



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 04:28 AM EST

PDB ID : 2R6G  
Title : The Crystal Structure of the E. coli Maltose Transporter  
Authors : Oldham, M.L.; Khare, D.; Quioco, F.A.; Davidson, A.L.; Chen, J.  
Deposited on : 2007-09-05  
Resolution : 2.80 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

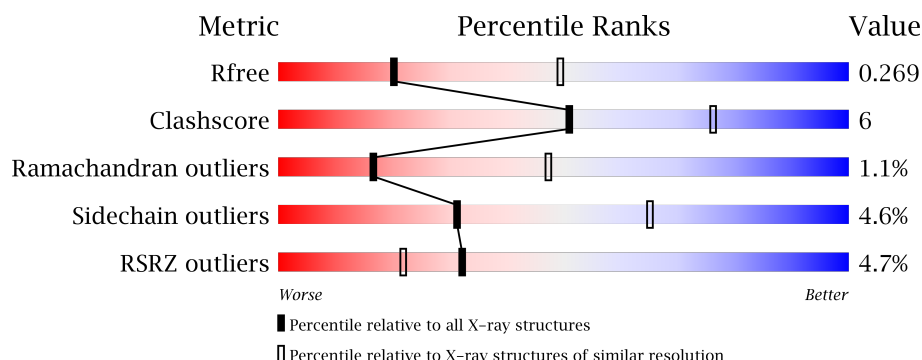
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	381	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	381	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>
2	E	370	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>•</div> </div> </div>
3	F	514	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div> </div>
4	G	296	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14713 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 Maltose/maltodextrin import ATP-binding protein malK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2876	1819	516	528	13			
1	B	372	Total	C	N	O	S	0	0	0
			2882	1822	517	530	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	GLN	GLU	ENGINEERED	UNP Q1R3Q1
A	372	ALA	-	EXPRESSION TAG	UNP Q1R3Q1
A	373	SER	-	EXPRESSION TAG	UNP Q1R3Q1
A	374	ALA	-	EXPRESSION TAG	UNP Q1R3Q1
A	375	SER	-	EXPRESSION TAG	UNP Q1R3Q1
A	376	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
A	377	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
A	378	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
A	379	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
A	380	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
A	381	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
B	159	GLN	GLU	ENGINEERED	UNP Q1R3Q1
B	372	ALA	-	EXPRESSION TAG	UNP Q1R3Q1
B	373	SER	-	EXPRESSION TAG	UNP Q1R3Q1
B	374	ALA	-	EXPRESSION TAG	UNP Q1R3Q1
B	375	SER	-	EXPRESSION TAG	UNP Q1R3Q1
B	376	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
B	377	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
B	378	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
B	379	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
B	380	HIS	-	EXPRESSION TAG	UNP Q1R3Q1
B	381	HIS	-	EXPRESSION TAG	UNP Q1R3Q1

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	370	Total	C	N	O	S	0	0	0
			2877	1853	469	549	6			

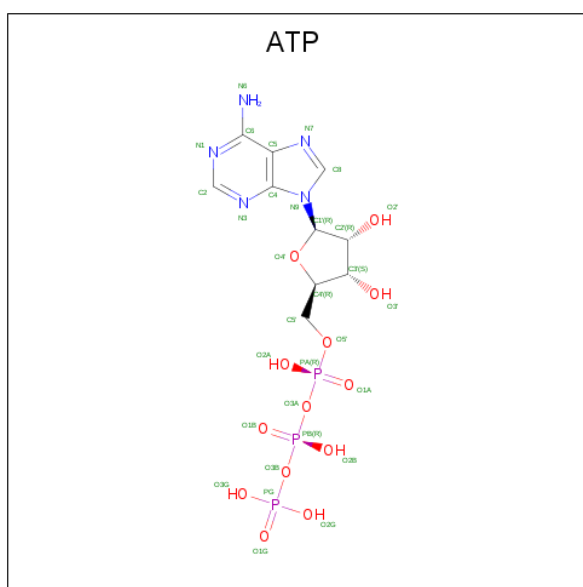
- Molecule 3 is a protein called Maltose transport system permease protein malF.

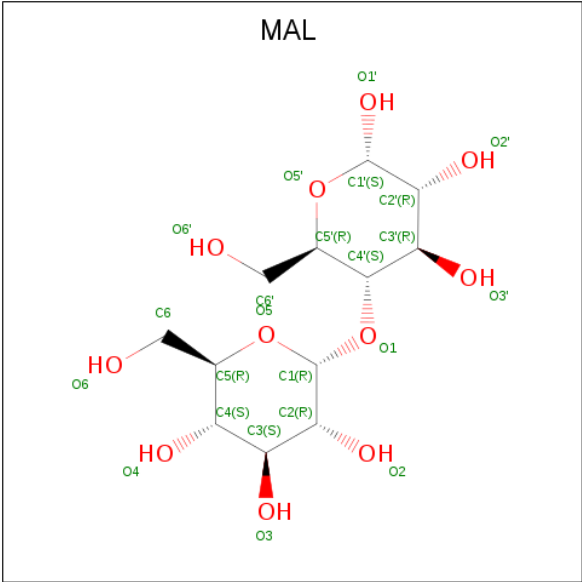
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	490	Total	C	N	O	S	0	0	0
			3806	2505	606	678	17			

- Molecule 4 is a protein called Maltose transport system permease protein malG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	284	Total	C	N	O	S	0	0	0
			2187	1468	348	363	8			

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



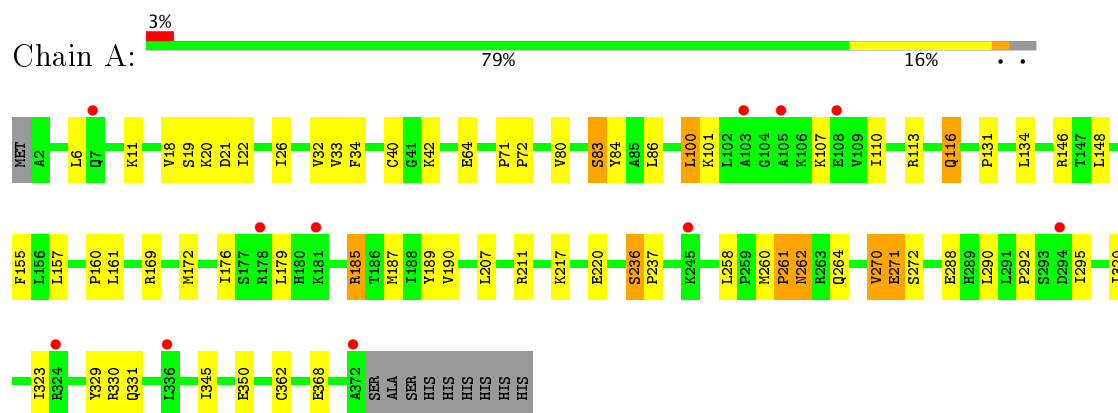


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			23	12	11		

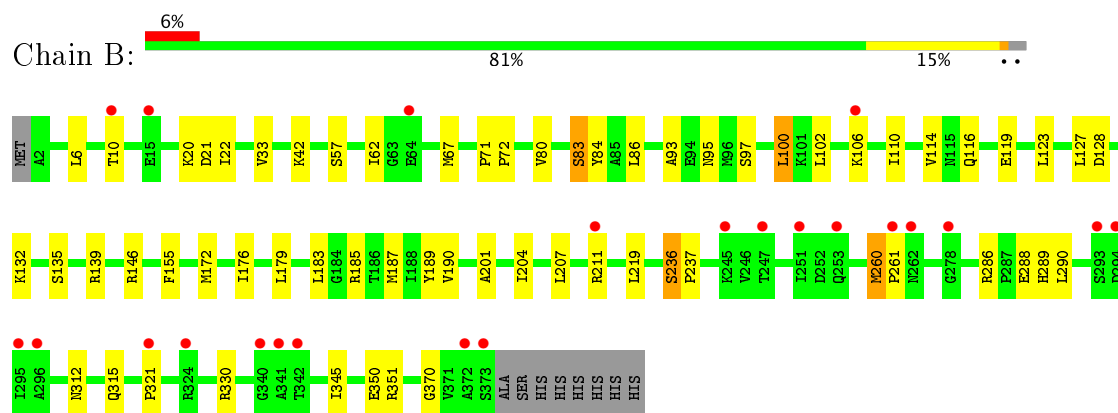
### 3 Residue-property plots

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.

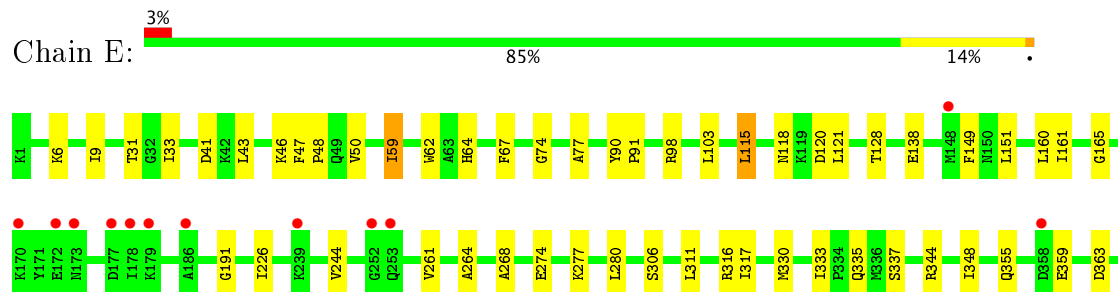
- Molecule 1: Maltose/maltodextrin import ATP-binding protein malK



- Molecule 1: Maltose/maltodextrin import ATP-binding protein malK



- Molecule 2: Maltose-binding periplasmic protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.26 Å   95.86 Å   109.99 Å 87.13°   82.43°   75.75°	Depositor
Resolution (Å)	47.40 – 2.80 35.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.8 (47.40-2.80) 83.4 (35.04-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.81 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.242   ,   0.271 0.240   ,   0.269	Depositor DCC
$R_{free}$ test set	1185 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAL, ATP

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	0.30	0/2926	0.51	0/3968
1	B	0.30	0/2932	0.49	0/3976
2	E	0.31	0/2946	0.45	0/3998
3	F	0.35	0/3901	0.51	0/5313
4	G	0.35	0/2247	0.49	0/3070
All	All	0.32	0/14952	0.49	0/20325

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2876	0	2944	45	0
1	B	2882	0	2949	41	0
2	E	2877	0	2859	29	0
3	F	3806	0	3836	55	0
4	G	2187	0	2277	34	0
5	A	31	0	12	4	0
5	B	31	0	12	0	0
6	F	23	0	22	0	0
All	All	14713	0	14911	191	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 (191) 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:A:236:SER:HB3	1:A:237:PRO:HD3	1.59	0.82
3:F:414:PHE:HA	3:F:418:THR:HG23	1.60	0.82
1:B:236:SER:HB3	1:B:237:PRO:HD3	1.63	0.80
1:B:260:MET:HB2	1:B:261:PRO:HD2	1.62	0.80
4:G:84:TRP:HB3	4:G:245:LEU:HA	1.68	0.76
1:A:217:LYS:HB2	1:A:220:GLU:HB2	1.73	0.71
1:A:236:SER:CB	1:A:237:PRO:HD3	2.22	0.69
2:E:64:HIS:CD2	2:E:261:VAL:H	2.11	0.69
4:G:173:HIS:O	4:G:177:ILE:HG22	1.94	0.68
1:A:18:VAL:HG21	5:A:1002:ATP:H4'	1.75	0.68
3:F:93:ASN:HD22	3:F:93:ASN:H	1.42	0.68
1:A:236:SER:HB3	1:A:237:PRO:CD	2.24	0.67
1:A:100:LEU:HD13	1:A:110:ILE:HG12	1.77	0.66
1:A:185:ARG:HH11	1:A:185:ARG:CG	2.08	0.66
2:E:64:HIS:HD2	2:E:261:VAL:H	1.42	0.66
4:G:84:TRP:HH2	4:G:240:VAL:HG12	1.62	0.64
1:B:236:SER:HB3	1:B:237:PRO:CD	2.27	0.63
2:E:62:TRP:HB3	2:E:67:PHE:HE1	1.64	0.63
1:B:236:SER:CB	1:B:237:PRO:HD3	2.29	0.62
1:B:20:LYS:HB3	1:B:211:ARG:HG2	1.82	0.61
3:F:394:ALA:HB1	4:G:183:THR:HG21	1.82	0.60
3:F:392:LEU:HD13	3:F:422:LEU:HD11	1.83	0.60
1:B:72:PRO:HB2	3:F:404:ALA:HB1	1.83	0.59
2:E:31:THR:HG22	3:F:177:THR:HG21	1.84	0.59
1:B:33:VAL:HG12	1:B:189:TYR:HB3	1.84	0.58
4:G:220:ILE:O	4:G:224:ILE:HG23	2.04	0.58
1:B:100:LEU:HD13	1:B:110:ILE:HG12	1.85	0.57
3:F:238:GLN:HG2	3:F:246:TRP:CE3	2.40	0.56
3:F:382:PRO:HA	3:F:385:MET:HG2	1.87	0.56
3:F:409:GLY:H	3:F:412:GLN:HB2	1.70	0.56
3:F:381:TYR:OH	4:G:27:ILE:HD13	2.06	0.56
3:F:387:LEU:HD21	3:F:429:LEU:HD13	1.88	0.56
1:A:290:LEU:HD22	1:A:345:ILE:HD13	1.88	0.55
2:E:9:ILE:HG12	2:E:59:ILE:HG23	1.89	0.55
2:E:337:SER:HB2	3:F:479:GLY:H	1.71	0.55
1:A:288:GLU:HG2	1:B:312:ASN:HB2	1.88	0.55
1:A:172:MET:O	1:A:176:ILE:HG12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:295:THR:HG22	3:F:384:MET:CG	2.37	0.54
1:A:262:ASN:HD22	1:A:264:GLN:H	1.55	0.54
1:B:86:LEU:HA	1:B:146:ARG:NH2	2.22	0.54
4:G:84:TRP:HB3	4:G:245:LEU:CA	2.38	0.54
1:A:40:CYS:SG	1:A:42:LYS:HG3	2.48	0.53
1:A:258:LEU:HB3	1:A:260:MET:SD	2.49	0.53
1:A:236:SER:CB	1:A:237:PRO:CD	2.86	0.53
3:F:86:THR:HA	3:F:89:ILE:HG22	1.91	0.53
3:F:323:LEU:N	3:F:324:PRO:HD2	2.23	0.53
3:F:259:THR:HG22	3:F:262:LYS:HD2	1.90	0.53
5:A:1002:ATP:H3'	1:B:135:SER:HB3	1.90	0.52
1:A:18:VAL:HG21	5:A:1002:ATP:C4'	2.39	0.52
1:B:183:LEU:HB3	1:B:185:ARG:HG2	1.92	0.52
1:B:155:PHE:HB2	1:B:187:MET:HG2	1.91	0.52
3:F:275:LYS:HB3	3:F:276:PRO:HD3	1.91	0.51
3:F:381:TYR:N	3:F:382:PRO:HD2	2.26	0.51
1:B:86:LEU:HA	1:B:146:ARG:HH21	1.76	0.51
1:B:286:ARG:HD2	1:B:289:HIS:CE1	2.46	0.51
2:E:333:ILE:HD12	2:E:335:GLN:HB2	1.93	0.50
3:F:83:LEU:HA	3:F:86:THR:HG22	1.94	0.50
4:G:37:ILE:HG22	4:G:40:ARG:NH1	2.25	0.50
1:A:329:TYR:HE2	1:A:331:GLN:HE21	1.59	0.50
1:B:260:MET:CB	1:B:261:PRO:HD2	2.39	0.50
1:A:288:GLU:HG3	1:A:330:ARG:HD3	1.93	0.50
3:F:484:PHE:HB3	4:G:135:LEU:HD11	1.93	0.50
4:G:224:ILE:HG22	4:G:274:ILE:HD12	1.93	0.50
2:E:41:ASP:O	2:E:46:LYS:HE2	2.12	0.50
1:A:83:SER:O	1:A:84:TYR:CD1	2.65	0.50
3:F:341:ASN:ND2	3:F:344:PHE:H	2.09	0.50
1:B:97:SER:HB3	1:B:114:VAL:HG21	1.93	0.50
3:F:290:ILE:HD11	3:F:373:ILE:HG21	1.93	0.49
1:A:113:ARG:HA	1:A:116:GLN:HB2	1.93	0.49
1:B:132:LYS:HA	1:B:139:ARG:HH21	1.76	0.49
3:F:139:GLU:O	3:F:141:GLY:N	2.40	0.49
4:G:88:SER:HB3	4:G:227:ILE:HD13	1.94	0.49
1:A:157:LEU:HB3	1:A:160:PRO:HG3	1.95	0.49
1:A:6:LEU:HD22	1:A:22:ILE:HD11	1.95	0.48
2:E:344:ARG:O	2:E:348:ILE:HG12	2.13	0.48
1:B:102:LEU:HD23	3:F:408:ALA:HB2	1.94	0.48
3:F:139:GLU:C	3:F:141:GLY:H	2.16	0.48
2:E:47:PHE:HB3	2:E:48:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:295:THR:HG22	3:F:384:MET:HG3	1.96	0.48
2:E:311:LEU:HB3	2:E:317:ILE:HD13	1.95	0.48
1:A:260:MET:HB2	1:A:261:PRO:HD2	1.94	0.48
1:B:236:SER:CB	1:B:237:PRO:CD	2.91	0.48
1:B:84:TYR:HD2	4:G:296:GLY:HA2	1.78	0.47
1:A:33:VAL:HG12	1:A:189:TYR:HB3	1.95	0.47
4:G:166:TYR:CZ	4:G:229:GLU:HG2	2.49	0.47
4:G:164:PHE:HA	4:G:167:LEU:HD22	1.97	0.47
1:B:10:THR:HB	1:B:57:SER:HB2	1.96	0.47
4:G:166:TYR:CE1	4:G:229:GLU:HG2	2.50	0.47
4:G:220:ILE:HG22	4:G:277:VAL:HG12	1.97	0.47
3:F:471:THR:HG23	3:F:490:ILE:HD13	1.97	0.47
1:A:320:ILE:HB	1:A:323:ILE:HD12	1.98	0.46
2:E:161:ILE:HA	2:E:191:GLY:HA3	1.97	0.46
3:F:280:ILE:O	3:F:284:THR:HG23	2.15	0.46
3:F:95:SER:HB2	3:F:483:ASP:HA	1.96	0.46
1:A:131:PRO:HA	1:A:134:LEU:HD12	1.98	0.46
1:A:292:PRO:HD2	1:A:295:ILE:HD12	1.96	0.46
2:E:46:LYS:O	2:E:50:VAL:HG22	2.15	0.46
1:A:270:VAL:HG13	1:A:362:CYS:HB3	1.98	0.46
2:E:59:ILE:HD13	2:E:280:LEU:HD11	1.98	0.46
1:A:42:LYS:HG2	1:A:207:LEU:HD12	1.97	0.46
3:F:212:THR:HG23	3:F:222:ASN:HD21	1.80	0.46
1:A:11:LYS:HB3	1:A:19:SER:HB2	1.97	0.46
1:B:93:ALA:HB2	1:B:127:LEU:HG	1.98	0.46
4:G:152:PRO:C	4:G:154:ILE:H	2.19	0.46
4:G:91:VAL:HG13	4:G:163:ILE:HG22	1.98	0.46
1:B:83:SER:O	1:B:84:TYR:CD1	2.69	0.45
2:E:64:HIS:HE1	2:E:330:MET:O	1.99	0.45
3:F:159:LEU:HD11	3:F:188:ALA:HB1	1.97	0.45
3:F:403:SER:HB3	3:F:413:ASN:HD21	1.82	0.45
4:G:198:THR:HG23	4:G:201:GLN:H	1.81	0.45
1:A:185:ARG:NH1	1:A:185:ARG:HG3	2.31	0.45
1:B:33:VAL:HG22	1:B:204:ILE:HG12	1.98	0.45
2:E:62:TRP:HB3	2:E:67:PHE:CE1	2.48	0.45
2:E:77:ALA:HB2	2:E:268:ALA:HA	1.99	0.45
4:G:16:THR:O	4:G:20:LEU:HB2	2.16	0.45
4:G:84:TRP:CZ3	4:G:240:VAL:O	2.70	0.45
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.81	0.45
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.82	0.45
2:E:59:ILE:HD11	2:E:264:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:62:ALA:HB1	3:F:65:TRP:CD1	2.52	0.45
1:A:185:ARG:NH1	1:A:185:ARG:CG	2.72	0.44
1:B:289:HIS:CD2	1:B:351:ARG:HD2	2.52	0.44
3:F:262:LYS:C	3:F:264:PHE:H	2.21	0.44
4:G:81:VAL:O	4:G:84:TRP:HB2	2.17	0.44
1:A:80:VAL:HG13	1:A:157:LEU:HA	1.99	0.44
3:F:93:ASN:HD21	3:F:257:VAL:H	1.64	0.44
4:G:166:TYR:OH	4:G:229:GLU:HG2	2.16	0.44
5:A:1002:ATP:O1A	1:B:135:SER:HB2	2.18	0.44
2:E:90:TYR:HA	2:E:91:PRO:HD3	1.84	0.44
4:G:45:ALA:HB2	4:G:260:TRP:CE2	2.53	0.44
1:B:172:MET:O	1:B:176:ILE:HG12	2.18	0.44
1:B:33:VAL:HG13	1:B:201:ALA:HB2	2.00	0.43
1:A:148:LEU:HD22	1:A:179:LEU:HD22	1.99	0.43
4:G:10:LYS:HA	4:G:13:LEU:HD12	2.01	0.43
3:F:62:ALA:HB1	3:F:65:TRP:HD1	1.82	0.43
1:A:271:GLU:O	1:A:272:SER:HB3	2.18	0.43
1:A:155:PHE:HB2	1:A:187:MET:HG2	1.99	0.43
1:A:34:PHE:HB2	1:A:190:VAL:HG22	1.99	0.43
3:F:448:THR:C	3:F:450:GLY:H	2.21	0.43
1:B:42:LYS:HD2	1:B:190:VAL:HG13	2.00	0.43
4:G:84:TRP:CZ3	4:G:243:TYR:HB2	2.54	0.43
4:G:81:VAL:HA	4:G:84:TRP:CD1	2.54	0.43
1:A:161:LEU:HB3	1:A:169:ARG:HG3	2.01	0.43
3:F:173:LEU:HG	3:F:202:ARG:HH21	1.84	0.43
1:B:315:GLN:HG2	1:B:330:ARG:HG2	2.01	0.43
3:F:422:LEU:O	3:F:426:LEU:HB2	2.19	0.43
2:E:244:VAL:HB	2:E:316:ARG:HA	2.01	0.42
3:F:295:THR:HG22	3:F:384:MET:HG2	1.99	0.42
2:E:149:PHE:O	2:E:151:LEU:HD12	2.19	0.42
3:F:213:LEU:HD12	3:F:219:LEU:HG	2.01	0.42
3:F:42:PHE:HA	3:F:45:THR:HG22	2.01	0.42
2:E:337:SER:HB3	3:F:477:GLU:HA	2.01	0.42
3:F:95:SER:CB	3:F:483:ASP:HA	2.49	0.42
1:B:6:LEU:HD22	1:B:22:ILE:HD11	2.02	0.42
1:B:290:LEU:HD22	1:B:345:ILE:HD13	2.01	0.42
1:B:95:ASN:O	1:B:146:ARG:HG3	2.19	0.42
3:F:364:ASP:HA	3:F:365:PRO:HD3	1.87	0.42
3:F:211:TYR:HB3	3:F:219:LEU:HD22	2.02	0.42
4:G:224:ILE:O	4:G:228:THR:HG22	2.19	0.42
1:A:83:SER:OG	1:A:84:TYR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:417:ILE:O	3:F:421:LEU:HB2	2.19	0.42
4:G:90:LYS:O	4:G:94:ILE:HG12	2.19	0.42
1:A:288:GLU:HG2	1:B:312:ASN:CB	2.48	0.42
1:B:71:PRO:HA	1:B:72:PRO:HD3	1.90	0.42
2:E:98:ARG:HB3	2:E:103:LEU:HD12	2.02	0.42
3:F:335:ILE:HD11	4:G:30:PRO:HB3	2.01	0.42
4:G:62:ALA:O	4:G:81:VAL:HB	2.20	0.42
1:A:86:LEU:HA	1:A:146:ARG:HH21	1.85	0.41
1:B:237:PRO:HG2	1:B:330:ARG:HD2	2.01	0.41
2:E:74:GLY:HA3	3:F:253:PRO:HG3	2.01	0.41
1:A:71:PRO:HA	1:A:72:PRO:HD3	1.98	0.41
1:B:260:MET:HB2	1:B:261:PRO:CD	2.40	0.41
1:B:219:LEU:HD22	1:B:370:GLY:HA3	2.02	0.41
4:G:230:VAL:HB	4:G:231:PRO:HD3	2.01	0.41
4:G:29:PHE:HB3	4:G:30:PRO:HD3	2.03	0.41
3:F:370:THR:O	3:F:374:ILE:HG23	2.21	0.41
3:F:441:PHE:CZ	3:F:445:GLN:HG3	2.54	0.41
2:E:363:ASP:O	2:E:367:ARG:HG2	2.20	0.41
1:B:62:ILE:HD12	1:B:67:MET:HG3	2.03	0.41
3:F:308:TRP:C	3:F:310:ALA:H	2.23	0.41
2:E:6:LYS:HA	2:E:33:ILE:HG23	2.02	0.41
3:F:34:MET:SD	3:F:46:THR:HG21	2.59	0.41
2:E:115:LEU:HA	2:E:226:ILE:HG22	2.03	0.41
2:E:118:ASN:HB3	2:E:121:LEU:HB2	2.03	0.41
3:F:308:TRP:O	3:F:310:ALA:N	2.46	0.41
4:G:180:TYR:CE2	4:G:211:SER:HA	2.55	0.41
1:A:20:LYS:HB3	1:A:211:ARG:HD2	2.01	0.40
3:F:31:VAL:HG22	3:F:46:THR:HG23	2.03	0.40
2:E:355:GLN:HE21	2:E:359:GLU:HG3	1.87	0.40
1:A:26:ILE:HG12	1:A:32:VAL:HG21	2.03	0.40
1:B:42:LYS:HG2	1:B:207:LEU:HD12	2.04	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	369/381 (97%)	350 (95%)	13 (4%)	6 (2%)	11	36
1	B	370/381 (97%)	343 (93%)	22 (6%)	5 (1%)	13	39
2	E	368/370 (100%)	350 (95%)	17 (5%)	1 (0%)	44	77
3	F	486/514 (95%)	449 (92%)	31 (6%)	6 (1%)	15	44
4	G	280/296 (95%)	268 (96%)	9 (3%)	3 (1%)	17	47
All	All	1873/1942 (96%)	1760 (94%)	92 (5%)	21 (1%)	17	47

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	83	SER
1	A	236	SER
1	A	271	GLU
3	F	309	GLU
4	G	153	PHE
1	B	83	SER
3	F	263	ASN
3	F	460	PRO
1	B	21	ASP
1	B	106	LYS
1	B	236	SER
1	B	321	PRO
1	A	64	GLU
3	F	121	ASN
3	F	140	THR
4	G	8	SER
1	A	261	PRO
2	E	165	GLY
4	G	230	VAL
3	F	253	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	314/323 (97%)	305 (97%)	9 (3%)	48	81
1	B	315/323 (98%)	305 (97%)	10 (3%)	44	78
2	E	297/297 (100%)	287 (97%)	10 (3%)	42	76
3	F	398/424 (94%)	365 (92%)	33 (8%)	13	36
4	G	227/237 (96%)	217 (96%)	10 (4%)	33	67
All	All	1551/1604 (97%)	1479 (95%)	72 (5%)	31	65

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	101	LYS
1	A	107	LYS
1	A	116	GLN
1	A	185	ARG
1	A	262	ASN
1	A	270	VAL
1	A	350	GLU
1	A	368	GLU
1	B	80	VAL
1	B	100	LEU
1	B	116	GLN
1	B	119	GLU
1	B	123	LEU
1	B	128	ASP
1	B	179	LEU
1	B	260	MET
1	B	288	GLU
1	B	350	GLU
2	E	43	LEU
2	E	59	ILE
2	E	115	LEU
2	E	120	ASP
2	E	128	THR
2	E	138	GLU
2	E	160	LEU
2	E	274	GLU
2	E	277	LYS
2	E	306	SER

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Mol	Chain	Res	Type
3	F	41	LEU
3	F	89	ILE
3	F	93	ASN
3	F	97	THR
3	F	99	GLN
3	F	115	GLN
3	F	124	LEU
3	F	129	ASP
3	F	133	LEU
3	F	173	LEU
3	F	186	ILE
3	F	187	THR
3	F	210	LEU
3	F	218	THR
3	F	259	THR
3	F	271	GLU
3	F	275	LYS
3	F	311	LEU
3	F	314	LYS
3	F	331	ILE
3	F	341	ASN
3	F	342	GLN
3	F	347	ILE
3	F	354	LEU
3	F	367	THR
3	F	374	ILE
3	F	406	ASP
3	F	413	ASN
3	F	418	THR
3	F	423	ILE
3	F	464	THR
3	F	467	LEU
3	F	496	LEU
4	G	27	ILE
4	G	49	LEU
4	G	83	LEU
4	G	84	TRP
4	G	164	PHE
4	G	167	LEU
4	G	177	ILE
4	G	212	VAL
4	G	224	ILE

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Mol	Chain	Res	Type
4	G	290	THR

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

Mol	Chain	Res	Type
1	A	82	GLN
1	A	163	ASN
1	A	253	GLN
1	A	255	GLN
1	A	262	ASN
1	A	264	GLN
1	A	309	GLN
1	A	331	GLN
1	B	82	GLN
1	B	255	GLN
1	B	265	GLN
1	B	289	HIS
2	E	64	HIS
2	E	218	ASN
2	E	335	GLN
2	E	349	ASN
2	E	355	GLN
3	F	93	ASN
3	F	99	GLN
3	F	222	ASN
3	F	341	ASN
3	F	413	ASN
4	G	58	HIS
4	G	250	GLN
4	G	282	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
5	ATP	A	1002	-	27,33,33	1.04	1 (3%)	25,52,52	1.70	2 (8%)
5	ATP	B	1001	-	27,33,33	1.06	1 (3%)	25,52,52	1.73	2 (8%)
6	MAL	F	3001	-	24,24,24	0.47	0	35,35,35	0.82	1 (2%)

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
5	ATP	A	1002	-	-	0/18/38/38	0/3/3/3
5	ATP	B	1001	-	-	0/18/38/38	0/3/3/3
6	MAL	F	3001	-	-	0/8/48/48	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	ATP	C5-C4	3.29	1.47	1.40
5	A	1002	ATP	C5-C4	3.30	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	ATP	N3-C2-N1	-6.65	123.06	128.86
5	A	1002	ATP	N3-C2-N1	-6.50	123.19	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	ATP	C4-C5-N7	-2.46	107.03	109.41
5	A	1002	ATP	C4-C5-N7	-2.35	107.14	109.41
6	F	3001	MAL	C1'-O5'-C5'	2.44	117.79	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	ATP	4	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	371/381 (97%)	-0.00	11 (2%) 51 39	55, 75, 96, 108	0
1	B	372/381 (97%)	0.16	23 (6%) 21 13	59, 87, 142, 163	0
2	E	370/370 (100%)	-0.08	12 (3%) 48 37	64, 84, 109, 120	0
3	F	490/514 (95%)	0.28	33 (6%) 19 11	60, 84, 123, 144	0
4	G	284/296 (95%)	-0.01	10 (3%) 44 33	55, 70, 102, 130	0
All	All	1887/1942 (97%)	0.09	89 (4%) 32 22	55, 81, 119, 163	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	59	ASN	11.7
1	B	293	SER	5.1
2	E	170	LYS	5.1
1	A	372	ALA	5.1
3	F	40	TYR	4.6
4	G	67	VAL	4.5
1	B	373	SER	4.5
1	B	295	ILE	4.4
3	F	271	GLU	4.1
3	F	246	TRP	4.1
3	F	269	THR	3.8
3	F	262	LYS	3.7
1	B	294	ASP	3.7
4	G	116	PRO	3.7
1	B	324	ARG	3.6
1	B	261	PRO	3.6
3	F	129	ASP	3.6
4	G	8	SER	3.6
4	G	9	GLN	3.6
3	F	224	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	278	GLY	3.4
3	F	17	TRP	3.4
1	A	105	ALA	3.3
2	E	173	ASN	3.3
2	E	177	ASP	3.2
4	G	133	ALA	3.2
3	F	266	ARG	3.2
2	E	178	ILE	3.1
2	E	239	LYS	3.1
1	A	108	GLU	3.1
3	F	268	PHE	3.0
1	B	340	GLY	3.0
3	F	213	LEU	3.0
3	F	239	SER	3.0
1	B	15	GLU	2.9
3	F	241	THR	2.9
4	G	114	ARG	2.9
3	F	38	GLY	2.9
1	B	253	GLN	2.8
2	E	179	LYS	2.8
2	E	172	GLU	2.8
3	F	240	ILE	2.8
3	F	39	GLU	2.8
1	B	296	ALA	2.8
3	F	242	ALA	2.7
3	F	223	GLN	2.7
4	G	10	LYS	2.7
1	B	372	ALA	2.7
1	A	336	LEU	2.6
3	F	18	SER	2.6
3	F	248	ASP	2.6
3	F	245	ASN	2.5
1	B	342	THR	2.5
1	A	103	ALA	2.5
3	F	37	GLN	2.5
3	F	358	LYS	2.4
3	F	227	LYS	2.4
3	F	35	TYR	2.4
1	B	247	THR	2.4
1	B	245	LYS	2.4
1	B	321	PRO	2.4
3	F	265	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	226	VAL	2.4
1	B	262	ASN	2.3
2	E	253	GLN	2.3
1	A	245	LYS	2.3
4	G	66	SER	2.3
1	A	294	ASP	2.3
1	B	211	ARG	2.2
1	A	324	ARG	2.2
2	E	148	MET	2.2
4	G	75	THR	2.2
2	E	252	GLY	2.2
1	B	251	ILE	2.2
3	F	58	ALA	2.2
1	A	7	GLN	2.2
4	G	284	TRP	2.2
1	B	341	ALA	2.2
3	F	29	TYR	2.1
1	A	181	LYS	2.1
2	E	358	ASP	2.1
1	A	178	ARG	2.1
3	F	456	GLY	2.1
1	B	106	LYS	2.1
1	B	64	GLU	2.0
3	F	263	ASN	2.0
2	E	186	ALA	2.0
3	F	503	ILE	2.0
1	B	10	THR	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	MAL	F	3001	23/23	0.93	0.30	1.31	76,77,77,78	0
5	ATP	A	1002	31/31	0.94	0.17	-0.40	58,64,65,65	0
5	ATP	B	1001	31/31	0.95	0.16	-0.60	63,66,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.