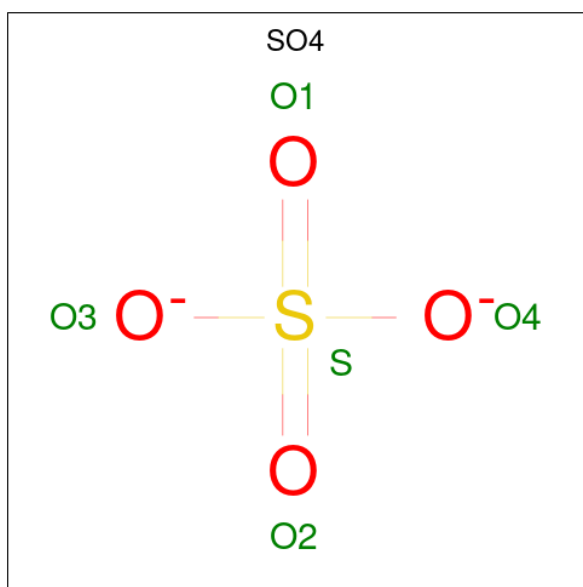
- Molecule 1 is a protein called Lethal(3)malignant brain tumor-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	Se	0	0	0
			2545	1638	432	463	7	5			
1	B	313	Total	C	N	O	S	Se	0	0	0
			2545	1638	432	463	7	5			
1	C	313	Total	C	N	O	S	Se	0	0	0
			2545	1638	432	463	7	5			

There are 15 discrepancies between the modelled and reference sequences:

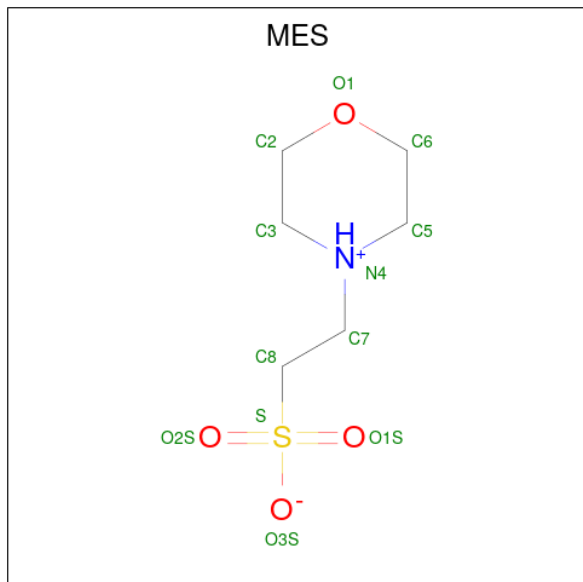
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	MSE	MET	modified residue	UNP Q9Y468
A	254	MSE	MET	modified residue	UNP Q9Y468
A	349	MSE	MET	modified residue	UNP Q9Y468
A	357	MSE	MET	modified residue	UNP Q9Y468
A	453	MSE	MET	modified residue	UNP Q9Y468
B	242	MSE	MET	modified residue	UNP Q9Y468
B	254	MSE	MET	modified residue	UNP Q9Y468
B	349	MSE	MET	modified residue	UNP Q9Y468
B	357	MSE	MET	modified residue	UNP Q9Y468
B	453	MSE	MET	modified residue	UNP Q9Y468
C	242	MSE	MET	modified residue	UNP Q9Y468
C	254	MSE	MET	modified residue	UNP Q9Y468
C	349	MSE	MET	modified residue	UNP Q9Y468
C	357	MSE	MET	modified residue	UNP Q9Y468
C	453	MSE	MET	modified residue	UNP Q9Y468

- 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	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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	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	B	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		

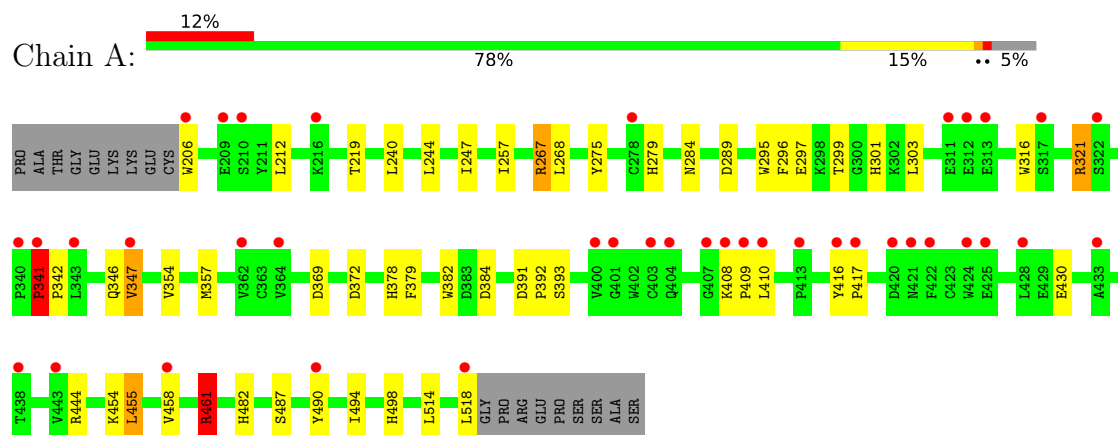
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	201	Total	O	0	0
			201	201		
4	C	188	Total	O	0	0
			188	188		

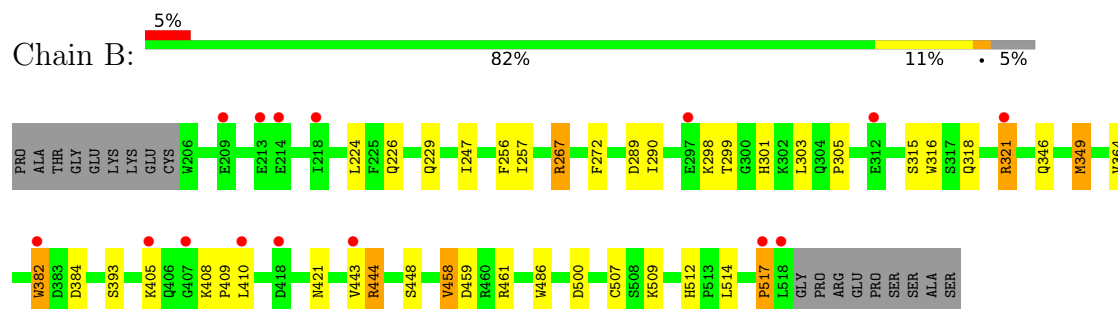
3 Residue-property plots [i](#)

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.

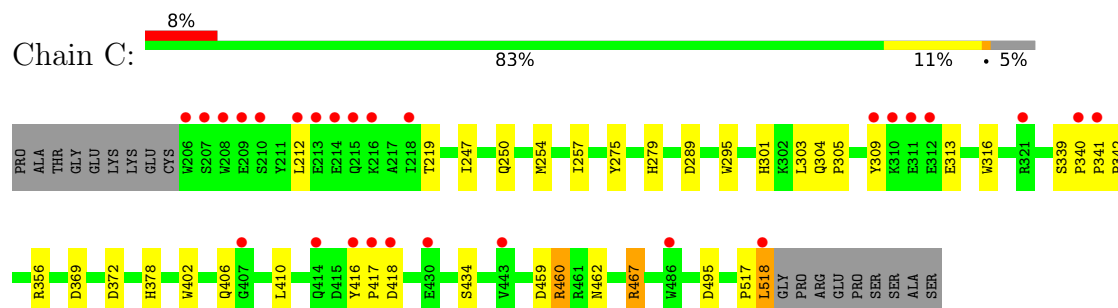
- Molecule 1: Lethal(3)malignant brain tumor-like protein



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	105.66Å 105.66Å 90.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 1.85 19.84 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.84-1.85) 96.9 (19.84-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.13	Depositor
R, R_{free}	0.207 , 0.238 0.231 , 0.253	Depositor DCC
R_{free} test set	4678 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.027 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8296	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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	0.88	2/2639 (0.1%)	0.95	1/3599 (0.0%)
1	B	1.05	3/2639 (0.1%)	1.74	3/3599 (0.1%)
1	C	0.98	0/2639	0.95	0/3599
All	All	0.97	5/7917 (0.1%)	1.27	4/10797 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	MSE	SE-CE	-9.07	1.68	1.95
1	B	305	PRO	C-O	-6.64	1.17	1.24
1	B	290	ILE	C-O	-6.54	1.17	1.24
1	A	267	ARG	CZ-NH1	5.18	1.40	1.32
1	A	347	VAL	CA-CB	5.18	1.59	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	517	PRO	O-C-N	-85.73	14.12	122.99
1	A	341	PRO	N-CA-C	7.06	119.31	110.70
1	B	349	MSE	CG-SE-CE	5.33	110.65	98.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ARG	NE-CZ-NH2	-5.08	114.63	119.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	517	PRO	Mainchain

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	34	0
1	B	2545	0	2380	38	0
1	C	2545	0	2380	26	0
2	A	20	0	0	1	0
2	B	30	0	0	0	0
2	C	20	0	0	0	0
3	A	24	0	25	6	0
3	B	36	0	39	12	0
3	C	24	0	25	3	0
4	A	118	0	0	4	0
4	B	201	0	0	5	0
4	C	188	0	0	3	0
All	All	8296	0	7229	98	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 7.

All (98) 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:346:GLN:CG	1:B:349:MSE:HE3	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLN:CB	1:B:349:MSE:HE3	2.05	0.86
1:B:272:PHE:CD2	3:B:1021:MES:H22	2.11	0.85
1:C:301:HIS:HE1	1:C:369:ASP:OD1	1.62	0.83
1:A:279:HIS:CE1	3:A:1011:MES:H82	2.13	0.82
1:B:272:PHE:CE2	3:B:1021:MES:H22	2.20	0.76
1:B:346:GLN:CG	1:B:349:MSE:CE	2.65	0.74
1:A:408:LYS:HG3	1:A:409:PRO:HD2	1.70	0.72
1:B:346:GLN:HB2	1:B:349:MSE:HE3	1.69	0.71
1:C:301:HIS:CE1	1:C:369:ASP:OD1	2.44	0.71
1:A:301:HIS:HE1	1:A:369:ASP:OD1	1.75	0.69
1:A:279:HIS:CD2	3:A:1011:MES:H51	2.28	0.69
1:B:346:GLN:HG3	1:B:349:MSE:CE	2.24	0.68
1:A:347:VAL:HG12	4:A:2091:HOH:O	1.94	0.67
1:B:346:GLN:HG2	1:B:349:MSE:HE3	1.77	0.65
1:A:391:ASP:HB2	1:A:392:PRO:HD2	1.79	0.64
1:A:454:LYS:NZ	4:A:2046:HOH:O	2.29	0.64
1:C:295:TRP:CH2	1:C:301:HIS:CD2	2.86	0.63
1:A:267:ARG:HD2	1:A:284:ASN:ND2	2.13	0.63
1:A:275:TYR:CD2	3:A:1011:MES:H81	2.34	0.62
1:A:267:ARG:HD2	1:A:284:ASN:HD22	1.64	0.62
1:B:382:TRP:HZ3	4:B:2179:HOH:O	1.83	0.61
1:C:517:PRO:O	1:C:518:LEU:HB2	1.99	0.61
1:A:295:TRP:CH2	1:A:301:HIS:CD2	2.89	0.60
1:A:275:TYR:HB3	3:A:1011:MES:H81	1.81	0.60
1:C:254:MSE:HE2	1:C:304:GLN:CD	2.26	0.60
1:C:460:ARG:HA	1:C:460:ARG:HE	1.65	0.60
1:A:341:PRO:HB3	1:A:342:PRO:HD2	1.84	0.59
1:A:455:LEU:HD12	1:A:455:LEU:C	2.29	0.58
1:B:364:VAL:HG23	1:B:410:LEU:HD11	1.86	0.58
1:B:298:LYS:NZ	4:B:2203:HOH:O	2.35	0.58
1:C:402:TRP:CE2	1:C:406:GLN:HG3	2.40	0.57
1:C:462:ASN:C	1:C:462:ASN:HD22	2.13	0.57
1:B:346:GLN:HG3	1:B:349:MSE:HE3	1.81	0.57
1:B:226:GLN:H	1:B:229:GLN:NE2	2.02	0.57
1:C:305:PRO:HB2	1:C:309:TYR:HB2	1.87	0.56
1:A:296:PHE:CZ	1:A:297:GLU:HG3	2.41	0.56
1:B:461:ARG:HD3	3:B:1023:MES:H31	1.86	0.56
1:B:272:PHE:CE2	3:B:1021:MES:C2	2.89	0.56
1:A:482:HIS:NE2	2:A:2005:SO4:O2	2.37	0.56
1:B:272:PHE:CG	3:B:1021:MES:H22	2.40	0.55
1:C:257:ILE:HD12	1:C:316:TRP:CZ2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ARG:CD	3:B:1023:MES:H31	2.36	0.55
1:A:301:HIS:CE1	1:A:369:ASP:OD1	2.60	0.54
1:A:408:LYS:HB2	4:A:2026:HOH:O	2.07	0.54
1:B:318:GLN:OE1	1:B:321:ARG:NH2	2.41	0.53
1:C:247:ILE:HG12	1:C:289:ASP:HB3	1.91	0.53
1:A:247:ILE:HG12	1:A:289:ASP:HB3	1.91	0.52
1:C:279:HIS:CD2	3:C:1031:MES:H62	2.44	0.52
1:B:349:MSE:HE1	4:B:2063:HOH:O	2.09	0.52
1:B:408:LYS:HG3	1:B:409:PRO:HD2	1.92	0.52
1:B:458:VAL:HG13	1:B:500:ASP:HB3	1.92	0.51
1:B:364:VAL:CG2	1:B:410:LEU:HD11	2.40	0.51
1:A:299:THR:OG1	1:A:301:HIS:HD2	1.92	0.51
1:C:341:PRO:HA	1:C:372:ASP:O	2.11	0.51
1:B:267:ARG:HD2	4:B:2126:HOH:O	2.10	0.50
1:B:272:PHE:CZ	3:B:1021:MES:H22	2.47	0.50
1:B:459:ASP:OD2	3:B:1023:MES:H22	2.12	0.50
1:C:339:SER:HB3	1:C:340:PRO:HD2	1.94	0.49
1:C:342:PRO:HD3	1:C:372:ASP:O	2.12	0.49
1:B:256:PHE:CZ	3:B:1021:MES:H31	2.48	0.48
1:C:250:GLN:NE2	4:C:2084:HOH:O	2.44	0.47
1:C:275:TYR:CD2	3:C:1031:MES:H51	2.48	0.47
1:C:212:LEU:HD11	1:C:219:THR:HG23	1.96	0.47
1:C:356:ARG:HD3	4:C:2122:HOH:O	2.15	0.46
1:B:346:GLN:HB2	1:B:349:MSE:CE	2.42	0.46
1:A:257:ILE:HD12	1:A:316:TRP:CZ2	2.51	0.46
1:A:296:PHE:CE2	1:A:297:GLU:HG3	2.51	0.46
1:B:272:PHE:CZ	3:B:1021:MES:C2	2.99	0.46
1:A:275:TYR:HD2	3:A:1011:MES:H81	1.78	0.46
1:C:459:ASP:OD1	1:C:467:ARG:NH1	2.49	0.45
1:B:247:ILE:HG12	1:B:289:ASP:HB3	1.98	0.45
1:A:393:SER:HB2	1:A:444:ARG:HB2	1.98	0.45
1:B:509:LYS:NZ	4:B:2107:HOH:O	2.50	0.45
1:C:378:HIS:HE1	4:C:2040:HOH:O	1.99	0.45
1:A:279:HIS:CG	3:A:1011:MES:H51	2.52	0.45
1:C:462:ASN:C	1:C:462:ASN:ND2	2.74	0.45
1:A:487:SER:HB3	1:A:490:TYR:CE2	2.53	0.43
1:A:494:ILE:HD11	1:A:498:HIS:CG	2.53	0.43
1:A:455:LEU:C	1:A:455:LEU:CD1	2.91	0.43
1:B:256:PHE:CE2	3:B:1021:MES:H31	2.54	0.43
1:B:507:CYS:HB3	1:B:512:HIS:O	2.18	0.43
1:C:416:TYR:CG	1:C:417:PRO:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:NH1	1:C:495:ASP:OD2	2.52	0.42
1:B:257:ILE:HD12	1:B:316:TRP:CZ2	2.54	0.42
1:B:299:THR:O	1:B:301:HIS:CE1	2.72	0.42
1:A:416:TYR:CD1	1:A:417:PRO:HD2	2.55	0.42
1:B:486:TRP:CE3	3:B:1023:MES:H51	2.54	0.42
1:B:443:VAL:O	1:B:443:VAL:HG23	2.21	0.41
1:A:461:ARG:HE	1:A:461:ARG:HB2	1.65	0.41
1:A:342:PRO:HD3	1:A:372:ASP:O	2.21	0.41
1:B:393:SER:O	1:B:444:ARG:HB3	2.20	0.41
1:B:224:LEU:HD22	1:B:448:SER:HB2	2.02	0.41
1:C:416:TYR:CD1	1:C:417:PRO:HD2	2.56	0.41
1:A:321:ARG:HD3	4:A:2054:HOH:O	2.20	0.41
1:A:378:HIS:CD2	1:A:379:PHE:N	2.89	0.40
1:C:275:TYR:CG	3:C:1031:MES:H51	2.56	0.40
1:A:212:LEU:HD11	1:A:219:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

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%)	306 (98%)	4 (1%)	1 (0%)	36	25
1	B	311/331 (94%)	308 (99%)	3 (1%)	0	100	100
1	C	311/331 (94%)	302 (97%)	9 (3%)	0	100	100
All	All	933/993 (94%)	916 (98%)	16 (2%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	PRO

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	277/286 (97%)	259 (94%)	18 (6%)	15	4
1	B	277/286 (97%)	268 (97%)	9 (3%)	34	19
1	C	277/286 (97%)	269 (97%)	8 (3%)	37	22
All	All	831/858 (97%)	796 (96%)	35 (4%)	26	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	TRP
1	A	240	LEU
1	A	244	LEU
1	A	268	LEU
1	A	303	LEU
1	A	321	ARG
1	A	346	GLN
1	A	354	VAL
1	A	357	MSE
1	A	382	TRP
1	A	384	ASP
1	A	410	LEU
1	A	430	GLU
1	A	455	LEU
1	A	458	VAL
1	A	461	ARG
1	A	514	LEU
1	A	518	LEU
1	B	303	LEU
1	B	315	SER
1	B	382	TRP
1	B	384	ASP
1	B	405	LYS
1	B	421	ASN
1	B	444	ARG
1	B	458	VAL

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Mol	Chain	Res	Type
1	B	514	LEU
1	C	303	LEU
1	C	313	GLU
1	C	410	LEU
1	C	418	ASP
1	C	434	SER
1	C	460	ARG
1	C	467	ARG
1	C	518	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	271	HIS
1	A	279	HIS
1	A	284	ASN
1	A	301	HIS
1	A	304	GLN
1	A	462	ASN
1	A	512	HIS
1	B	215	GLN
1	B	229	GLN
1	B	279	HIS
1	B	304	GLN
1	B	398	HIS
1	B	406	GLN
1	B	414	GLN
1	B	421	ASN
1	B	452	ASN
1	B	477	HIS
1	B	488	HIS
1	C	271	HIS
1	C	301	HIS
1	C	378	HIS
1	C	406	GLN
1	C	462	ASN
1	C	498	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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	C	2002	-	4,4,4	0.28	0	6,6,6	0.46	0
2	SO4	B	2013	-	4,4,4	0.37	0	6,6,6	1.04	1 (16%)
2	SO4	C	2003	-	4,4,4	1.82	1 (25%)	6,6,6	1.86	2 (33%)
2	SO4	B	2001	-	4,4,4	0.25	0	6,6,6	0.74	0
2	SO4	C	2007	-	4,4,4	1.15	0	6,6,6	0.71	0
3	MES	A	1012	-	12,12,12	1.18	1 (8%)	15,16,16	1.74	3 (20%)
2	SO4	B	2014	-	4,4,4	0.23	0	6,6,6	0.45	0
3	MES	B	1021	-	12,12,12	1.10	1 (8%)	15,16,16	1.83	2 (13%)
3	MES	C	1031	-	12,12,12	0.93	1 (8%)	15,16,16	2.00	5 (33%)
2	SO4	B	2011	-	4,4,4	1.34	1 (25%)	6,6,6	1.24	0
3	MES	C	1032	-	12,12,12	1.04	1 (8%)	15,16,16	1.20	0
3	MES	A	1011	-	12,12,12	2.31	3 (25%)	15,16,16	2.15	8 (53%)
2	SO4	B	2004	-	4,4,4	0.26	0	6,6,6	0.40	0
2	SO4	A	2008	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	A	2010	-	4,4,4	0.37	0	6,6,6	0.46	0
2	SO4	B	2009	-	4,4,4	0.28	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	2012	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	C	2006	-	4,4,4	0.25	0	6,6,6	0.62	0
3	MES	B	1023	-	12,12,12	1.31	1 (8%)	15,16,16	1.83	3 (20%)
2	SO4	A	2005	-	4,4,4	0.21	0	6,6,6	0.31	0
3	MES	B	1022	-	12,12,12	0.75	0	15,16,16	1.52	2 (13%)

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	B	1023	-	-	5/6/14/14	0/1/1/1
3	MES	A	1011	-	-	5/6/14/14	0/1/1/1
3	MES	B	1021	-	-	3/6/14/14	0/1/1/1
3	MES	C	1031	-	-	2/6/14/14	0/1/1/1
3	MES	B	1022	-	-	4/6/14/14	0/1/1/1
3	MES	A	1012	-	-	5/6/14/14	0/1/1/1
3	MES	C	1032	-	-	1/6/14/14	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1011	MES	C8-S	6.79	1.87	1.77
3	B	1023	MES	C8-S	3.90	1.83	1.77
3	A	1012	MES	C8-S	3.67	1.82	1.77
3	B	1021	MES	C8-S	3.22	1.82	1.77
3	C	1032	MES	C8-S	3.04	1.81	1.77
3	A	1011	MES	C7-N4	2.92	1.54	1.47
2	C	2003	SO4	O1-S	2.68	1.60	1.44
3	C	1031	MES	C8-S	2.59	1.81	1.77
3	A	1011	MES	C7-C8	2.19	1.58	1.52
2	B	2011	SO4	O1-S	2.19	1.57	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1021	MES	O1-C6-C5	-4.09	102.97	111.77
3	B	1023	MES	C2-C3-N4	3.96	116.14	110.12
3	A	1012	MES	C5-N4-C3	3.85	117.14	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1031	MES	C2-C3-N4	3.59	115.58	110.12
3	A	1011	MES	C6-C5-N4	3.59	115.58	110.12
3	C	1031	MES	C5-N4-C3	3.41	116.18	108.84
3	B	1022	MES	C7-N4-C5	-3.36	102.29	111.24
3	B	1021	MES	C5-N4-C3	3.23	115.80	108.84
3	A	1011	MES	C8-C7-N4	3.22	124.56	112.36
2	C	2003	SO4	O4-S-O1	-2.98	94.00	109.56
3	B	1023	MES	C6-C5-N4	2.92	114.56	110.12
3	A	1011	MES	O1-C6-C5	-2.85	105.63	111.77
3	A	1011	MES	C2-C3-N4	2.77	114.33	110.12
3	A	1011	MES	C7-N4-C5	2.76	118.60	111.24
3	B	1022	MES	O3S-S-C8	2.70	111.28	106.00
3	C	1031	MES	O1-C6-C5	-2.57	106.23	111.77
2	C	2003	SO4	O3-S-O2	2.45	122.36	109.56
3	A	1011	MES	C5-N4-C3	2.26	113.71	108.84
3	A	1011	MES	O2S-S-C8	2.20	110.06	106.73
3	C	1031	MES	C7-N4-C5	-2.17	105.45	111.24
3	A	1012	MES	C8-C7-N4	2.14	120.45	112.36
3	A	1011	MES	O3S-S-C8	2.12	110.15	106.00
3	B	1023	MES	C8-C7-N4	2.10	120.29	112.36
3	A	1012	MES	C2-C3-N4	2.10	113.30	110.12
2	B	2013	SO4	O3-S-O2	2.04	120.22	109.56
3	C	1031	MES	O2S-S-C8	2.00	109.75	106.73

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1011	MES	C8-C7-N4-C3
3	A	1011	MES	C8-C7-N4-C5
3	A	1011	MES	C7-C8-S-O2S
3	A	1011	MES	C7-C8-S-O3S
3	A	1012	MES	C8-C7-N4-C3
3	B	1022	MES	C8-C7-N4-C3
3	B	1022	MES	C7-C8-S-O2S
3	B	1022	MES	C7-C8-S-O3S
3	B	1023	MES	C8-C7-N4-C3
3	B	1023	MES	C7-C8-S-O1S
3	C	1031	MES	C8-C7-N4-C3
3	C	1032	MES	C8-C7-N4-C3
3	A	1012	MES	C8-C7-N4-C5
3	B	1023	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
3	A	1012	MES	C7-C8-S-O3S
3	A	1011	MES	C7-C8-S-O1S
3	A	1012	MES	C7-C8-S-O2S
3	B	1021	MES	C7-C8-S-O1S
3	B	1022	MES	C7-C8-S-O1S
3	B	1023	MES	C7-C8-S-O2S
3	B	1021	MES	N4-C7-C8-S
3	C	1031	MES	C8-C7-N4-C5
3	B	1023	MES	C7-C8-S-O3S
3	A	1012	MES	C7-C8-S-O1S
3	B	1021	MES	C7-C8-S-O3S

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1021	MES	8	0
3	C	1031	MES	3	0
3	A	1011	MES	6	0
3	B	1023	MES	4	0
2	A	2005	SO4	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

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, 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	308/331 (93%)	0.88	39 (12%) 8 7	13, 37, 67, 81	0
1	B	308/331 (93%)	0.38	15 (4%) 35 38	13, 29, 46, 60	0
1	C	308/331 (93%)	0.62	27 (8%) 15 15	13, 32, 53, 65	0
All	All	924/993 (93%)	0.63	81 (8%) 15 15	13, 32, 57, 81	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	418	ASP	4.6
1	B	518	LEU	4.4
1	A	343	LEU	4.2
1	C	340	PRO	4.0
1	A	417	PRO	4.0
1	C	310	LYS	3.9
1	B	312	GLU	3.9
1	C	209	GLU	3.6
1	C	216	LYS	3.6
1	C	210	SER	3.6
1	A	518	LEU	3.5
1	A	312	GLU	3.5
1	A	443	VAL	3.4
1	B	443	VAL	3.4
1	C	312	GLU	3.3
1	C	213	GLU	3.2
1	A	421	ASN	3.2
1	C	311	GLU	3.2
1	C	518	LEU	3.1
1	A	210	SER	3.1
1	A	206	TRP	3.1
1	A	422	PHE	3.1
1	A	216	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	340	PRO	3.0
1	C	417	PRO	3.0
1	B	382	TRP	2.9
1	B	209	GLU	2.9
1	A	410	LEU	2.9
1	B	407	GLY	2.8
1	C	414	GLN	2.8
1	C	407	GLY	2.8
1	A	209	GLU	2.8
1	A	311	GLU	2.7
1	B	517	PRO	2.7
1	C	341	PRO	2.7
1	A	341	PRO	2.7
1	A	404	GLN	2.7
1	A	313	GLU	2.7
1	C	214	GLU	2.7
1	A	490	TYR	2.6
1	A	413	PRO	2.6
1	A	401	GLY	2.6
1	A	416	TYR	2.6
1	A	403	CYS	2.6
1	A	424	TRP	2.6
1	C	443	VAL	2.6
1	C	309	TYR	2.5
1	C	208	TRP	2.5
1	A	322	SER	2.5
1	A	347	VAL	2.5
1	B	214	GLU	2.4
1	B	418	ASP	2.4
1	B	218	ILE	2.4
1	B	213	GLU	2.3
1	A	428	LEU	2.3
1	A	433	ALA	2.3
1	C	218	ILE	2.3
1	A	407	GLY	2.3
1	B	405	LYS	2.3
1	A	364	VAL	2.3
1	C	416	TYR	2.3
1	A	400	VAL	2.3
1	C	321	ARG	2.2
1	C	212	LEU	2.2
1	C	430	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	317	SER	2.2
1	C	206	TRP	2.2
1	A	362	VAL	2.2
1	B	410	LEU	2.1
1	A	420	ASP	2.1
1	A	438	THR	2.1
1	A	425	GLU	2.1
1	C	486	TRP	2.1
1	A	278	CYS	2.1
1	A	408	LYS	2.0
1	A	409	PRO	2.0
1	A	458	VAL	2.0
1	B	297	GLU	2.0
1	C	207	SER	2.0
1	C	215	GLN	2.0
1	B	321	ARG	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	SO4	A	2012	5/5	0.55	0.13	102,103,104,104	0
3	MES	B	1021	12/12	0.61	0.25	86,88,95,95	0
2	SO4	B	2011	5/5	0.62	0.34	33,33,35,38	0
2	SO4	C	2003	5/5	0.63	0.42	27,29,29,35	0
2	SO4	A	2005	5/5	0.64	0.14	88,89,90,90	0
3	MES	C	1031	12/12	0.69	0.23	76,79,89,89	0
3	MES	A	1011	12/12	0.70	0.25	71,74,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	2010	5/5	0.71	0.12	76,77,80,80	0
2	SO4	A	2008	5/5	0.75	0.16	92,93,93,94	0
3	MES	A	1012	12/12	0.79	0.15	66,67,71,71	0
3	MES	B	1023	12/12	0.80	0.16	76,78,89,90	0
2	SO4	B	2013	5/5	0.80	0.12	51,53,56,59	0
2	SO4	C	2006	5/5	0.83	0.12	74,74,75,78	0
3	MES	C	1032	12/12	0.83	0.14	48,51,54,55	0
2	SO4	B	2014	5/5	0.84	0.12	82,83,84,85	0
2	SO4	C	2007	5/5	0.84	0.28	32,33,37,40	0
3	MES	B	1022	12/12	0.87	0.11	32,37,50,50	0
2	SO4	B	2004	5/5	0.87	0.09	69,69,70,71	0
2	SO4	B	2009	5/5	0.88	0.10	68,69,71,72	0
2	SO4	C	2002	5/5	0.91	0.11	62,63,64,64	0
2	SO4	B	2001	5/5	0.94	0.08	49,51,53,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.