



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 AM GMT

PDB ID : 2O8F  
Title : human MutSalpha (MSH2/MSH6) bound to DNA with a single base T insert  
Authors : Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.  
Deposited on : 2006-12-12  
Resolution : 3.25 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 (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

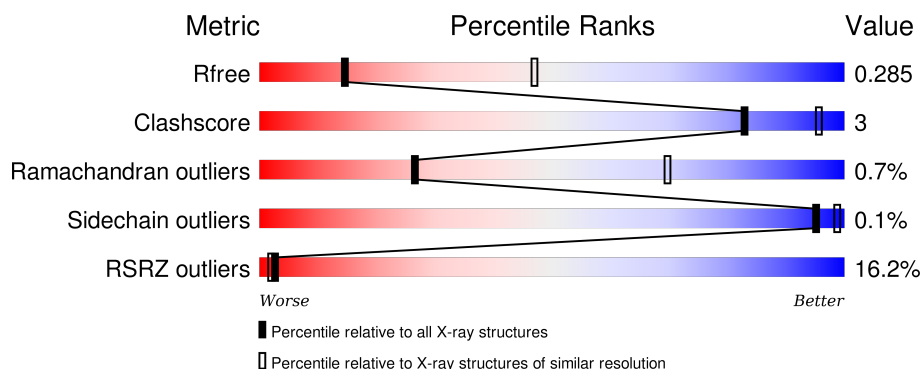
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	E	17	<div> <div>6%</div> <div> <div>71%</div> <div>24%</div> <div>6%</div> </div> </div>
2	F	18	<div> <div>17%</div> <div> <div>78%</div> <div>11%</div> <div>11%</div> </div> </div>
3	A	934	<div> <div>18%</div> <div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
4	B	1022	<div> <div>12%</div> <div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14708 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 DNA chain called 5'-D(\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*GP\*CP\*CP\*GP\*C P\*TP\*AP\*GP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	17	Total	C	N	O	P	0	0	0
			346	163	68	99	16			

- Molecule 2 is a DNA chain called 5'-D(\*CP\*GP\*CP\*TP\*AP\*GP\*CP\*GP\*TP\*GP\*CP\*G P\*GP\*CP\*CP\*GP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	18	Total	C	N	O	P	0	0	0
			365	173	67	108	17			

- Molecule 3 is a protein called DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	832	Total	C	N	O	S	0	0	0
			6494	4119	1103	1238	34			

- Molecule 4 is a protein called DNA mismatch repair protein MSH6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	933	Total	C	N	O	S	0	0	0
			7456	4730	1279	1396	51			

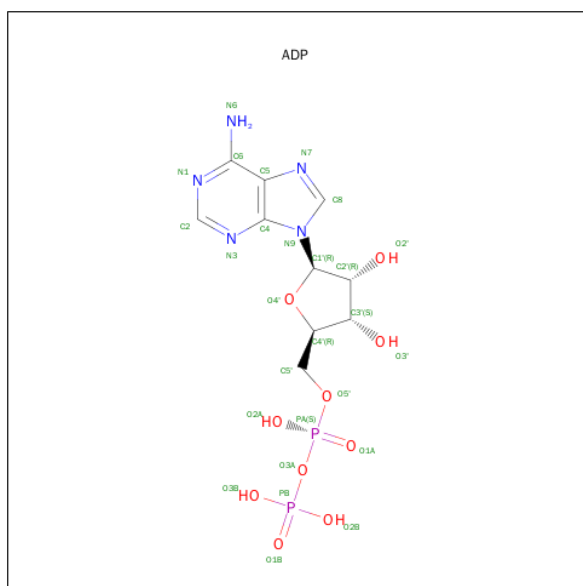
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	MET	-	INITIATING METHIONINE	UNP P52701
B	340	GLY	-	CLONING ARTIFACT	UNP P52701

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

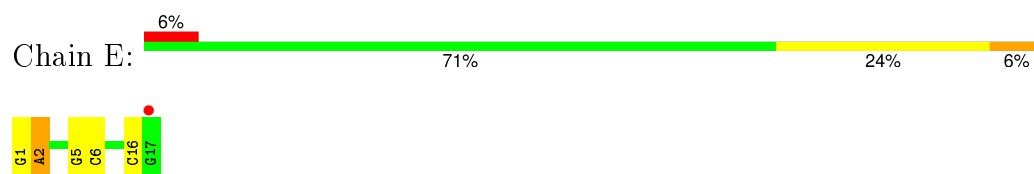
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



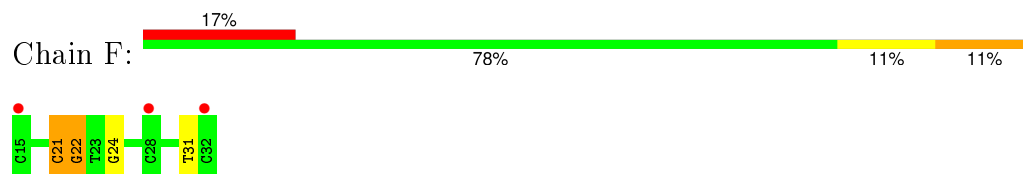
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

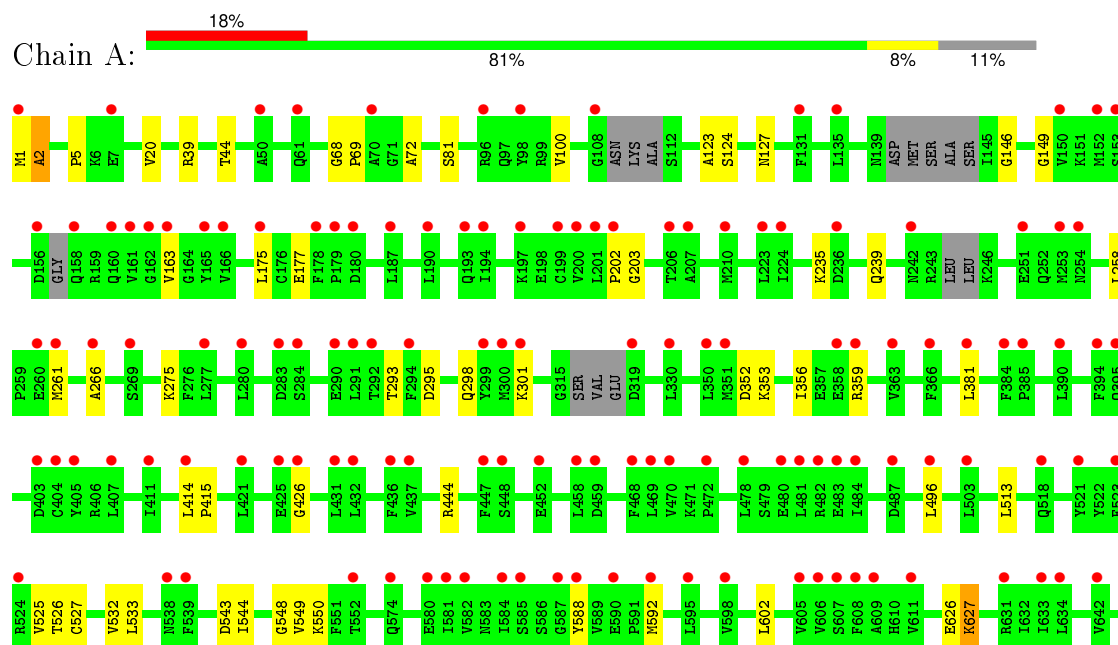
- Molecule 1: 5'-D(\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*TP\*AP\*GP\*CP\*G)-3',

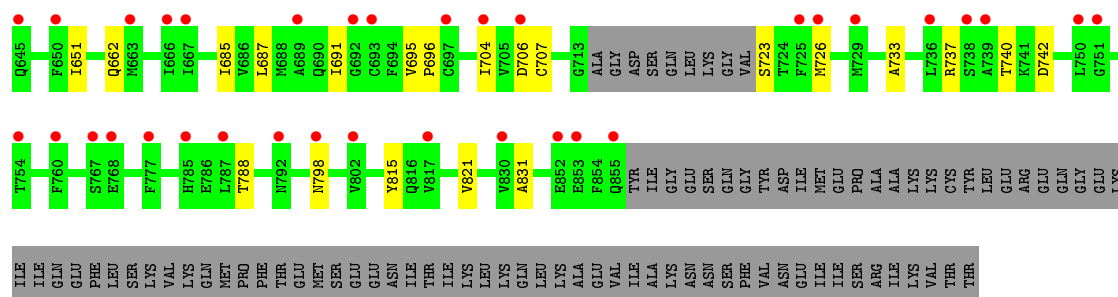


- Molecule 2: 5'-D(\*CP\*GP\*CP\*TP\*AP\*GP\*CP\*GP\*TP\*GP\*CP\*GP\*GP\*CP\*CP\*GP\*TP\*C)-3'

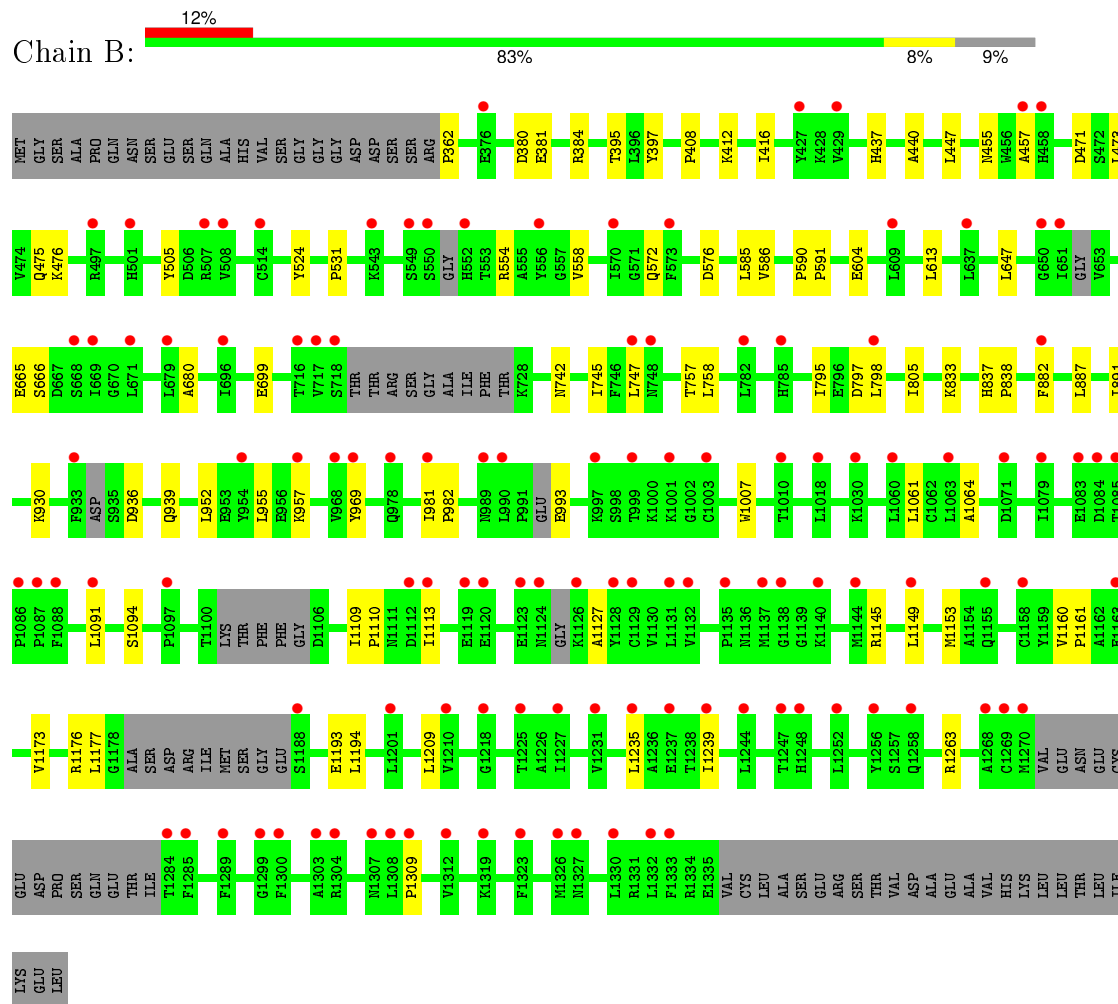


- Molecule 3: DNA mismatch repair protein Msh2





• Molecule 4: DNA mismatch repair protein MSH6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.55Å 259.55Å 259.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 82.08 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.25) 99.5 (82.08-3.25)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.243 , 0.293 0.241 , 0.285	Depositor DCC
$R_{free}$ test set	2373 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 135.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 47211 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	14708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ADP

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	E	0.61	0/388	1.32	5/597 (0.8%)
2	F	0.61	0/408	1.46	6/628 (1.0%)
3	A	0.30	0/6595	0.56	0/8898
4	B	0.32	0/7600	0.58	0/10244
All	All	0.33	0/14991	0.65	11/20367 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	22	DG	O3'-P-O5'	-11.73	81.71	104.00
2	F	22	DG	OP1-P-O3'	-7.96	87.68	105.20
2	F	22	DG	OP2-P-O3'	-7.58	88.53	105.20
1	E	2	DA	P-O3'-C3'	7.20	128.34	119.70
1	E	1	DG	P-O3'-C3'	7.11	128.23	119.70
1	E	5	DG	P-O3'-C3'	7.10	128.22	119.70
1	E	6	DC	O4'-C1'-N1	6.83	112.78	108.00
1	E	16	DC	P-O3'-C3'	6.20	127.14	119.70
2	F	21	DC	P-O3'-C3'	5.97	126.86	119.70
2	F	21	DC	O4'-C1'-N1	5.50	111.85	108.00
2	F	24	DG	O4'-C1'-N9	-5.15	104.39	108.00

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	E	346	0	190	1	0
2	F	365	0	203	2	0
3	A	6494	0	6491	43	0
4	B	7456	0	7431	48	0
5	A	1	0	0	0	0
6	A	27	0	12	0	0
7	A	1	0	0	0	0
7	B	17	0	0	0	0
7	E	1	0	0	0	0
All	All	14708	0	14327	90	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 3.

All (90) 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)
3:A:39:ARG:HE	3:A:44:THR:HG21	1.52	0.74
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.70	0.73
4:B:747:LEU:HA	4:B:757:THR:HG21	1.70	0.73
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.55	0.72
4:B:699:GLU:HG2	4:B:833:LYS:HD2	1.75	0.67
4:B:993:GLU:HB3	4:B:1007:TRP:HD1	1.62	0.65
3:A:175:LEU:H	3:A:293:THR:HG21	1.63	0.64
3:A:588:TYR:O	3:A:592:MET:HG2	1.98	0.63
4:B:380:ASP:HB2	4:B:384:ARG:H	1.64	0.62
3:A:627:LYS:HA	3:A:704:ILE:HB	1.80	0.62
3:A:651:ILE:HD12	3:A:815:TYR:HB2	1.83	0.61
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.66	0.61
4:B:797:ASP:HB3	4:B:882:PHE:CD1	2.37	0.60
3:A:359:ARG:NH2	3:A:691:ILE:O	2.34	0.59
3:A:20:VAL:HG21	3:A:68:GLY:HA2	1.84	0.59
4:B:380:ASP:O	4:B:397:TYR:HB2	2.02	0.58
3:A:301:LYS:HB2	3:A:707:CYS:HB3	1.86	0.57
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.85	0.57
4:B:437:HIS:HA	4:B:457:ALA:HB3	1.86	0.57
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.86	0.57
3:A:175:LEU:HB2	3:A:266:ALA:HB1	1.87	0.56
3:A:415:PRO:HB3	3:A:444:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:527:CYS:HB2	3:A:548:GLY:HA2	1.88	0.55
4:B:758:LEU:HD22	4:B:1149:LEU:HD22	1.89	0.54
4:B:1173:VAL:HG22	4:B:1209:LEU:HB3	1.91	0.53
3:A:740:THR:HG23	3:A:742:ASP:H	1.75	0.52
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.91	0.52
3:A:543:ASP:HB3	3:A:550:LYS:HD2	1.92	0.51
4:B:1149:LEU:O	4:B:1153:MET:HG2	2.11	0.51
4:B:981:ILE:HD12	4:B:982:PRO:HD2	1.94	0.50
4:B:412:LYS:O	4:B:416:ILE:HG12	2.11	0.50
4:B:447:LEU:HD21	4:B:473:LEU:HG	1.94	0.49
3:A:525:VAL:C	3:A:527:CYS:H	2.16	0.49
4:B:952:LEU:HD23	4:B:955:LEU:HD12	1.92	0.49
3:A:124:SER:HB2	3:A:127:ASN:HB3	1.95	0.49
3:A:100:VAL:HB	3:A:123:ALA:HB3	1.95	0.49
4:B:742:ASN:HB3	4:B:1177:LEU:HD12	1.94	0.49
3:A:381:LEU:HD21	3:A:602:LEU:HD22	1.94	0.49
3:A:788:THR:HG21	3:A:821:VAL:HG21	1.95	0.48
1:E:2:DA:H61	2:F:31:DT:H3	1.60	0.48
3:A:177:GLU:HG3	3:A:266:ALA:HB2	1.96	0.47
4:B:665:GLU:HG3	4:B:666:SER:H	1.79	0.47
4:B:798:LEU:HB3	4:B:805:ILE:HD11	1.97	0.47
4:B:957:LYS:HE3	4:B:969:TYR:CD2	2.50	0.47
3:A:258:LEU:H	3:A:261:MET:HB2	1.80	0.47
3:A:544:ILE:HG12	3:A:549:VAL:HG13	1.97	0.47
3:A:295:ASP:HB3	3:A:298:GLN:HG3	1.96	0.47
4:B:440:ALA:HB3	4:B:457:ALA:HB1	1.97	0.46
4:B:1127:ALA:HB1	4:B:1263:ARG:HD2	1.96	0.46
4:B:471:ASP:O	4:B:475:GLN:HG2	2.16	0.45
3:A:695:VAL:HA	3:A:696:PRO:HD3	1.86	0.45
3:A:39:ARG:HE	3:A:44:THR:CG2	2.27	0.44
3:A:175:LEU:N	3:A:293:THR:HG21	2.31	0.44
3:A:235:LYS:HB2	3:A:239:GLN:HG3	1.98	0.44
3:A:69:PRO:HG2	3:A:72:ALA:HB3	1.99	0.44
4:B:524:TYR:CE1	4:B:531:PRO:HA	2.53	0.44
3:A:733:ALA:O	3:A:737:ARG:HG2	2.17	0.44
3:A:687:LEU:O	3:A:691:ILE:HG13	2.18	0.43
4:B:586:VAL:HG11	4:B:613:LEU:HD11	1.99	0.43
4:B:837:HIS:HA	4:B:838:PRO:HD3	1.87	0.43
3:A:1:MET:H2	4:B:476:LYS:HG3	1.83	0.43
4:B:381:GLU:HB2	4:B:395:THR:HB	2.00	0.43
4:B:993:GLU:HB3	4:B:1007:TRP:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2:ALA:H	4:B:476:LYS:HE2	1.84	0.43
3:A:831:ALA:HA	4:B:1194:LEU:HD13	1.99	0.43
4:B:408:PRO:HA	4:B:505:TYR:HD1	1.84	0.43
4:B:1091:LEU:HB3	4:B:1094:SER:HB3	2.00	0.43
3:A:353:LYS:HE2	3:A:626:GLU:HG2	2.01	0.42
4:B:590:PRO:HA	4:B:591:PRO:HD3	1.81	0.42
3:A:352:ASP:O	3:A:356:ILE:HG13	2.19	0.42
3:A:662:GLN:OE1	3:A:798:ASN:HB2	2.19	0.42
4:B:887:LEU:O	4:B:891:ILE:HG12	2.18	0.42
3:A:723:SER:HB2	3:A:726:MET:H	1.85	0.42
3:A:414:LEU:N	3:A:415:PRO:HD2	2.34	0.42
4:B:1091:LEU:HB2	4:B:1113:ILE:HB	2.02	0.42
3:A:496:LEU:HB2	3:A:513:LEU:HD12	2.01	0.42
4:B:742:ASN:O	4:B:1145:ARG:NH1	2.53	0.42
4:B:572:GLN:HB2	4:B:680:ALA:HB2	2.01	0.42
4:B:362:PRO:HG2	4:B:455:ASN:HA	2.02	0.42
4:B:1160:VAL:HA	4:B:1161:PRO:HD3	1.88	0.42
4:B:554:ARG:NH2	4:B:604:GLU:HG3	2.29	0.41
4:B:1109:ILE:HA	4:B:1110:PRO:HD3	1.91	0.41
4:B:1235:LEU:HD23	4:B:1239:ILE:HD12	2.03	0.41
4:B:797:ASP:HB3	4:B:882:PHE:HD1	1.84	0.41
4:B:558:VAL:HG21	4:B:585:LEU:HD11	2.03	0.41
3:A:706:ASP:HB2	3:A:742:ASP:HB2	2.03	0.40
3:A:685:ILE:HG12	3:A:696:PRO:HD2	2.04	0.40
2:F:21:DC:H4'	2:F:22:DG:OP1	2.21	0.40
3:A:235:LYS:HE2	3:A:275:LYS:HE3	2.03	0.40
3:A:149:GLY:O	3:A:163:VAL:HA	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	
3	A	818/934 (88%)	723 (88%)	86 (10%)	9 (1%)	17	60
4	B	913/1022 (89%)	830 (91%)	80 (9%)	3 (0%)	46	83
All	All	1731/1956 (88%)	1553 (90%)	166 (10%)	12 (1%)	26	70

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	533	LEU
3	A	526	THR
3	A	627	LYS
3	A	2	ALA
4	B	930	LYS
4	B	1309	PRO
3	A	426	GLY
3	A	146	GLY
3	A	532	VAL
4	B	745	ILE
3	A	203	GLY
3	A	202	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	
3	A	704/808 (87%)	704 (100%)	0	100	100
4	B	821/899 (91%)	819 (100%)	2 (0%)	95	98
All	All	1525/1707 (89%)	1523 (100%)	2 (0%)	95	99

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	576	ASP
4	B	647	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	798	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
6	ADP	A	936	5	22,29,29	1.09	2 (9%)	27,45,45	1.86	4 (14%)

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
6	ADP	A	936	5	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	O4'-C1'	2.06	1.43	1.41
6	A	936	ADP	C5-C4	3.29	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	936	ADP	N3-C2-N1	-7.00	123.54	128.89
6	A	936	ADP	PA-O3A-PB	-3.17	122.03	132.67
6	A	936	ADP	C4-C5-N7	-2.93	106.78	109.48
6	A	936	ADP	C2'-C1'-N9	-2.92	109.83	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	E	17/17 (100%)	0.76	1 (5%) 26 18	105, 113, 127, 132	0
2	F	18/18 (100%)	1.14	3 (16%) 2 2	102, 112, 118, 118	0
3	A	832/934 (89%)	1.11	167 (20%) 1 1	38, 111, 114, 120	0
4	B	933/1022 (91%)	0.88	120 (12%) 5 3	38, 110, 121, 126	0
All	All	1800/1991 (90%)	0.99	291 (16%) 3 2	38, 111, 118, 132	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	550	SER	11.3
3	A	153	SER	9.0
3	A	426	GLY	7.3
4	B	1308	LEU	6.9
3	A	366	PHE	6.8
3	A	206	THR	6.3
3	A	152	MET	6.2
4	B	1330	LEU	5.9
4	B	1285	PHE	5.9
3	A	284	SER	5.6
3	A	131	PHE	5.6
4	B	1269	CYS	5.5
3	A	166	VAL	5.4
3	A	291	LEU	5.4
3	A	692	GLY	5.4
3	A	852	GLU	5.2
3	A	469	LEU	5.2
4	B	651	ILE	5.2
1	E	17	DG	5.2
4	B	954	TYR	5.0
3	A	395	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
3	A	161	VAL	4.9
2	F	15	DC	4.9
3	A	587	GLY	4.8
3	A	421	LEU	4.8
3	A	202	PRO	4.8
4	B	669	ILE	4.8
4	B	1284	THR	4.8
4	B	716	THR	4.7
3	A	693	CYS	4.7
3	A	319	ASP	4.7
3	A	292	THR	4.6
3	A	706	ASP	4.6
4	B	717	VAL	4.5
3	A	798	ASN	4.4
3	A	480	GLU	4.4
4	B	997	LYS	4.3
3	A	236	ASP	4.3
3	A	750	LEU	4.2
4	B	1309	PRO	4.1
4	B	1087	PRO	4.1
4	B	1235	LEU	4.1
3	A	726	MET	4.1
3	A	242	ASN	4.1
4	B	552	HIS	4.1
4	B	1137	MET	4.0
3	A	478	LEU	4.0
3	A	156	ASP	4.0
4	B	1085	THR	4.0
3	A	390	LEU	4.0
3	A	574	GLN	3.9
3	A	108	GLY	3.9
3	A	384	PHE	3.9
3	A	330	LEU	3.9
3	A	608	PHE	3.8
4	B	1323	PHE	3.8
3	A	598	VAL	3.8
4	B	1135	PRO	3.8
3	A	1	MET	3.8
4	B	1303	ALA	3.8
4	B	1300	PHE	3.8
3	A	767	SER	3.8
3	A	394	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
4	B	1131	LEU	3.7
4	B	1138	GLY	3.6
3	A	585	SER	3.6
3	A	436	PHE	3.6
4	B	1129	CYS	3.6
3	A	582	VAL	3.6
4	B	747	LEU	3.6
3	A	350	LEU	3.6
4	B	989	ASN	3.5
3	A	754	THR	3.5
3	A	736	LEU	3.5
4	B	679	LEU	3.5
4	B	1120	GLU	3.5
3	A	197	LYS	3.5
3	A	179	PRO	3.5
3	A	175	LEU	3.5
4	B	1332	LEU	3.5
4	B	508	VAL	3.4
3	A	404	CYS	3.4
3	A	704	ILE	3.4
4	B	637	LEU	3.4
4	B	1091	LEU	3.4
4	B	556	TYR	3.4
3	A	254	ASN	3.4
3	A	483	GLU	3.3
3	A	458	LEU	3.3
3	A	224	ILE	3.3
3	A	201	LEU	3.3
3	A	431	LEU	3.3
3	A	751	GLY	3.3
3	A	269	SER	3.2
3	A	363	VAL	3.2
3	A	830	VAL	3.2
4	B	1248	HIS	3.2
2	F	32	DC	3.2
3	A	452	GLU	3.2
2	F	28	DC	3.2
3	A	414	LEU	3.2
3	A	251	GLU	3.1
3	A	459	ASP	3.1
3	A	777	PHE	3.1
4	B	1268	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
4	B	1132	VAL	3.1
3	A	817	VAL	3.1
4	B	543	LYS	3.1
3	A	785	HIS	3.1
3	A	787	LEU	3.1
4	B	507	ARG	3.1
4	B	1299	GLY	3.1
3	A	738	SER	3.0
4	B	1252	LEU	3.0
3	A	425	GLU	3.0
4	B	1270	MET	3.0
3	A	768	GLU	3.0
4	B	1327	ASN	3.0
3	A	437	VAL	3.0
3	A	187	LEU	3.0
4	B	981	ILE	3.0
3	A	359	ARG	3.0
4	B	990	LEU	2.9
3	A	180	ASP	2.9
3	A	725	PHE	2.9
4	B	1128	TYR	2.9
3	A	158	GLN	2.9
3	A	468	PHE	2.9
4	B	501	HIS	2.9
4	B	1258	GLN	2.9
3	A	689	ALA	2.9
4	B	1304	ARG	2.9
4	B	1086	PRO	2.8
4	B	1144	MET	2.8
3	A	150	VAL	2.8
3	A	518	GLN	2.8
4	B	1001	LYS	2.8
4	B	1149	LEU	2.8
3	A	351	MET	2.8
4	B	1113	ILE	2.8
3	A	223	LEU	2.8
4	B	1312	VAL	2.8
4	B	1231	VAL	2.8
4	B	933	PHE	2.8
3	A	667	ILE	2.8
3	A	190	LEU	2.8
3	A	163	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
4	B	1003	CYS	2.8
3	A	484	ILE	2.7
3	A	588	TYR	2.7
3	A	482	ARG	2.7
4	B	514	CYS	2.7
3	A	666	ILE	2.7
4	B	1126	LYS	2.7
3	A	194	ILE	2.7
3	A	470	VAL	2.7
3	A	283	ASP	2.7
3	A	448	SER	2.7
4	B	1289	PHE	2.7
4	B	1307	ASN	2.7
3	A	50	ALA	2.7
3	A	260	GLU	2.7
3	A	301	LYS	2.7
3	A	381	LEU	2.7
3	A	294	PHE	2.6
3	A	631	ARG	2.6
4	B	1326	MET	2.6
4	B	1333	PHE	2.6
3	A	592	MET	2.6
3	A	496	LEU	2.6
4	B	549	SER	2.6
3	A	135	LEU	2.6
3	A	253	MET	2.6
3	A	405	TYR	2.6
3	A	538	ASN	2.6
3	A	634	LEU	2.6
3	A	207	ALA	2.5
4	B	1158	CYS	2.5
3	A	266	ALA	2.5
3	A	760	PHE	2.5
3	A	523	PHE	2.5
4	B	1218	GLY	2.5
4	B	1247	THR	2.5
3	A	200	VAL	2.5
4	B	1237	GLU	2.5
4	B	1227	ILE	2.5
3	A	447	PHE	2.5
4	B	978	GLN	2.5
4	B	1155	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	300	MET	2.5
3	A	407	LEU	2.5
3	A	61	GLN	2.4
3	A	358	GLU	2.4
4	B	1079	ILE	2.4
4	B	668	SER	2.4
3	A	411	ILE	2.4
3	A	584	ILE	2.4
4	B	1140	LYS	2.4
4	B	1010	THR	2.4
4	B	1063	LEU	2.4
4	B	1256	TYR	2.4
3	A	739	ALA	2.4
4	B	497	ARG	2.4
3	A	261	MET	2.4
4	B	957	LYS	2.4
3	A	178	PHE	2.4
3	A	595	LEU	2.4
3	A	642	VAL	2.4
4	B	696	ILE	2.4
4	B	1239	ILE	2.4
3	A	280	LEU	2.4
3	A	524	ARG	2.3
4	B	609	LEU	2.3
4	B	882	PHE	2.3
3	A	199	CYS	2.3
4	B	1225	THR	2.3
3	A	472	PRO	2.3
4	B	427	TYR	2.3
4	B	376	GLU	2.3
4	B	718	SER	2.3
3	A	580	GLU	2.3
3	A	581	ILE	2.3
4	B	1244	LEU	2.3
3	A	96	ARG	2.3
3	A	162	GLY	2.3
3	A	792	ASN	2.3
3	A	432	LEU	2.3
4	B	1088	PHE	2.3
3	A	165	TYR	2.2
3	A	605	VAL	2.2
4	B	1124	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	539	PHE	2.2
4	B	650	GLY	2.2
3	A	606	VAL	2.2
3	A	290	GLU	2.2
4	B	1083	GLU	2.2
3	A	607	SER	2.2
4	B	570	ILE	2.2
3	A	521	TYR	2.2
4	B	1188	SER	2.2
3	A	403	ASP	2.2
3	A	503	LEU	2.2
3	A	385	PRO	2.2
3	A	650	PHE	2.2
4	B	1112	ASP	2.2
4	B	1210	VAL	2.2
4	B	1097	PRO	2.2
3	A	633	ILE	2.2
4	B	1123	GLU	2.1
3	A	663	MET	2.1
3	A	160	GLN	2.1
3	A	611	VAL	2.1
4	B	785	HIS	2.1
4	B	968	VAL	2.1
4	B	969	TYR	2.1
3	A	98	TYR	2.1
4	B	671	LEU	2.1
3	A	193	GLN	2.1
3	A	277	LEU	2.1
3	A	481	LEU	2.1
3	A	855	GLN	2.1
3	A	70	ALA	2.1
4	B	1030	LYS	2.1
3	A	645	GLN	2.1
4	B	429	VAL	2.1
4	B	1071	ASP	2.1
3	A	7	GLU	2.1
4	B	782	LEU	2.1
4	B	1201	LEU	2.1
4	B	457	ALA	2.1
4	B	999	THR	2.1
3	A	729	MET	2.1
4	B	1163	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	748	ASN	2.1
3	A	590	GLU	2.0
4	B	458	HIS	2.0
4	B	573	PHE	2.0
4	B	1084	ASP	2.0
3	A	299	TYR	2.0
3	A	552	THR	2.0
3	A	210	MET	2.0
4	B	1319	LYS	2.0
3	A	853	GLU	2.0
4	B	1119	GLU	2.0
3	A	487	ASP	2.0
3	A	609	ALA	2.0
3	A	697	CYS	2.0
4	B	798	LEU	2.0
4	B	1018	LEU	2.0
4	B	1060	LEU	2.0
3	A	802	VAL	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	ADP	A	936	27/27	0.95	0.22	-0.99	110,110,111,111	0
5	MG	A	935	1/1	0.94	0.25	-	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.