Full wwPDB X-ray Structure Validation Report

May 25, 2020 – 07:33 am BST

PDB ID	:	1OYX
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

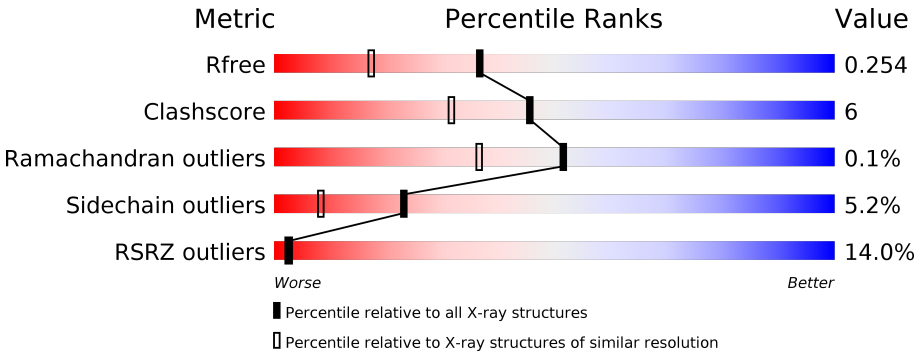
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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 <=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	17% 76% 16% • 5%
1	B	331	8% 79% 12% • 5%
1	C	331	14% 80% 13% • 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	B	2011	-	-	-	X
2	SO4	C	2003	-	X	-	X
3	MES	A	1011	-	-	X	-
3	MES	B	1021	-	-	X	X

2 Entry composition (i)

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.

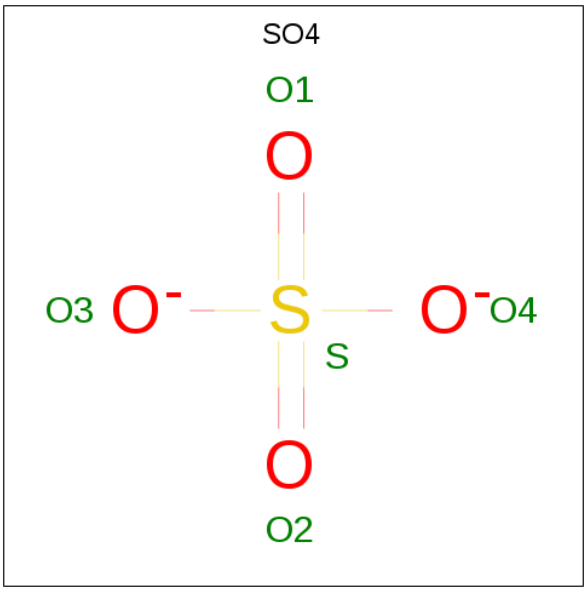
- Molecule 1 is a protein called Lethal(3)malignant brain tumor-like protein.

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:

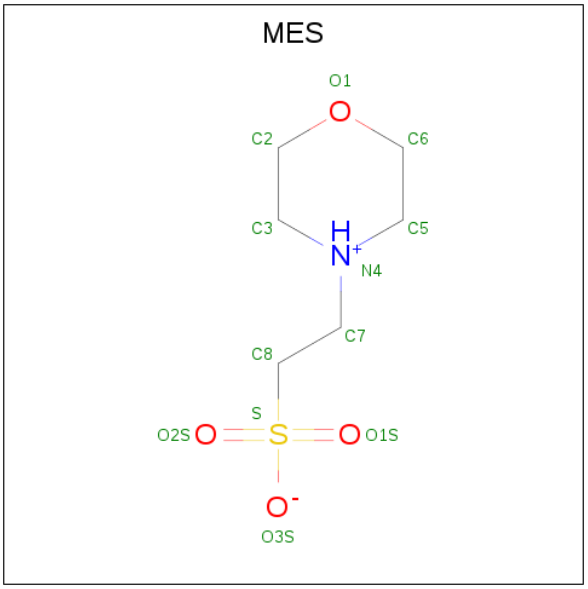
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	MSE	MET	MODIFIED RESIDUE	UNP Q9Y468
A	254	MSE	MET	MODIFIED RESIDUE	UNP Q9Y468
A	349	MSE	MET	MODIFIED RESIDUE	UNP Q9Y468
A	357	MSE	MET	MODIFIED RESIDUE	UNP Q9Y468
A	453	MSE	MET	MODIFIED RESIDUE	UNP Q9Y468
B	242	MSE	MET	MODIFIED RESIDUE	UNP Q9Y468
B	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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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.

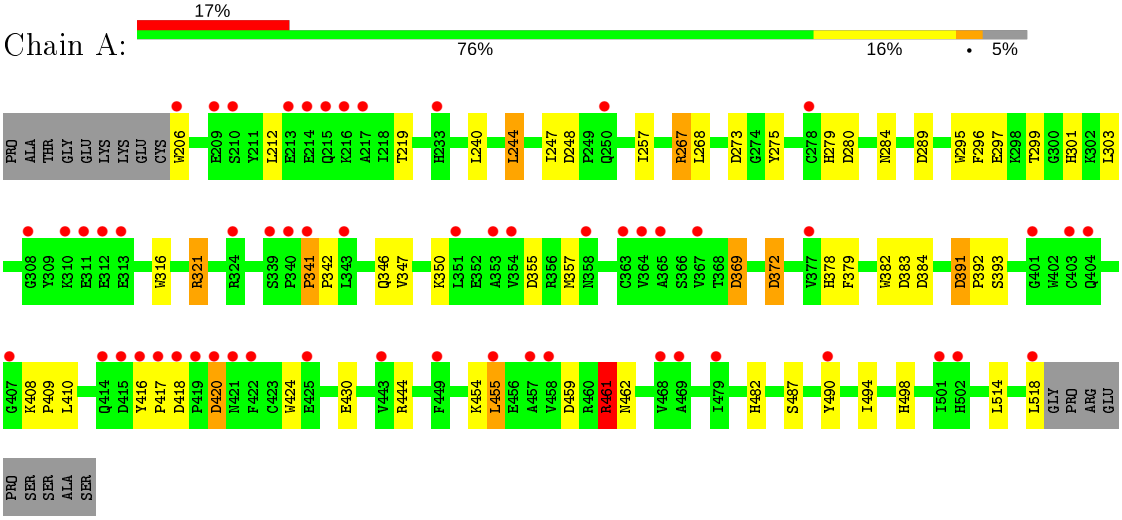
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	201	Total	O	0	0
			201	201		
4	C	188	Total	O	0	0
			188	188		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

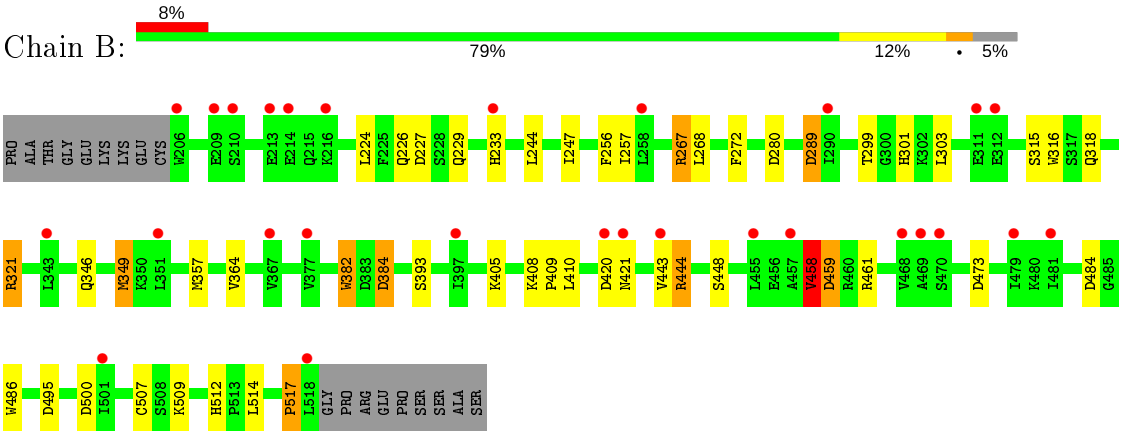
- Molecule 1: Lethal(3)malignant brain tumor-like protein

Chain A:



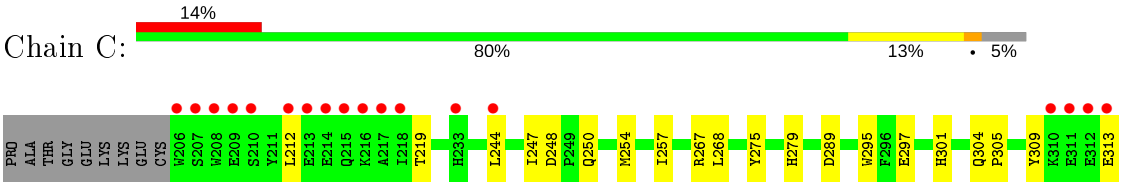
- Molecule 1: Lethal(3)malignant brain tumor-like protein

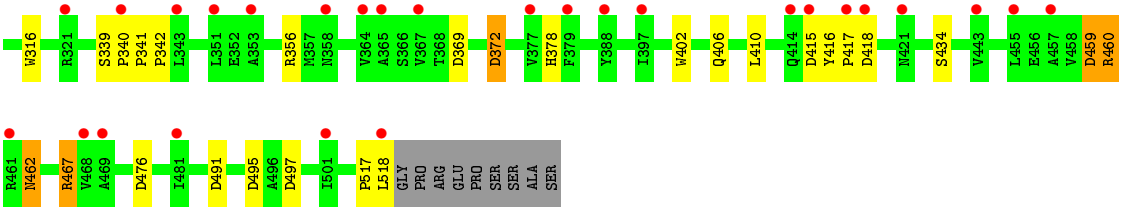
Chain B:



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

Chain C:




W316
R321
S339
P340
P341
P342
L343
L351
E352
A353
R356
M357
N358
V364
A365
S366
V367
T368
D369
D372
V377
H378
F379
Y388
I397
W402
Q406
L410
Q414
D415
Y416
P417
D418
N421
S434
V443
L455
E456
A457
V458
D459
R460
R461
N462
R467
V468
A469
D476
I481
D491
D495
A496
D497
I501
P517
L518
GLY
PRO
ARG
GLU
PRO
SER
SER
ALA
SER

4 Data and refinement statistics (i)

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 19.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.84-1.85) 97.0 (19.50-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.13	Depositor
R, R_{free}	0.207 , 0.238 0.231 , 0.254	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 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.70	1/2639 (0.0%)	0.86	12/3599 (0.3%)
1	B	0.86	1/2639 (0.0%)	1.48	14/3599 (0.4%)
1	C	0.80	1/2639 (0.0%)	0.87	7/3599 (0.2%)
All	All	0.79	3/7917 (0.0%)	1.11	33/10797 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	GLU	CD-OE1	5.87	1.32	1.25
1	B	458	VAL	CB-CG2	-5.70	1.40	1.52
1	A	267	ARG	CZ-NH1	5.35	1.40	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	517	PRO	O-C-N	-67.86	14.12	122.70
1	B	267	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	B	267	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	A	459	ASP	CB-CG-OD2	8.08	125.57	118.30
1	B	459	ASP	CB-CG-OD2	7.96	125.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	248	ASP	CB-CG-OD2	7.79	125.31	118.30
1	B	384	ASP	CB-CG-OD2	7.72	125.25	118.30
1	B	473	ASP	CB-CG-OD2	7.51	125.06	118.30
1	B	227	ASP	CB-CG-OD2	7.46	125.02	118.30
1	C	267	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	384	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	C	459	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	248	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	267	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	280	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	369	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	280	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	372	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	497	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	355	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	289	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	484	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	391	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	476	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	420	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	420	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	349	MSE	CG-SE-CE	5.34	110.65	98.90
1	B	495	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	491	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	244	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	273	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	418	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	372	ASP	CB-CG-OD2	5.02	122.81	118.30

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	37	0
1	C	2545	0	2380	25	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	5	0
4	B	201	0	0	4	0
4	C	188	0	0	3	0
All	All	8296	0	7229	96	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 6.

All (96) 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
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	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:460:ARG:HE	1:C:460:ARG:HA	1.65	0.60
1:A:341:PRO:HB3	1:A:342:PRO:HD2	1.84	0.59
1:B:364:VAL:HG23	1:B:410:LEU:HD11	1.86	0.58
1:C:402:TRP:CE2	1:C:406:GLN:HG3	2.40	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:C:254:MSE:HE2	1:C:304:GLN:CD	2.26	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
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:A:455:LEU:C	1:A:455:LEU:HD12	2.29	0.53
1:C:247:ILE:HG12	1:C:289:ASP:HB3	1.91	0.53
1:C:462:ASN:C	1:C:462:ASN:HD22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:350:LYS:NZ	4:A:2034:HOH:O	2.52	0.42
1:C:416:TYR:CG	1:C:417:PRO:HD2	2.55	0.42
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:HB2	1:A:461:ARG:HE	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:C:416:TYR:CD1	1:C:417:PRO:HD2	2.56	0.41
1:B:224:LEU:HD22	1:B:448:SER:HB2	2.02	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 (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%)	306 (98%)	4 (1%)	1 (0%)	41 26
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%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	PRO

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	277/286 (97%)	257 (93%)	20 (7%)	14 3
1	B	277/286 (97%)	264 (95%)	13 (5%)	26 10
1	C	277/286 (97%)	267 (96%)	10 (4%)	35 18
All	All	831/858 (97%)	788 (95%)	43 (5%)	23 8

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	TRP
1	A	240	LEU

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Mol	Chain	Res	Type
1	A	244	LEU
1	A	268	LEU
1	A	303	LEU
1	A	321	ARG
1	A	346	GLN
1	A	357	MSE
1	A	382	TRP
1	A	383	ASP
1	A	384	ASP
1	A	410	LEU
1	A	420	ASP
1	A	424	TRP
1	A	430	GLU
1	A	455	LEU
1	A	461	ARG
1	A	462	ASN
1	A	514	LEU
1	A	518	LEU
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	405	LYS
1	B	421	ASN
1	B	444	ARG
1	B	458	VAL
1	B	514	LEU
1	C	244	LEU
1	C	268	LEU
1	C	313	GLU
1	C	410	LEU
1	C	415	ASP
1	C	418	ASP
1	C	434	SER
1	C	460	ARG
1	C	462	ASN
1	C	467	ARG

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	HIS
1	A	284	ASN
1	A	301	HIS
1	A	304	GLN
1	A	378	HIS
1	A	462	ASN
1	B	215	GLN
1	B	229	GLN
1	B	406	GLN
1	B	488	HIS
1	C	271	HIS
1	C	301	HIS
1	C	378	HIS
1	C	406	GLN
1	C	462	ASN

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 carbohydrates 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	B	2009	-	4,4,4	0.17	0	6,6,6	0.44	0
3	MES	C	1032	-	12,12,12	1.05	1 (8%)	14,16,16	1.32	2 (14%)
2	SO4	C	2006	-	4,4,4	0.18	0	6,6,6	0.62	0
2	SO4	A	2012	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	B	2013	-	4,4,4	0.28	0	6,6,6	1.14	1 (16%)
2	SO4	B	2001	-	4,4,4	0.19	0	6,6,6	0.80	0
2	SO4	C	2003	-	4,4,4	1.83	1 (25%)	6,6,6	1.94	3 (50%)
2	SO4	C	2007	-	4,4,4	1.12	0	6,6,6	0.76	0
2	SO4	B	2014	-	4,4,4	0.17	0	6,6,6	0.44	0
2	SO4	B	2004	-	4,4,4	0.15	0	6,6,6	0.40	0
3	MES	B	1023	-	12,12,12	1.31	1 (8%)	14,16,16	1.90	5 (35%)
3	MES	B	1022	-	12,12,12	0.75	0	14,16,16	1.69	2 (14%)
3	MES	C	1031	-	12,12,12	0.92	1 (8%)	14,16,16	2.12	7 (50%)
3	MES	A	1012	-	12,12,12	1.18	1 (8%)	14,16,16	1.78	5 (35%)
2	SO4	A	2008	-	4,4,4	0.23	0	6,6,6	0.28	0
2	SO4	B	2011	-	4,4,4	1.32	1 (25%)	6,6,6	1.25	0
3	MES	A	1011	-	12,12,12	2.28	3 (25%)	14,16,16	2.14	7 (50%)
3	MES	B	1021	-	12,12,12	1.09	1 (8%)	14,16,16	1.88	4 (28%)
2	SO4	A	2010	-	4,4,4	0.26	0	6,6,6	0.53	0
2	SO4	A	2005	-	4,4,4	0.13	0	6,6,6	0.33	0
2	SO4	C	2002	-	4,4,4	0.18	0	6,6,6	0.44	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	1032	-	-	1/6/14/14	0/1/1/1
3	MES	B	1023	-	-	5/6/14/14	0/1/1/1
3	MES	B	1022	-	-	4/6/14/14	0/1/1/1
3	MES	C	1031	-	-	2/6/14/14	0/1/1/1
3	MES	A	1012	-	-	5/6/14/14	0/1/1/1
3	MES	A	1011	-	-	5/6/14/14	0/1/1/1
3	MES	B	1021	-	-	2/6/14/14	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	6.76	1.87	1.77
3	B	1023	MES	C8-S	3.90	1.83	1.77
3	A	1012	MES	C8-S	3.68	1.82	1.77
3	B	1021	MES	C8-S	3.23	1.82	1.77
3	C	1032	MES	C8-S	3.06	1.81	1.77
3	A	1011	MES	C7-N4	2.89	1.54	1.47
2	C	2003	SO4	O1-S	2.72	1.60	1.46
3	C	1031	MES	C8-S	2.62	1.81	1.77
2	B	2011	SO4	O1-S	2.19	1.57	1.46
3	A	1011	MES	C7-C8	2.06	1.58	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1021	MES	O1-C6-C5	-4.01	102.97	111.80
3	B	1023	MES	C2-C3-N4	3.98	116.14	110.10
3	A	1012	MES	C5-N4-C3	3.69	117.14	108.83
3	C	1031	MES	C2-C3-N4	3.61	115.58	110.10
3	A	1011	MES	C6-C5-N4	3.61	115.58	110.10
3	B	1022	MES	C7-N4-C5	-3.50	102.29	111.23
3	B	1022	MES	O3S-S-C8	3.41	111.28	105.77
3	C	1031	MES	C5-N4-C3	3.27	116.18	108.83
3	B	1021	MES	C5-N4-C3	3.10	115.80	108.83
3	B	1023	MES	C6-C5-N4	2.94	114.56	110.10
2	C	2003	SO4	O4-S-O1	-2.93	94.00	109.31
3	A	1011	MES	C7-N4-C5	2.88	118.60	111.23
3	A	1011	MES	O1-C6-C5	-2.80	105.63	111.80
3	A	1011	MES	C2-C3-N4	2.79	114.33	110.10
3	A	1011	MES	O3S-S-C8	2.71	110.15	105.77
3	A	1011	MES	O2S-S-C8	2.61	110.06	106.92
3	C	1031	MES	O1-C6-C5	-2.53	106.23	111.80
2	C	2003	SO4	O3-S-O2	2.50	122.36	109.31
3	B	1023	MES	O3S-S-C8	2.43	109.70	105.77
2	C	2003	SO4	O4-S-O3	2.43	119.42	109.06
3	A	1012	MES	O3S-S-C8	2.42	109.68	105.77
3	B	1021	MES	O3S-S-C8	2.39	109.63	105.77
3	C	1031	MES	O2S-S-C8	2.36	109.75	106.92
3	B	1023	MES	O1S-S-C8	2.30	109.69	106.92
3	C	1031	MES	O3S-S-C8	2.27	109.43	105.77
3	C	1031	MES	C7-N4-C5	-2.26	105.45	111.23
3	C	1032	MES	O3S-S-C8	2.17	109.28	105.77
3	A	1011	MES	C5-N4-C3	2.17	113.71	108.83
3	B	1021	MES	O1S-S-C8	2.15	109.51	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1023	MES	O2S-S-C8	2.15	109.50	106.92
3	C	1031	MES	O1S-S-C8	2.15	109.50	106.92
3	A	1012	MES	C2-C3-N4	2.11	113.30	110.10
3	A	1012	MES	O1S-S-C8	2.10	109.44	106.92
2	B	2013	SO4	O3-S-O2	2.09	120.22	109.31
3	C	1032	MES	O2S-S-C8	2.03	109.36	106.92
3	A	1012	MES	C7-N4-C3	2.03	116.42	111.23

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1032	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	A	1012	MES	C8-C7-N4-C3
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	B	1021	MES	N4-C7-C8-S
3	A	1012	MES	C7-C8-S-O3S
3	B	1023	MES	C8-C7-N4-C5
3	A	1012	MES	C8-C7-N4-C5
3	B	1022	MES	C7-C8-S-O1S
3	B	1023	MES	C7-C8-S-O2S
3	A	1012	MES	C7-C8-S-O2S
3	A	1011	MES	C7-C8-S-O1S
3	B	1021	MES	C7-C8-S-O1S
3	C	1031	MES	C8-C7-N4-C5
3	B	1023	MES	C7-C8-S-O3S
3	A	1012	MES	C7-C8-S-O1S

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1023	MES	4	0
3	C	1031	MES	3	0
3	A	1011	MES	6	0
3	B	1021	MES	8	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, 95^{th} 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%)	0.99	56 (18%) 1 1	13, 37, 67, 81	0
1	B	308/331 (93%)	0.55	28 (9%) 9 8	13, 29, 46, 60	0
1	C	308/331 (93%)	0.76	45 (14%) 2 2	13, 32, 53, 65	0
All	All	924/993 (93%)	0.77	129 (13%) 2 3	13, 33, 57, 81	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	VAL	8.9
1	A	421	ASN	7.5
1	A	417	PRO	6.9
1	A	312	GLU	6.4
1	C	340	PRO	5.7
1	C	310	LYS	5.7
1	A	455	LEU	5.6
1	A	418	ASP	5.6
1	A	420	ASP	5.4
1	C	455	LEU	5.4
1	B	312	GLU	5.3
1	C	216	LYS	5.1
1	B	455	LEU	5.1
1	C	312	GLU	5.1
1	C	418	ASP	5.0
1	A	343	LEU	5.0
1	A	216	LYS	4.8
1	A	210	SER	4.7
1	B	469	ALA	4.6
1	A	340	PRO	4.5
1	C	469	ALA	4.4
1	A	425	GLU	4.4
1	C	209	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	311	GLU	4.3
1	A	209	GLU	4.3
1	C	210	SER	4.3
1	B	443	VAL	4.2
1	A	351	LEU	4.1
1	A	313	GLU	4.1
1	A	206	TRP	4.1
1	C	351	LEU	4.1
1	C	518	LEU	4.0
1	A	469	ALA	3.9
1	B	518	LEU	3.9
1	A	419	PRO	3.8
1	A	339	SER	3.8
1	A	213	GLU	3.8
1	B	457	ALA	3.7
1	C	417	PRO	3.7
1	C	311	GLU	3.7
1	A	310	LYS	3.5
1	C	218	ILE	3.5
1	C	213	GLU	3.5
1	A	353	ALA	3.5
1	C	206	TRP	3.4
1	A	416	TYR	3.4
1	C	501	ILE	3.3
1	A	490	TYR	3.2
1	C	321	ARG	3.2
1	C	457	ALA	3.2
1	C	212	LEU	3.2
1	C	377	VAL	3.2
1	A	415	ASP	3.1
1	B	481	ILE	3.1
1	C	468	VAL	3.0
1	A	214	GLU	3.0
1	C	214	GLU	3.0
1	B	421	ASN	3.0
1	A	457	ALA	3.0
1	B	351	LEU	3.0
1	B	397	ILE	3.0
1	A	414	GLN	3.0
1	C	365	ALA	3.0
1	B	209	GLU	2.9
1	C	343	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	468	VAL	2.9
1	B	468	VAL	2.9
1	A	501	ILE	2.8
1	C	443	VAL	2.8
1	C	353	ALA	2.8
1	B	213	GLU	2.8
1	B	501	ILE	2.8
1	B	367	VAL	2.8
1	C	364	VAL	2.8
1	C	379	PHE	2.7
1	A	217	ALA	2.7
1	A	215	GLN	2.7
1	A	458	VAL	2.7
1	A	518	LEU	2.7
1	C	414	GLN	2.7
1	A	278	CYS	2.7
1	C	233	HIS	2.7
1	A	354	VAL	2.7
1	C	215	GLN	2.6
1	A	364	VAL	2.6
1	C	207	SER	2.5
1	A	403	CYS	2.5
1	C	388	TYR	2.5
1	A	341	PRO	2.5
1	A	365	ALA	2.5
1	B	258	LEU	2.5
1	A	404	GLN	2.4
1	B	377	VAL	2.4
1	B	214	GLU	2.4
1	C	217	ALA	2.4
1	C	461	ARG	2.4
1	A	377	VAL	2.4
1	B	216	LYS	2.4
1	B	479	ILE	2.4
1	A	422	PHE	2.3
1	B	206	TRP	2.3
1	C	313	GLU	2.3
1	B	233	HIS	2.3
1	B	210	SER	2.3
1	A	358	ASN	2.3
1	A	250	GLN	2.2
1	B	311	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	208	TRP	2.2
1	A	367	VAL	2.2
1	A	449	PHE	2.2
1	B	420	ASP	2.2
1	C	358	ASN	2.1
1	C	421	ASN	2.1
1	A	407	GLY	2.1
1	B	470	SER	2.1
1	A	502	HIS	2.1
1	C	367	VAL	2.1
1	A	363	CYS	2.1
1	A	479	ILE	2.1
1	B	290	ILE	2.1
1	A	308	GLY	2.1
1	A	324	ARG	2.1
1	B	343	LEU	2.1
1	C	481	ILE	2.1
1	A	401	GLY	2.1
1	C	415	ASP	2.0
1	A	233	HIS	2.0
1	C	244	LEU	2.0
1	C	397	ILE	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, 95^{th} 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	B	1021	12/12	0.51	0.44	86,88,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	C	1031	12/12	0.61	0.40	76,79,89,89	0
2	SO4	A	2012	5/5	0.64	0.32	102,103,104,104	0
2	SO4	B	2011	5/5	0.64	0.49	33,33,35,38	0
3	MES	B	1023	12/12	0.68	0.34	76,78,89,90	0
2	SO4	C	2003	5/5	0.74	0.60	27,29,29,35	0
3	MES	A	1011	12/12	0.75	0.35	71,74,76,76	0
3	MES	A	1012	12/12	0.75	0.22	66,67,71,71	0
3	MES	C	1032	12/12	0.76	0.18	48,51,54,55	0
2	SO4	A	2010	5/5	0.77	0.21	76,77,80,80	0
2	SO4	A	2005	5/5	0.80	0.26	88,89,90,90	0
2	SO4	C	2007	5/5	0.85	0.47	32,33,37,40	0
3	MES	B	1022	12/12	0.90	0.14	32,37,50,50	0
2	SO4	B	2009	5/5	0.91	0.15	68,69,71,72	0
2	SO4	B	2013	5/5	0.92	0.20	51,53,56,59	0
2	SO4	C	2006	5/5	0.93	0.17	74,74,75,78	0
2	SO4	B	2004	5/5	0.94	0.20	69,69,70,71	0
2	SO4	B	2014	5/5	0.95	0.21	82,83,84,85	0
2	SO4	C	2002	5/5	0.95	0.12	62,63,64,64	0
2	SO4	A	2008	5/5	0.96	0.23	92,93,93,94	0
2	SO4	B	2001	5/5	0.97	0.13	49,51,53,55	0

6.5 Other polymers

There are no such residues in this entry.