



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:10 am BST

PDB ID : 1OZ3
Title : Crystal Structure of 3-MBT repeats of lethal (3) malignant Brain Tumor (Native-I) 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 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 : 2.11
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) : 2.11

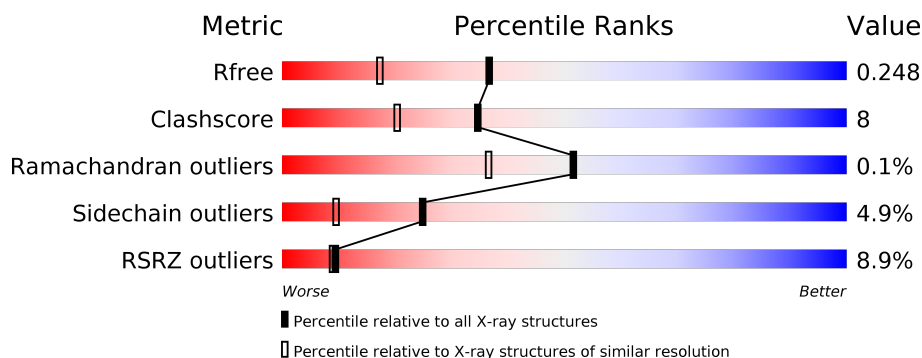
1 Overall quality at a glance

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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 on 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	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	331	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	C	331	<div> <div>13%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 5%</div> </div> </div>

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	A	1005	-	-	X	-
3	MES	C	1011	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8232 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			

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



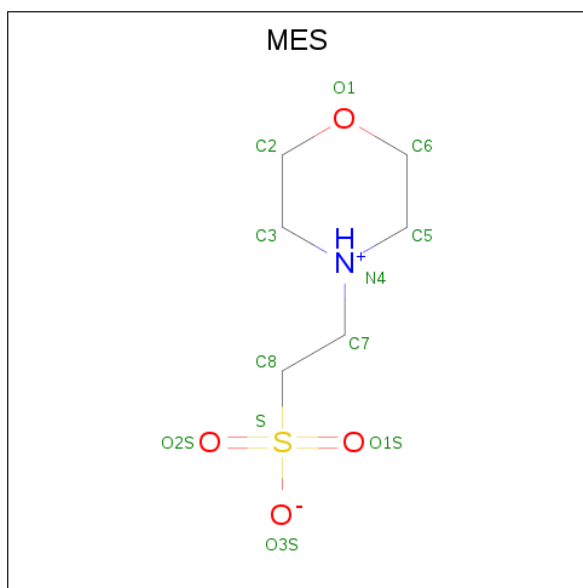
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- 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	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

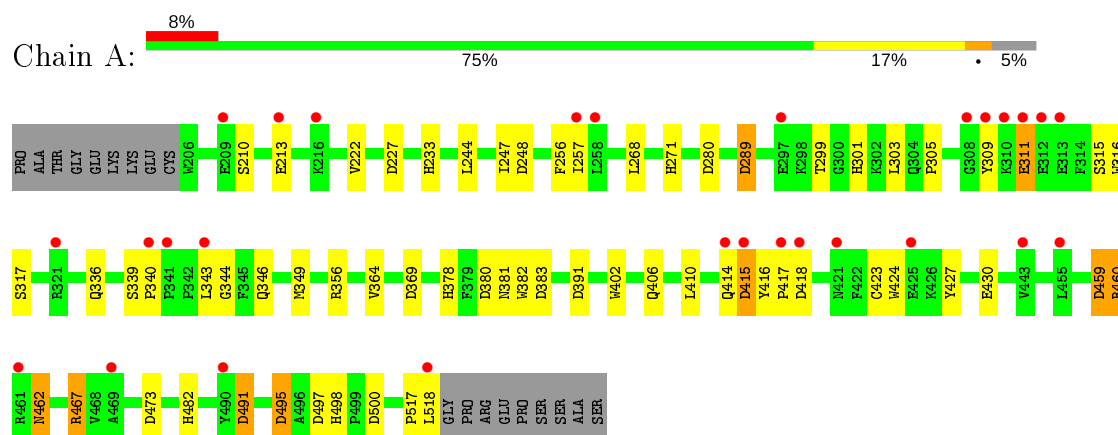
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total	O	0	0
			172	172		
4	B	189	Total	O	0	0
			189	189		
4	C	114	Total	O	0	0
			114	114		

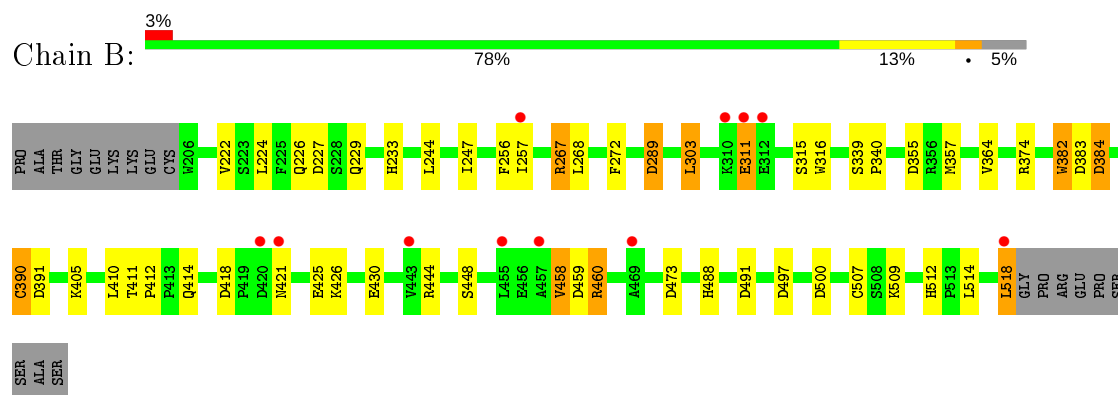
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

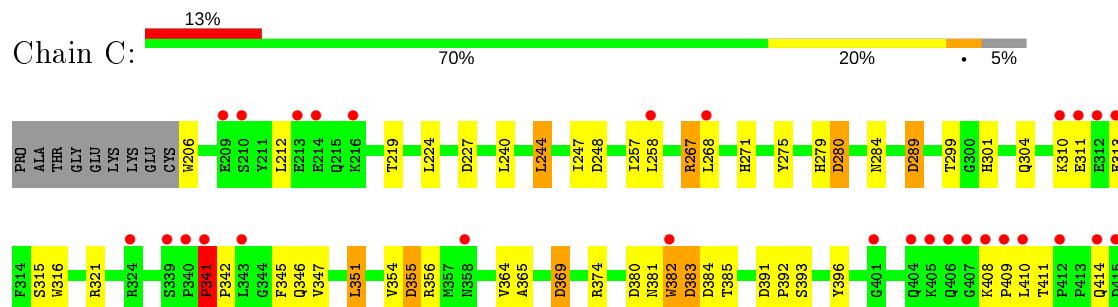
- Molecule 1: Lethal(3)malignant brain tumor-like protein

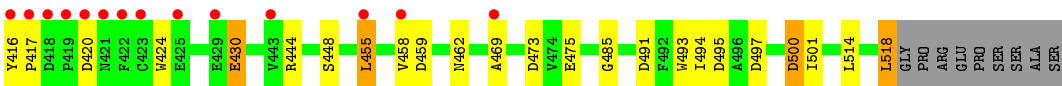


- Molecule 1: Lethal(3)malignant brain tumor-like protein



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	105.25Å 105.25Å 90.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 1.85 19.83 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-1.85) 100.0 (19.83-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.13	Depositor
R, R_{free}	0.211 , 0.245 0.216 , 0.248	Depositor DCC
R_{free} test set	4822 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.026 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8232	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 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	0.79	0/2639	0.95	12/3599 (0.3%)
1	B	0.82	2/2639 (0.1%)	1.03	17/3599 (0.5%)
1	C	0.77	0/2639	1.09	19/3599 (0.5%)
All	All	0.79	2/7917 (0.0%)	1.03	48/10797 (0.4%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	VAL	CB-CG2	-8.57	1.34	1.52
1	B	311	GLU	CD-OE2	5.52	1.31	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	ARG	NE-CZ-NH2	-19.44	110.58	120.30
1	B	267	ARG	NE-CZ-NH2	-15.82	112.39	120.30
1	C	267	ARG	NE-CZ-NH1	14.37	127.48	120.30
1	B	267	ARG	NE-CZ-NH1	14.13	127.36	120.30
1	A	491	ASP	CB-CG-OD2	10.87	128.08	118.30
1	C	374	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	B	473	ASP	CB-CG-OD2	8.82	126.24	118.30
1	C	280	ASP	CB-CG-OD2	8.45	125.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ASP	CB-CG-OD2	8.38	125.84	118.30
1	C	473	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	473	ASP	CB-CG-OD2	7.92	125.43	118.30
1	C	355	ASP	CB-CG-OD2	7.54	125.09	118.30
1	B	459	ASP	CB-CG-OD2	7.51	125.06	118.30
1	B	374	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	C	369	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	459	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	497	ASP	CB-CG-OD2	6.92	124.53	118.30
1	C	289	ASP	CB-CG-OD2	6.52	124.16	118.30
1	C	459	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	248	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	227	ASP	CB-CG-OD2	6.42	124.07	118.30
1	A	415	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	355	ASP	CB-CG-OD2	6.25	123.92	118.30
1	C	267	ARG	CD-NE-CZ	6.17	132.24	123.60
1	C	227	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	420	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	289	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	289	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	267	ARG	CD-NE-CZ	5.65	131.50	123.60
1	A	391	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	374	ARG	CG-CD-NE	-5.54	100.16	111.80
1	B	418	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	500	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	267	ARG	CG-CD-NE	-5.50	100.25	111.80
1	B	460	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	248	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	497	ASP	CB-CG-OD1	5.42	123.17	118.30
1	C	518	LEU	CA-CB-CG	5.40	127.72	115.30
1	B	384	ASP	CB-CG-OD1	-5.36	113.47	118.30
1	C	497	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	491	ASP	CB-CG-OD2	5.21	122.98	118.30
1	B	383	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	227	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	495	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	383	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	418	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	390	CYS	CA-CB-SG	5.01	123.02	114.00
1	B	391	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	321	ARG	Sidechain

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	38	0
1	B	2545	0	2380	29	0
1	C	2545	0	2380	57	0
2	A	10	0	0	2	0
2	B	25	0	0	1	0
2	C	15	0	0	1	0
3	A	24	0	25	1	0
3	B	24	0	25	4	0
3	C	24	0	25	11	0
4	A	172	0	0	4	0
4	B	189	0	0	5	0
4	C	114	0	0	6	0
All	All	8232	0	7215	124	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 8.

All (124) 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:C:275:TYR:CD2	3:C:1011:MES:H81	2.08	0.88
1:A:301:HIS:HE1	1:A:369:ASP:OD1	1.63	0.82
1:C:301:HIS:HE1	1:C:369:ASP:OD1	1.62	0.81
1:C:347:VAL:HG12	4:C:1091:HOH:O	1.80	0.80
1:C:408:LYS:HG3	1:C:409:PRO:HD2	1.62	0.80
1:C:458:VAL:CG2	1:C:500:ASP:HB3	2.12	0.79
1:C:275:TYR:HD2	3:C:1011:MES:H81	1.47	0.77
1:A:498:HIS:HD2	1:A:500:ASP:H	1.34	0.73
1:B:509:LYS:NZ	4:B:1114:HOH:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:NH2	1:C:495:ASP:OD2	2.22	0.72
1:C:458:VAL:HG22	1:C:500:ASP:HB3	1.71	0.71
1:C:279:HIS:CE1	3:C:1011:MES:H82	2.28	0.69
1:A:460:ARG:HD3	4:A:1080:HOH:O	1.93	0.69
1:A:305:PRO:HB2	1:A:309:TYR:HB2	1.76	0.68
1:B:364:VAL:HG23	1:B:410:LEU:HD11	1.78	0.65
1:C:416:TYR:CD1	1:C:417:PRO:HD2	2.32	0.65
1:B:272:PHE:CE2	3:B:1021:MES:H22	2.32	0.64
1:A:257:ILE:HD12	1:A:316:TRP:CZ2	2.32	0.64
1:C:455:LEU:HD12	1:C:469:ALA:HB3	1.78	0.63
1:B:339:SER:HB2	1:B:340:PRO:HD2	1.80	0.63
1:A:459:ASP:OD1	1:A:467:ARG:NH1	2.30	0.62
1:C:391:ASP:HB2	1:C:392:PRO:HD2	1.83	0.61
1:C:310:LYS:HB2	1:C:313:GLU:HG3	1.82	0.61
1:C:244:LEU:HD22	1:C:258:LEU:HB2	1.83	0.60
1:C:382:TRP:CG	3:C:1012:MES:H21	2.37	0.60
1:B:267:ARG:HD2	4:B:1131:HOH:O	2.01	0.60
1:C:458:VAL:HG21	1:C:500:ASP:HB3	1.83	0.60
1:C:304:GLN:HG3	4:C:1058:HOH:O	2.02	0.60
1:C:382:TRP:CE3	3:C:1012:MES:H62	2.36	0.60
1:A:271:HIS:HE1	4:A:1060:HOH:O	1.85	0.59
1:A:339:SER:HB3	1:A:340:PRO:HD2	1.83	0.59
1:A:402:TRP:CE2	1:A:406:GLN:HG3	2.38	0.59
1:A:344:GLY:O	1:A:349:MSE:SE	2.72	0.57
1:A:416:TYR:CG	1:A:417:PRO:HD2	2.39	0.57
1:B:458:VAL:HG22	1:B:500:ASP:HB3	1.85	0.57
1:C:299:THR:OG1	1:C:301:HIS:HD2	1.87	0.57
1:C:458:VAL:HG22	4:C:1029:HOH:O	2.05	0.57
1:C:275:TYR:HB3	3:C:1011:MES:H81	1.87	0.56
1:A:299:THR:OG1	1:A:301:HIS:HD2	1.89	0.56
1:B:272:PHE:CZ	3:B:1021:MES:H22	2.40	0.56
1:A:517:PRO:O	1:A:518:LEU:HB2	2.07	0.55
1:B:222:VAL:HG12	2:B:1009:SO4:O4	2.07	0.55
1:A:378:HIS:HE1	4:A:1065:HOH:O	1.89	0.54
1:A:303:LEU:C	1:A:303:LEU:HD13	2.28	0.54
1:B:410:LEU:HD13	1:B:410:LEU:C	2.28	0.54
1:A:460:ARG:HA	1:A:460:ARG:HE	1.73	0.53
1:B:426:LYS:O	1:B:430:GLU:HG3	2.09	0.53
1:B:226:GLN:H	1:B:229:GLN:NE2	2.07	0.53
1:C:301:HIS:CE1	1:C:369:ASP:OD1	2.53	0.52
1:B:382:TRP:HZ3	4:B:1181:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LEU:HD11	1:C:219:THR:HG23	1.92	0.51
1:C:380:ASP:O	1:C:381:ASN:HB2	2.09	0.51
1:C:393:SER:O	1:C:444:ARG:HB2	2.11	0.50
1:C:271:HIS:HE1	4:C:1114:HOH:O	1.94	0.50
1:A:315:SER:HB2	2:A:1005:SO4:O2	2.12	0.49
1:B:247:ILE:HG12	1:B:289:ASP:HB3	1.93	0.49
1:A:301:HIS:CE1	1:A:369:ASP:OD1	2.55	0.48
1:C:244:LEU:CD2	1:C:258:LEU:HB2	2.43	0.48
1:A:427:TYR:HA	1:A:430:GLU:HG2	1.94	0.48
1:B:272:PHE:CD2	3:B:1021:MES:H22	2.49	0.48
1:C:475:GLU:HG3	1:C:493:TRP:CZ3	2.48	0.48
1:A:381:ASN:O	1:A:414:GLN:NE2	2.47	0.48
1:B:226:GLN:H	1:B:229:GLN:HE21	1.61	0.48
1:B:364:VAL:CG2	1:B:410:LEU:HD11	2.42	0.48
1:C:304:GLN:NE2	4:C:1037:HOH:O	2.32	0.48
1:C:341:PRO:HB3	1:C:342:PRO:HD2	1.94	0.48
1:A:380:ASP:O	1:A:381:ASN:HB2	2.13	0.48
1:C:279:HIS:CG	3:C:1011:MES:H51	2.49	0.47
1:C:351:LEU:HD12	1:C:365:ALA:HB3	1.96	0.47
1:C:364:VAL:HG23	1:C:410:LEU:HD21	1.96	0.47
1:A:303:LEU:O	1:A:311:GLU:HG2	2.15	0.47
1:A:482:HIS:ND1	1:A:491:ASP:OD2	2.44	0.47
1:A:462:ASN:C	1:A:462:ASN:HD22	2.18	0.47
1:B:488:HIS:HD2	1:B:491:ASP:OD2	1.96	0.47
1:A:247:ILE:HG12	1:A:289:ASP:HB3	1.95	0.47
1:C:383:ASP:HB3	1:C:385:THR:HB	1.96	0.47
1:B:458:VAL:CG2	1:B:500:ASP:HB3	2.45	0.47
1:C:275:TYR:CD2	3:C:1011:MES:C8	2.89	0.47
1:A:356:ARG:NH1	1:A:495:ASP:OD2	2.48	0.46
1:C:271:HIS:HD2	1:C:280:ASP:OD2	1.98	0.46
1:C:416:TYR:CG	1:C:417:PRO:HD2	2.50	0.46
1:A:317:SER:N	2:A:1005:SO4:O2	2.33	0.46
1:A:415:ASP:O	1:A:415:ASP:OD1	2.34	0.46
1:B:257:ILE:HD12	1:B:316:TRP:CZ2	2.51	0.46
1:B:460:ARG:HD2	4:B:1158:HOH:O	2.16	0.46
1:C:345:PHE:CE1	1:C:392:PRO:HB3	2.50	0.46
1:C:354:VAL:HG22	1:C:396:TYR:HB3	1.97	0.46
1:C:414:GLN:HA	1:C:414:GLN:OE1	2.16	0.46
1:A:416:TYR:CD1	1:A:417:PRO:HD2	2.51	0.46
1:A:305:PRO:HB2	1:A:309:TYR:CB	2.44	0.46
1:B:303:LEU:O	1:B:311:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:C	1:C:455:LEU:HD12	2.37	0.45
1:A:256:PHE:CZ	3:A:1031:MES:H72	2.51	0.45
1:B:224:LEU:HD22	1:B:448:SER:HB2	1.98	0.45
1:B:382:TRP:CE2	1:B:414:GLN:HB2	2.52	0.45
1:C:316:TRP:HB2	2:C:1006:SO4:O4	2.17	0.45
1:A:382:TRP:CE2	1:A:414:GLN:HB2	2.52	0.44
1:C:355:ASP:OD1	3:C:1012:MES:H32	2.18	0.44
1:C:257:ILE:HD12	1:C:316:TRP:CZ2	2.52	0.44
1:C:410:LEU:HD23	1:C:411:THR:N	2.33	0.44
1:A:222:VAL:HG22	4:A:1173:HOH:O	2.16	0.44
1:C:267:ARG:HD3	1:C:284:ASN:ND2	2.33	0.43
1:C:224:LEU:HD22	1:C:448:SER:HB2	2.00	0.43
1:C:494:ILE:HD13	1:C:501:ILE:HG23	2.01	0.43
1:A:271:HIS:HD2	1:A:280:ASP:OD1	2.01	0.42
1:B:425:GLU:HG2	4:B:1162:HOH:O	2.19	0.42
1:C:455:LEU:C	1:C:455:LEU:CD1	2.88	0.42
1:A:343:LEU:N	1:A:343:LEU:HD12	2.35	0.42
1:B:507:CYS:HB3	1:B:512:HIS:O	2.20	0.41
1:C:444:ARG:HD3	4:C:1036:HOH:O	2.19	0.41
1:B:256:PHE:CE2	3:B:1021:MES:H81	2.56	0.41
1:C:247:ILE:HG12	1:C:289:ASP:HB3	2.01	0.41
1:C:408:LYS:CG	1:C:409:PRO:HD2	2.40	0.41
1:C:430:GLU:O	1:C:430:GLU:HG3	2.19	0.41
1:A:364:VAL:HG13	1:A:424:TRP:CH2	2.56	0.41
1:B:411:THR:HA	1:B:412:PRO:HD3	1.85	0.41
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.86	0.41
1:C:279:HIS:ND1	3:C:1011:MES:H51	2.36	0.41
1:C:275:TYR:CB	3:C:1011:MES:H81	2.49	0.41
1:C:485:GLY:HA3	1:C:518:LEU:O	2.21	0.41
1:A:346:GLN:HG3	1:A:349:MSE:HE3	2.03	0.41
1:C:455:LEU:CD1	1:C:469:ALA:HB3	2.46	0.41
1:B:458:VAL:CG2	1:B:460:ARG:HH21	2.35	0.40
1:A:210:SER:O	1:A:213:GLU:HB2	2.22	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%)	304 (98%)	7 (2%)	0	100	100
1	B	311/331 (94%)	307 (99%)	4 (1%)	0	100	100
1	C	311/331 (94%)	303 (97%)	7 (2%)	1 (0%)	41	26
All	All	933/993 (94%)	914 (98%)	18 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	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%)	267 (96%)	10 (4%)	35	18
1	B	277/286 (97%)	263 (95%)	14 (5%)	24	9
1	C	277/286 (97%)	260 (94%)	17 (6%)	18	5
All	All	831/858 (97%)	790 (95%)	41 (5%)	25	9

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	244	LEU

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Mol	Chain	Res	Type
1	A	268	LEU
1	A	311	GLU
1	A	336	GLN
1	A	410	LEU
1	A	423	CYS
1	A	460	ARG
1	A	462	ASN
1	A	467	ARG
1	B	233	HIS
1	B	244	LEU
1	B	268	LEU
1	B	303	LEU
1	B	315	SER
1	B	357	MSE
1	B	382	TRP
1	B	384	ASP
1	B	390	CYS
1	B	405	LYS
1	B	421	ASN
1	B	444	ARG
1	B	514	LEU
1	B	518	LEU
1	C	206	TRP
1	C	240	LEU
1	C	244	LEU
1	C	268	LEU
1	C	311	GLU
1	C	315	SER
1	C	341	PRO
1	C	346	GLN
1	C	351	LEU
1	C	382	TRP
1	C	383	ASP
1	C	384	ASP
1	C	424	TRP
1	C	430	GLU
1	C	455	LEU
1	C	462	ASN
1	C	514	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	A	271	HIS
1	A	301	HIS
1	A	336	GLN
1	A	378	HIS
1	A	414	GLN
1	A	462	ASN
1	A	488	HIS
1	A	498	HIS
1	B	215	GLN
1	B	229	GLN
1	B	358	ASN
1	B	406	GLN
1	B	488	HIS
1	C	271	HIS
1	C	284	ASN
1	C	301	HIS
1	C	452	ASN
1	C	462	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	1009	-	4,4,4	0.16	0	6,6,6	1.35	2 (33%)
2	SO4	A	1002	-	4,4,4	0.26	0	6,6,6	0.58	0
3	MES	B	1022	-	12,12,12	0.86	0	14,16,16	1.82	4 (28%)
2	SO4	B	1007	-	4,4,4	0.37	0	6,6,6	0.98	1 (16%)
2	SO4	C	1008	-	4,4,4	0.51	0	6,6,6	0.81	0
2	SO4	A	1005	-	4,4,4	0.37	0	6,6,6	0.81	0
2	SO4	B	1003	-	4,4,4	0.20	0	6,6,6	1.02	0
3	MES	C	1011	-	12,12,12	2.72	3 (25%)	14,16,16	2.15	5 (35%)
2	SO4	C	1004	-	4,4,4	0.27	0	6,6,6	0.89	0
3	MES	C	1012	-	12,12,12	1.23	1 (8%)	14,16,16	1.41	2 (14%)
2	SO4	B	1001	-	4,4,4	0.24	0	6,6,6	0.82	0
3	MES	A	1031	-	12,12,12	1.10	1 (8%)	14,16,16	2.25	6 (42%)
3	MES	B	1021	-	12,12,12	0.94	1 (8%)	14,16,16	2.57	6 (42%)
3	MES	A	1032	-	12,12,12	1.08	1 (8%)	14,16,16	1.80	3 (21%)
2	SO4	B	1010	-	4,4,4	0.25	0	6,6,6	0.59	0
2	SO4	C	1006	-	4,4,4	0.29	0	6,6,6	0.52	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	1012	-	-	2/6/14/14	0/1/1/1
3	MES	B	1022	-	-	5/6/14/14	0/1/1/1
3	MES	B	1021	-	-	1/6/14/14	0/1/1/1
3	MES	A	1032	-	-	1/6/14/14	0/1/1/1
3	MES	A	1031	-	-	4/6/14/14	0/1/1/1
3	MES	C	1011	-	-	5/6/14/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1011	MES	C8-S	7.38	1.88	1.77
3	C	1011	MES	C7-N4	4.12	1.56	1.47
3	C	1012	MES	C8-S	3.84	1.83	1.77
3	C	1011	MES	C7-C8	3.28	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1032	MES	C8-S	3.08	1.81	1.77
3	A	1031	MES	C8-S	2.95	1.81	1.77
3	B	1021	MES	C8-S	2.08	1.80	1.77

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1021	MES	O1-C6-C5	-6.17	98.20	111.80
3	A	1031	MES	O1-C2-C3	-5.07	100.63	111.80
3	C	1011	MES	C7-N4-C5	4.27	122.16	111.23
3	B	1021	MES	C5-N4-C3	4.25	118.39	108.83
3	A	1032	MES	C7-N4-C3	3.63	120.51	111.23
3	C	1011	MES	O2S-S-C8	3.49	111.12	106.92
3	A	1031	MES	C7-N4-C3	-3.47	102.35	111.23
3	A	1032	MES	C5-N4-C3	3.44	116.57	108.83
3	B	1022	MES	C7-N4-C5	-3.34	102.70	111.23
3	B	1022	MES	O3S-S-C8	3.17	110.90	105.77
3	C	1011	MES	C6-C5-N4	3.14	114.86	110.10
3	B	1021	MES	O1-C2-C3	-2.99	105.21	111.80
3	B	1022	MES	C7-N4-C3	2.88	118.61	111.23
3	B	1021	MES	C7-N4-C3	-2.85	103.94	111.23
3	C	1012	MES	C5-N4-C3	2.85	115.25	108.83
3	C	1011	MES	O1-C6-C5	-2.59	106.09	111.80
3	B	1022	MES	O1-C6-C5	-2.53	106.21	111.80
3	C	1012	MES	O3S-S-C8	2.47	109.77	105.77
3	C	1011	MES	O3S-S-C8	2.46	109.74	105.77
3	A	1031	MES	O3S-S-C8	2.45	109.73	105.77
3	B	1021	MES	O3S-S-C8	2.35	109.57	105.77
2	B	1009	SO4	O4-S-O2	-2.34	97.07	109.31
3	A	1031	MES	O1S-S-C8	2.30	109.69	106.92
2	B	1009	SO4	O3-S-O2	2.24	121.00	109.31
3	A	1031	MES	C7-N4-C5	-2.19	105.64	111.23
3	A	1031	MES	O1-C6-C5	-2.18	106.98	111.80
3	B	1021	MES	O1S-S-C8	2.11	109.45	106.92
3	A	1032	MES	O2S-S-C8	2.11	109.45	106.92
2	B	1007	SO4	O4-S-O2	-2.01	98.84	109.31

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1021	MES	N4-C7-C8-S

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

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1009	SO4	1	0
2	A	1005	SO4	2	0
3	C	1011	MES	8	0
3	C	1012	MES	3	0
3	A	1031	MES	1	0
3	B	1021	MES	4	0
2	C	1006	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%)	0.46	28 (9%) 9 8	17, 26, 39, 47	0
1	B	308/331 (93%)	0.22	11 (3%) 42 40	13, 23, 34, 42	0
1	C	308/331 (93%)	0.68	43 (13%) 2 3	17, 28, 44, 50	0
All	All	924/993 (93%)	0.45	82 (8%) 9 9	13, 25, 39, 50	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	443	VAL	7.4
1	C	421	ASN	7.2
1	C	417	PRO	7.0
1	A	310	LYS	6.7
1	A	312	GLU	5.6
1	C	343	LEU	5.3
1	C	340	PRO	5.2
1	C	418	ASP	5.0
1	C	425	GLU	4.9
1	C	404	GLN	4.8
1	C	420	ASP	4.7
1	A	343	LEU	4.6
1	A	311	GLU	4.5
1	C	312	GLU	4.3
1	B	421	ASN	4.2
1	C	416	TYR	4.2
1	A	518	LEU	4.1
1	C	313	GLU	4.1
1	C	407	GLY	4.0
1	B	312	GLU	4.0
1	B	443	VAL	4.0
1	C	419	PRO	3.9
1	C	414	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	339	SER	3.9
1	C	422	PHE	3.6
1	A	469	ALA	3.6
1	A	418	ASP	3.6
1	C	423	CYS	3.6
1	C	382	TRP	3.5
1	A	340	PRO	3.4
1	C	409	PRO	3.3
1	C	310	LYS	3.3
1	C	311	GLU	3.3
1	B	455	LEU	3.2
1	C	401	GLY	3.2
1	B	469	ALA	3.2
1	C	341	PRO	3.1
1	C	415	ASP	3.1
1	A	216	LYS	3.1
1	C	405	LYS	3.1
1	A	213	GLU	3.0
1	B	311	GLU	3.0
1	A	308	GLY	3.0
1	C	209	GLU	3.0
1	A	455	LEU	2.9
1	C	429	GLU	2.9
1	C	324	ARG	2.8
1	A	309	TYR	2.8
1	A	321	ARG	2.7
1	A	415	ASP	2.7
1	A	490	TYR	2.7
1	C	216	LYS	2.7
1	B	518	LEU	2.6
1	B	310	LYS	2.6
1	C	210	SER	2.5
1	A	313	GLU	2.5
1	A	258	LEU	2.5
1	A	443	VAL	2.5
1	C	455	LEU	2.5
1	C	469	ALA	2.4
1	C	214	GLU	2.3
1	A	257	ILE	2.3
1	A	425	GLU	2.3
1	B	420	ASP	2.3
1	C	268	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	458	VAL	2.3
1	A	417	PRO	2.3
1	C	412	PRO	2.2
1	A	461	ARG	2.2
1	C	258	LEU	2.2
1	C	213	GLU	2.2
1	B	457	ALA	2.2
1	A	414	GLN	2.2
1	C	406	GLN	2.1
1	A	209	GLU	2.1
1	C	358	ASN	2.1
1	C	410	LEU	2.1
1	A	341	PRO	2.1
1	A	297	GLU	2.1
1	B	257	ILE	2.1
1	C	408	LYS	2.1
1	A	421	ASN	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 carbohydrates 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(\AA^2)	Q<0.9
3	MES	B	1021	12/12	0.64	0.36	40,42,50,51	0
3	MES	A	1031	12/12	0.73	0.33	37,39,49,49	0
2	SO4	C	1008	5/5	0.77	0.34	36,40,45,46	0
2	SO4	B	1007	5/5	0.78	0.28	42,43,46,49	0
3	MES	C	1011	12/12	0.79	0.31	36,41,48,48	0
2	SO4	A	1005	5/5	0.85	0.35	47,47,49,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MES	C	1012	12/12	0.85	0.23	33,37,41,42	0
2	SO4	C	1004	5/5	0.89	0.29	40,42,43,46	0
3	MES	B	1022	12/12	0.91	0.14	20,25,37,39	0
3	MES	A	1032	12/12	0.91	0.12	24,29,35,36	0
2	SO4	B	1010	5/5	0.91	0.35	37,41,41,43	0
2	SO4	C	1006	5/5	0.91	0.48	49,51,54,54	0
2	SO4	B	1003	5/5	0.94	0.18	37,40,43,43	0
2	SO4	B	1009	5/5	0.95	0.16	33,33,37,38	0
2	SO4	A	1002	5/5	0.98	0.13	37,41,41,43	0
2	SO4	B	1001	5/5	0.98	0.15	30,31,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.