Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:19 PM GMT

PDB ID	:	3TKU
Title	:	MRCK beta in complex with fasudil
Authors	:	Heikkila, T.J.; Turnbull, A.; Wheatley, E.; Schroder, E.; Crighton, D.; Olson, M.F.
Deposited on	:	2011-08-29
Resolution	:	2.15 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

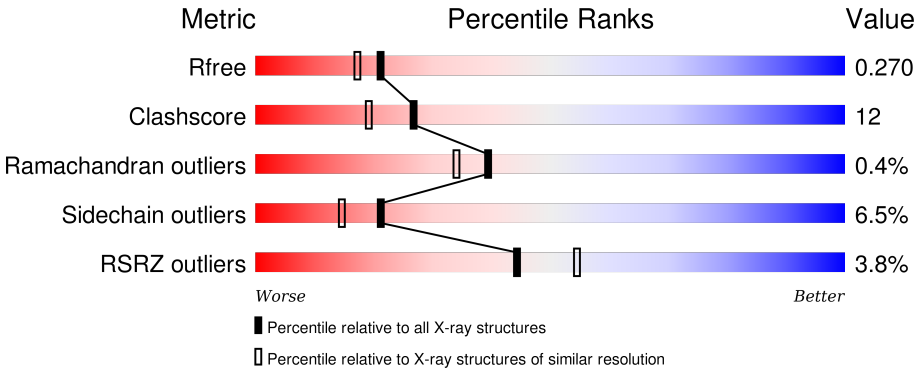
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	433	4% 70% 18% • 9%
1	B	433	3% 71% 17% •• 9%

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	M77	A	419	-	-	-	X
2	M77	B	419	-	-	-	X
3	EDO	A	420	-	-	-	X
3	EDO	B	420	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6531 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 Serine/threonine-protein kinase MRCK beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3110	1998	511	581	20			
1	B	395	Total	C	N	O	S	0	0	0
			3115	2005	507	583	20			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q9Y5S2
A	-14	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
A	-13	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
A	-12	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
A	-11	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
A	-10	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
A	-9	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
A	-8	SER	-	EXPRESSION TAG	UNP Q9Y5S2
A	-7	SER	-	EXPRESSION TAG	UNP Q9Y5S2
A	-6	GLY	-	EXPRESSION TAG	UNP Q9Y5S2
A	-5	GLU	-	EXPRESSION TAG	UNP Q9Y5S2
A	-4	ASN	-	EXPRESSION TAG	UNP Q9Y5S2
A	-3	LEU	-	EXPRESSION TAG	UNP Q9Y5S2
A	-2	TYR	-	EXPRESSION TAG	UNP Q9Y5S2
A	-1	PHE	-	EXPRESSION TAG	UNP Q9Y5S2
A	0	GLN	-	EXPRESSION TAG	UNP Q9Y5S2
A	1	GLY	-	EXPRESSION TAG	UNP Q9Y5S2
B	-15	MET	-	EXPRESSION TAG	UNP Q9Y5S2
B	-14	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
B	-13	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
B	-12	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
B	-11	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
B	-10	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
B	-9	HIS	-	EXPRESSION TAG	UNP Q9Y5S2
B	-8	SER	-	EXPRESSION TAG	UNP Q9Y5S2

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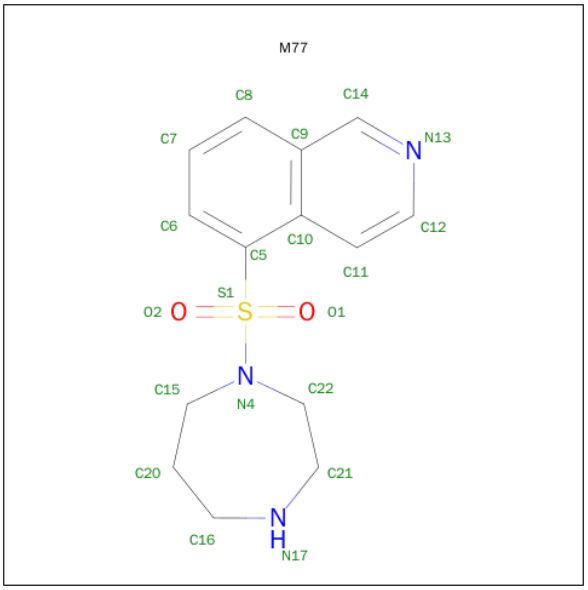
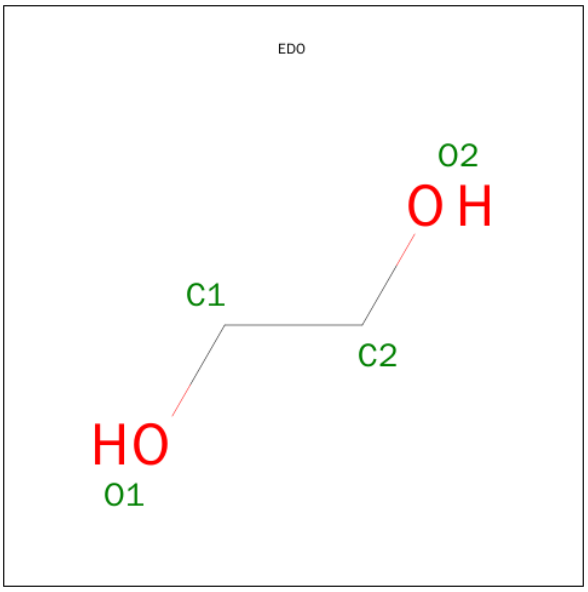
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	SER	-	EXPRESSION TAG	UNP Q9Y5S2
B	-6	GLY	-	EXPRESSION TAG	UNP Q9Y5S2
B	-5	GLU	-	EXPRESSION TAG	UNP Q9Y5S2
B	-4	ASN	-	EXPRESSION TAG	UNP Q9Y5S2
B	-3	LEU	-	EXPRESSION TAG	UNP Q9Y5S2
B	-2	TYR	-	EXPRESSION TAG	UNP Q9Y5S2
B	-1	PHE	-	EXPRESSION TAG	UNP Q9Y5S2
B	0	GLN	-	EXPRESSION TAG	UNP Q9Y5S2
B	1	GLY	-	EXPRESSION TAG	UNP Q9Y5S2

- Molecule 2 is 5-(1,4-DIAZEPAN-1-SULFONYL)ISOQUINOLINE (three-letter code: M77) (formula: $C_{14}H_{17}N_3O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	14	3	2	1		
2	A	1	Total	C	N	O	S	0	0
			20	14	3	2	1		
2	B	1	Total	C	N	O	S	0	0
			20	14	3	2	1		
2	B	1	Total	C	N	O	S	0	0
			20	14	3	2	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

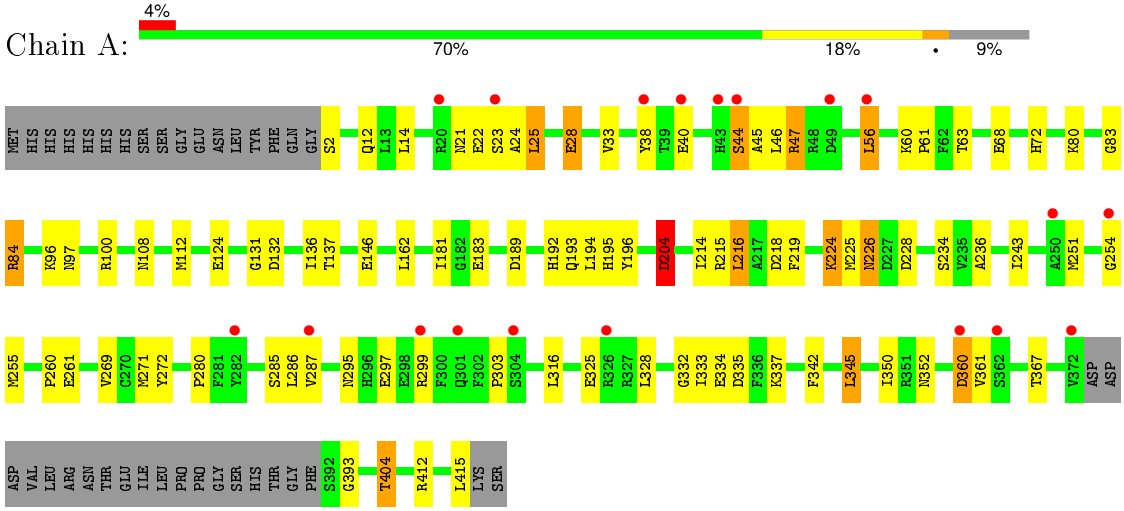
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	109	Total O 109 109	0	0
4	B	109	Total O 109 109	0	0

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 errors 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.

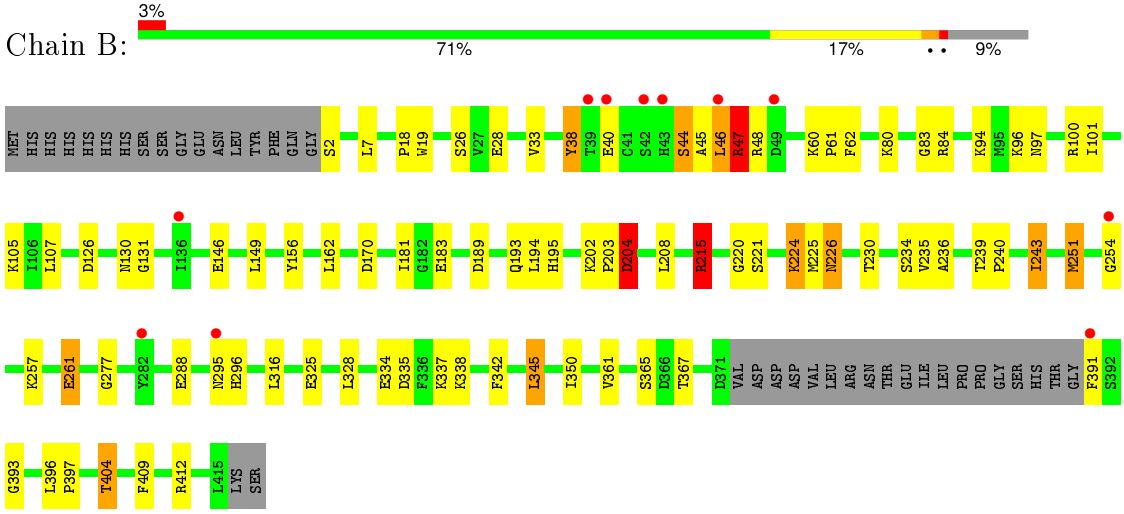
- Molecule 1: Serine/threonine-protein kinase MRCK beta

Chain A:



- Molecule 1: Serine/threonine-protein kinase MRCK beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.95Å 123.52Å 84.77Å 90.00° 101.13° 90.00°	Depositor
Resolution (Å)	40.00 – 2.15 49.59 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (40.00-2.15) 97.3 (49.59-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.221 , 0.273 0.220 , 0.270	Depositor DCC
R_{free} test set	2412 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 47927 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6531	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: M77, EDO

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	1.06	5/3182 (0.2%)	1.02	13/4315 (0.3%)
1	B	1.06	5/3188 (0.2%)	1.01	12/4322 (0.3%)
All	All	1.06	10/6370 (0.2%)	1.02	25/8637 (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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	VAL	CB-CG1	-7.70	1.36	1.52
1	B	33	VAL	CB-CG2	-7.04	1.38	1.52
1	A	33	VAL	CB-CG1	-6.63	1.39	1.52
1	B	215	ARG	CZ-NH1	-5.72	1.25	1.33
1	A	33	VAL	CB-CG2	-5.63	1.41	1.52
1	A	219	PHE	CG-CD1	-5.46	1.30	1.38
1	B	183	GLU	CB-CG	5.40	1.62	1.52
1	B	261	GLU	CD-OE2	-5.29	1.19	1.25
1	A	215	ARG	CZ-NH1	-5.10	1.26	1.33
1	A	261	GLU	CD-OE1	-5.03	1.20	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	VAL	CG1-CB-CG2	-10.39	94.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	84	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	A	100	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	B	215	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	33	VAL	CG1-CB-CG2	-8.86	96.72	110.90
1	A	215	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	B	84	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	B	84	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	B	100	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	412	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	100	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	204	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	226	ASN	CB-CA-C	-6.37	97.66	110.40
1	A	84	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	261	GLU	CA-CB-CG	6.16	126.95	113.40
1	A	28	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	B	204	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	226	ASN	CB-CA-C	-5.91	98.58	110.40
1	A	360	ASP	CB-CG-OD1	5.88	123.60	118.30
1	B	243	ILE	CG1-CB-CG2	-5.68	98.90	111.40
1	B	84	ARG	CD-NE-CZ	5.48	131.27	123.60
1	A	261	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	A	218	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	261	GLU	OE1-CD-OE2	-5.11	117.17	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3110	0	2950	58	0
1	B	3115	0	2955	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	0	34	8	0
2	B	40	0	34	8	0
3	A	4	0	6	1	0
3	B	4	0	6	7	0
4	A	109	0	0	7	0
4	B	109	0	0	5	0
All	All	6531	0	5985	149	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 12.

All (149) 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:234:SER:CB	1:B:254:GLY:O	1.91	1.18
1:B:45:ALA:HA	1:B:47:ARG:HH12	1.14	1.08
1:B:45:ALA:HA	1:B:47:ARG:NH1	1.69	1.07
1:A:80:LYS:HD3	1:A:367:THR:HG21	1.32	1.07
1:B:220:GLY:HA3	3:B:420:EDO:H21	1.36	1.05
1:B:80:LYS:HD3	1:B:367:THR:HG21	1.39	1.03
1:B:234:SER:HB3	1:B:254:GLY:O	1.57	1.02
2:B:419:M77:O2	2:B:419:M77:H11	1.67	0.95
1:A:131:GLY:HA2	1:A:194:LEU:HD11	1.47	0.94
1:A:131:GLY:O	4:A:457:HOH:O	1.84	0.93
1:B:131:GLY:HA2	1:B:194:LEU:HD11	1.50	0.93
1:A:28:GLU:OE2	1:A:404:THR:HG22	1.75	0.86
1:B:234:SER:HB2	1:B:254:GLY:O	1.76	0.85
2:A:418:M77:H6	2:A:418:M77:H222	1.59	0.84
1:B:105:LYS:NZ	3:B:420:EDO:H22	1.95	0.82
2:A:418:M77:C6	2:A:418:M77:H222	2.09	0.82
1:B:195:HIS:HA	1:B:225:MET:HE3	1.63	0.80
1:B:40:GLU:OE2	1:B:393:GLY:N	2.14	0.80
1:A:195:HIS:HA	1:A:225:MET:HE3	1.62	0.79
2:B:418:M77:H6	2:B:418:M77:H222	1.68	0.76
1:B:296:HIS:HD2	4:B:438:HOH:O	1.68	0.75
1:B:19:TRP:HZ3	1:B:130:ASN:OD1	1.69	0.75
1:B:47:ARG:HH11	1:B:47:ARG:CG	2.00	0.74
2:A:419:M77:O2	2:A:419:M77:H11	1.87	0.74
1:A:136:ILE:HD11	4:A:463:HOH:O	1.88	0.74
1:B:28:GLU:OE1	1:B:404:THR:HG22	1.87	0.73
1:B:224:LYS:O	4:B:495:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:M77:C6	2:B:418:M77:H222	2.20	0.72
1:A:22:GLU:O	1:A:23:SER:CB	2.37	0.71
1:B:105:LYS:HZ1	3:B:420:EDO:C2	2.04	0.70
1:B:44:SER:C	1:B:46:LEU:H	1.94	0.70
1:B:220:GLY:CA	3:B:420:EDO:H21	2.20	0.69
1:B:45:ALA:CA	1:B:47:ARG:HH12	1.99	0.69
1:B:230:THR:OG1	1:B:257:LYS:HG2	1.93	0.68
1:B:367:THR:O	1:B:367:THR:HG22	1.93	0.68
1:A:367:THR:HG22	1:A:367:THR:O	1.94	0.68
1:B:105:LYS:HZ3	3:B:420:EDO:H22	1.57	0.66
1:A:28:GLU:OE2	1:A:404:THR:CG2	2.43	0.66
1:B:126:ASP:OD2	4:B:517:HOH:O	2.14	0.66
1:A:189:ASP:O	1:A:193:GLN:HG2	1.96	0.65
1:B:44:SER:O	1:B:47:ARG:NH1	2.30	0.65
2:A:418:M77:H6	2:A:418:M77:C22	2.26	0.64
1:A:23:SER:O	4:A:495:HOH:O	2.14	0.64
1:A:80:LYS:CD	1:A:367:THR:HG21	2.20	0.64
1:A:38:TYR:HD2	1:A:63:THR:HG21	1.62	0.64
1:B:226:ASN:HB2	1:B:230:THR:O	1.98	0.64
1:B:234:SER:CA	1:B:254:GLY:O	2.45	0.63
1:B:334:GLU:OE2	1:B:337:LYS:HD2	1.99	0.63
1:B:189:ASP:O	1:B:193:GLN:HG2	1.98	0.63
1:A:25:LEU:HD22	1:B:62:PHE:CD2	2.34	0.63
1:B:38:TYR:OH	1:B:60:LYS:HG3	2.01	0.61
1:A:124:GLU:OE1	3:A:420:EDO:H12	2.00	0.60
1:A:40:GLU:OE2	1:A:393:GLY:N	2.34	0.60
1:B:337:LYS:NZ	4:B:528:HOH:O	2.34	0.59
1:A:334:GLU:OE2	1:A:337:LYS:HD2	2.04	0.58
1:B:28:GLU:OE1	1:B:404:THR:CG2	2.52	0.57
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.69	0.57
1:B:195:HIS:HA	1:B:225:MET:CE	2.32	0.56
1:A:44:SER:HB3	1:A:46:LEU:HD13	1.86	0.56
1:B:47:ARG:NH1	1:B:47:ARG:CG	2.60	0.56
1:B:45:ALA:CA	1:B:47:ARG:NH1	2.58	0.56
2:B:419:M77:H222	2:B:419:M77:H6	1.87	0.56
1:A:328:LEU:HD22	1:A:335:ASP:HB3	1.89	0.55
1:B:47:ARG:HG3	1:B:47:ARG:NH1	2.21	0.55
1:B:80:LYS:HD3	1:B:367:THR:CG2	2.24	0.54
1:B:44:SER:CB	1:B:46:LEU:HD22	2.38	0.54
1:B:96:LYS:O	1:B:97:ASN:HB2	2.07	0.54
1:B:44:SER:C	1:B:46:LEU:N	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LYS:NZ	3:B:420:EDO:C2	2.63	0.54
1:B:38:TYR:HE2	1:B:60:LYS:HA	1.72	0.53
1:B:46:LEU:O	1:B:48:ARG:N	2.40	0.53
2:B:418:M77:C22	2:B:418:M77:H6	2.37	0.53
1:A:80:LYS:HD3	1:A:367:THR:CG2	2.22	0.53
1:B:345:LEU:HD21	1:B:350:ILE:HD12	1.89	0.53
1:B:40:GLU:OE2	1:B:393:GLY:CA	2.56	0.53
1:A:226:ASN:HB3	1:A:228:ASP:H	1.73	0.53
1:B:131:GLY:HA2	1:B:194:LEU:CD1	2.32	0.53
1:A:352:ASN:OD1	4:A:471:HOH:O	2.19	0.52
1:A:236:ALA:HB2	1:A:251:MET:SD	2.49	0.52
1:A:136:ILE:CD1	4:A:463:HOH:O	2.53	0.51
1:A:195:HIS:HA	1:A:225:MET:CE	2.37	0.51
1:B:60:LYS:HB3	1:B:61:PRO:HD3	1.91	0.51
1:B:412:ARG:NH2	4:B:447:HOH:O	2.34	0.51
1:A:60:LYS:HB3	1:A:61:PRO:HD3	1.92	0.51
1:A:132:ASP:N	1:A:136:ILE:HD12	2.26	0.50
1:A:137:THR:HG23	1:A:216:LEU:O	2.11	0.50
1:A:181:ILE:HG22	1:A:342:PHE:HZ	1.76	0.50
1:A:38:TYR:HE1	1:A:56:LEU:HD13	1.76	0.50
1:A:234:SER:HB3	1:A:255:MET:SD	2.52	0.50
1:A:44:SER:C	1:A:46:LEU:H	2.15	0.49
1:A:38:TYR:CD2	1:A:63:THR:HG21	2.45	0.49
1:B:38:TYR:O	1:B:38:TYR:HD1	1.95	0.49
1:B:234:SER:HA	1:B:254:GLY:O	2.12	0.48
1:A:367:THR:CG2	1:A:367:THR:O	2.60	0.48
1:A:272:TYR:OH	1:A:303:PRO:HD3	2.13	0.48
1:A:96:LYS:O	1:A:97:ASN:HB2	2.13	0.48
1:B:204:ASP:OD1	1:B:204:ASP:N	2.39	0.48
1:B:44:SER:HG	1:B:391:PHE:N	2.12	0.48
1:B:38:TYR:CD1	1:B:38:TYR:C	2.87	0.48
1:A:38:TYR:OH	1:A:60:LYS:HG3	2.14	0.48
2:A:419:M77:H6	2:A:419:M77:H222	1.96	0.47
1:A:183:GLU:HB3	1:A:214:ILE:HG12	1.97	0.47
1:B:44:SER:HB3	1:B:46:LEU:HD22	1.96	0.47
1:B:236:ALA:HB2	1:B:251:MET:SD	2.55	0.47
1:B:181:ILE:HG22	1:B:342:PHE:HZ	1.80	0.46
1:A:332:GLY:HA3	4:A:467:HOH:O	2.15	0.46
1:B:18:PRO:HG2	1:B:26:SER:HB3	1.97	0.46
1:B:38:TYR:C	1:B:38:TYR:HD1	2.19	0.46
1:A:295:ASN:OD1	1:A:299:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:418:M77:H11	2:A:418:M77:O1	2.16	0.45
1:A:12:GLN:OE1	1:A:12:GLN:HA	2.15	0.45
1:A:68:GLU:O	1:A:72:HIS:HE1	1.99	0.45
1:A:192:HIS:CE1	1:A:260:PRO:HB2	2.51	0.45
1:B:83:GLY:HA3	2:B:418:M77:H151	1.99	0.44
2:A:419:M77:O2	2:A:419:M77:C11	2.63	0.44
1:A:24:ALA:HA	1:B:62:PHE:CD1	2.52	0.44
1:A:269:VAL:HG13	1:A:280:PRO:HD2	1.99	0.44
1:B:396:LEU:N	1:B:397:PRO:CD	2.81	0.44
1:B:105:LYS:HZ1	3:B:420:EDO:H22	1.65	0.44
1:B:94:LYS:HB3	1:B:101:ILE:HD13	2.00	0.43
1:B:367:THR:CG2	1:B:367:THR:O	2.63	0.43
2:B:419:M77:O2	2:B:419:M77:C11	2.44	0.43
1:B:46:LEU:C	1:B:48:ARG:N	2.70	0.43
1:A:189:ASP:HB2	1:A:333:ILE:HG21	2.00	0.43
1:A:415:LEU:C	4:A:429:HOH:O	2.57	0.43
1:A:108:ASN:O	1:A:112:MET:HG2	2.19	0.43
1:B:334:GLU:O	1:B:338:LYS:HG2	2.19	0.42
1:B:295:ASN:CG	1:B:295:ASN:O	2.58	0.42
1:A:345:LEU:HD21	1:A:350:ILE:HD12	2.00	0.42
1:A:196:TYR:CE2	1:A:224:LYS:HB2	2.55	0.42
1:A:204:ASP:OD1	1:A:204:ASP:N	2.49	0.42
1:B:328:LEU:HD22	1:B:335:ASP:HB3	2.00	0.42
1:A:243:ILE:HG21	1:A:243:ILE:HD13	1.89	0.42
1:A:44:SER:C	1:A:46:LEU:N	2.73	0.41
1:A:271:MET:HE1	1:A:316:LEU:HD23	2.02	0.41
1:B:107:LEU:HB2	1:B:149:LEU:HB2	2.03	0.41
1:B:316:LEU:HD12	1:B:328:LEU:HD12	2.01	0.41
1:A:14:LEU:HB2	1:B:409:PHE:CE1	2.56	0.41
1:B:239:THR:HA	1:B:240:PRO:HD3	1.96	0.41
1:B:156:TYR:CZ	1:B:215:ARG:HG2	2.56	0.41
1:B:170:ASP:O	1:B:277:GLY:HA2	2.20	0.41
1:A:25:LEU:HD22	1:B:62:PHE:CG	2.55	0.41
1:A:316:LEU:HD12	1:A:328:LEU:HD12	2.01	0.41
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.84	0.41
1:B:243:ILE:HD13	1:B:243:ILE:HG21	1.87	0.41
1:B:202:LYS:HB2	1:B:203:PRO:CD	2.51	0.41
1:B:46:LEU:C	1:B:48:ARG:H	2.25	0.40
2:B:418:M77:H11	2:B:418:M77:O1	2.20	0.40
1:A:83:GLY:HA3	2:A:418:M77:H151	2.02	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	391/433 (90%)	374 (96%)	15 (4%)	2 (0%)	34	26
1	B	391/433 (90%)	373 (95%)	17 (4%)	1 (0%)	46	42
All	All	782/866 (90%)	747 (96%)	32 (4%)	3 (0%)	39	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	45	ALA
1	B	47	ARG

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	321/384 (84%)	300 (94%)	21 (6%)	21	15
1	B	322/384 (84%)	301 (94%)	21 (6%)	21	15
All	All	643/768 (84%)	601 (94%)	42 (6%)	21	15

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	21	ASN
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	44	SER
1	A	47	ARG
1	A	56	LEU
1	A	84	ARG
1	A	146	GLU
1	A	162	LEU
1	A	204	ASP
1	A	216	LEU
1	A	224	LYS
1	A	285	SER
1	A	286	LEU
1	A	287	VAL
1	A	297	GLU
1	A	325	GLU
1	A	345	LEU
1	A	360	ASP
1	A	361	VAL
1	A	404	THR
1	B	2	SER
1	B	7	LEU
1	B	38	TYR
1	B	44	SER
1	B	46	LEU
1	B	47	ARG
1	B	146	GLU
1	B	162	LEU
1	B	204	ASP
1	B	215	ARG
1	B	221	SER
1	B	224	LYS
1	B	235	VAL
1	B	251	MET
1	B	261	GLU
1	B	288	GLU
1	B	325	GLU
1	B	345	LEU
1	B	361	VAL
1	B	365	SER
1	B	404	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	97	ASN
1	B	130	ASN
1	B	195	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	M77	A	418	-	20,22,22	4.53	10 (50%)	27,31,31	3.41	9 (33%)
2	M77	A	419	-	20,22,22	3.03	6 (30%)	27,31,31	2.27	10 (37%)
3	EDO	A	420	-	3,3,3	0.64	0	2,2,2	0.73	0
2	M77	B	418	-	20,22,22	2.44	8 (40%)	27,31,31	3.28	11 (40%)
2	M77	B	419	-	20,22,22	2.87	6 (30%)	27,31,31	2.06	8 (29%)
3	EDO	B	420	-	3,3,3	0.72	0	2,2,2	0.77	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
2	M77	A	418	-	-	0/12/21/21	0/3/3/3
2	M77	A	419	-	-	0/12/21/21	0/3/3/3
3	EDO	A	420	-	-	0/1/1/1	0/0/0/0
2	M77	B	418	-	-	0/12/21/21	0/3/3/3
2	M77	B	419	-	-	0/12/21/21	0/3/3/3
3	EDO	B	420	-	-	0/1/1/1	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	418	M77	S1-N4	-13.76	1.43	1.63
2	A	418	M77	C5-S1	-8.19	1.65	1.77
2	A	418	M77	C15-N4	-6.72	1.41	1.47
2	A	418	M77	O2-S1	-5.32	1.36	1.43
2	A	418	M77	C22-N4	-4.41	1.43	1.47
2	A	418	M77	C10-C9	-4.39	1.34	1.42
2	B	419	M77	C10-C9	-3.54	1.36	1.42
2	A	418	M77	C5-C10	-3.50	1.38	1.43
2	A	418	M77	C14-C9	-3.17	1.35	1.41
2	A	419	M77	C10-C9	-2.82	1.37	1.42
2	B	418	M77	C15-N4	-2.65	1.45	1.47
2	B	418	M77	C22-N4	-2.65	1.45	1.47
2	A	418	M77	C8-C9	-2.50	1.35	1.41
2	A	418	M77	C11-C10	-2.20	1.37	1.42
2	B	418	M77	C10-C9	-2.03	1.39	1.42
2	B	419	M77	C15-N4	2.00	1.49	1.47
2	B	418	M77	C20-C15	2.17	1.59	1.51
2	B	418	M77	O2-S1	2.22	1.46	1.43
2	B	418	M77	C11-C12	2.94	1.40	1.36
2	B	419	M77	C11-C12	3.14	1.40	1.36
2	A	419	M77	C5-S1	3.22	1.82	1.77
2	B	418	M77	S1-N4	4.39	1.69	1.63
2	A	419	M77	O2-S1	4.65	1.49	1.43
2	A	419	M77	C11-C12	4.88	1.42	1.36
2	B	419	M77	O2-S1	5.38	1.50	1.43
2	B	419	M77	S1-N4	6.20	1.72	1.63
2	A	419	M77	O1-S1	6.67	1.52	1.43
2	B	418	M77	O1-S1	6.92	1.52	1.43
2	B	419	M77	O1-S1	7.22	1.52	1.43
2	A	419	M77	S1-N4	7.52	1.74	1.63

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	418	M77	C21-C22-N4	-11.58	96.93	113.16
2	A	418	M77	C21-C22-N4	-7.83	102.19	113.16
2	A	418	M77	O2-S1-O1	-7.76	106.08	119.47
2	A	418	M77	C20-C15-N4	-7.29	99.52	112.28
2	A	418	M77	C11-C12-N13	-6.63	117.81	123.91
2	B	418	M77	O2-S1-O1	-5.79	109.48	119.47
2	B	419	M77	O2-S1-O1	-5.49	110.00	119.47
2	A	418	M77	O1-S1-N4	-5.37	101.38	106.69
2	B	418	M77	C20-C15-N4	-5.00	103.52	112.28
2	A	419	M77	O2-S1-O1	-4.85	111.10	119.47
2	B	418	M77	C11-C12-N13	-4.72	119.56	123.91
2	B	418	M77	O1-S1-N4	-4.17	102.57	106.69
2	A	419	M77	C11-C10-C9	-3.22	113.68	117.91
2	A	419	M77	O2-S1-C5	-2.85	101.85	107.92
2	B	419	M77	O2-S1-C5	-2.72	102.12	107.92
2	B	419	M77	C11-C12-N13	-2.45	121.65	123.91
2	B	418	M77	C10-C5-S1	-2.42	117.78	121.79
2	B	419	M77	C7-C6-C5	-2.25	118.28	120.41
2	A	419	M77	C11-C12-N13	-2.20	121.88	123.91
2	B	419	M77	C15-N4-S1	-2.10	110.91	118.05
2	B	419	M77	C10-C5-S1	-2.04	118.40	121.79
2	A	419	M77	C11-C10-C5	2.03	126.52	123.83
2	A	418	M77	C12-N13-C14	2.27	122.84	117.20
2	B	418	M77	C12-N13-C14	2.30	122.94	117.20
2	B	418	M77	O2-S1-C5	2.32	112.87	107.92
2	A	419	M77	C5-C10-C9	2.35	119.69	117.47
2	B	418	M77	C6-C5-S1	2.37	120.43	117.30
2	B	418	M77	O2-S1-N4	2.60	109.26	106.69
2	A	418	M77	C5-C10-C9	2.65	119.97	117.47
2	B	418	M77	C5-S1-N4	2.84	113.36	106.54
2	A	418	M77	O2-S1-N4	2.94	109.59	106.69
2	A	419	M77	O2-S1-N4	3.02	109.67	106.69
2	A	419	M77	C14-C9-C10	3.08	120.25	117.70
2	A	419	M77	C12-C11-C10	3.09	122.72	119.80
2	B	419	M77	O2-S1-N4	3.20	109.85	106.69
2	A	418	M77	C5-S1-N4	4.72	117.88	106.54
2	B	419	M77	C5-S1-N4	4.97	118.48	106.54
2	A	419	M77	C5-S1-N4	6.30	121.69	106.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	418	M77	5	0
2	A	419	M77	3	0
3	A	420	EDO	1	0
2	B	418	M77	5	0
2	B	419	M77	3	0
3	B	420	EDO	7	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	395/433 (91%)	0.50	19 (4%) 34 45	22, 39, 62, 76	0
1	B	395/433 (91%)	0.45	11 (2%) 56 66	22, 39, 63, 78	0
All	All	790/866 (91%)	0.48	30 (3%) 44 54	22, 39, 63, 78	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	HIS	5.4
1	A	360	ASP	3.7
1	A	254	GLY	3.5
1	B	49	ASP	3.4
1	A	44	SER	3.4
1	A	299	ARG	3.0
1	B	43	HIS	2.9
1	B	46	LEU	2.8
1	A	20	ARG	2.7
1	A	372	VAL	2.7
1	A	23	SER	2.7
1	A	38	TYR	2.4
1	B	254	GLY	2.4
1	A	282	TYR	2.4
1	B	282	TYR	2.4
1	B	39	THR	2.3
1	A	250	ALA	2.3
1	A	49	ASP	2.3
1	A	40	GLU	2.3
1	A	304	SER	2.2
1	B	42	SER	2.2
1	A	301	GLN	2.1
1	A	326	ARG	2.1
1	B	40	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	391	PHE	2.1
1	A	287	VAL	2.1
1	A	56	LEU	2.1
1	B	295	ASN	2.1
1	A	362	SER	2.1
1	B	136	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	EDO	B	420	4/4	0.80	0.27	6.02	32,36,39,39	0
2	M77	A	419	20/20	0.64	0.23	3.71	88,93,96,99	0
2	M77	B	419	20/20	0.67	0.20	2.38	89,92,95,97	0
3	EDO	A	420	4/4	0.94	0.16	2.05	26,29,31,38	0
2	M77	B	418	20/20	0.96	0.14	-0.47	26,32,37,41	0
2	M77	A	418	20/20	0.95	0.13	-0.95	26,33,43,46	0

6.5 Other polymers (i)

There are no such residues in this entry.