



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 AM GMT

PDB ID : 2O8D  
Title : human MutSalpha (MSH2/MSH6) bound to ADP and a G dU mispair  
Authors : Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.  
Deposited on : 2006-12-12  
Resolution : 3.00 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



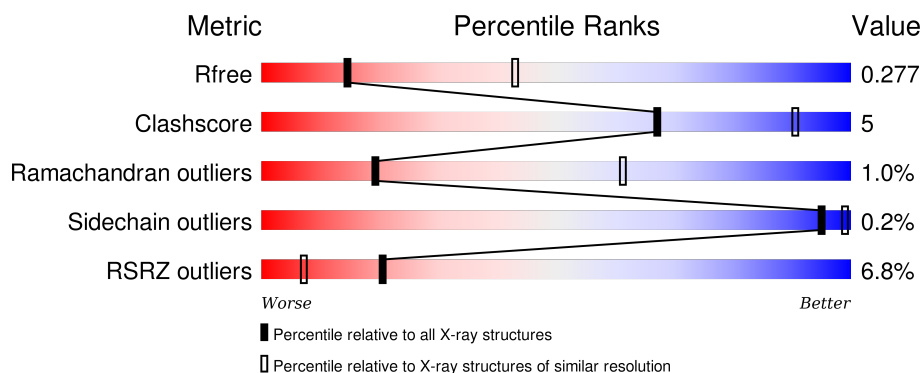
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	15	<div> <div>7%</div> <div>80% 13% 7%</div> </div>
2	F	15	<div> <div>7%</div> <div>67% 33%</div> </div>
3	A	934	<div> <div>7%</div> <div>77% 12% 11%</div> </div>
4	B	1022	<div> <div>5%</div> <div>79% 12% 9%</div> </div>



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14593 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\*AP\*CP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*T  
P\*AP\*GP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total	C	N	O	P	0	0	0
			307	145	62	86	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			302	144	53	91	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	830	Total	C	N	O	S	0	0	0
			6439	4085	1092	1228	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	932	Total	C	N	O	S	0	0	0
			7443	4721	1277	1394	51			

There are 2 discrepancies between the modelled and reference sequences:

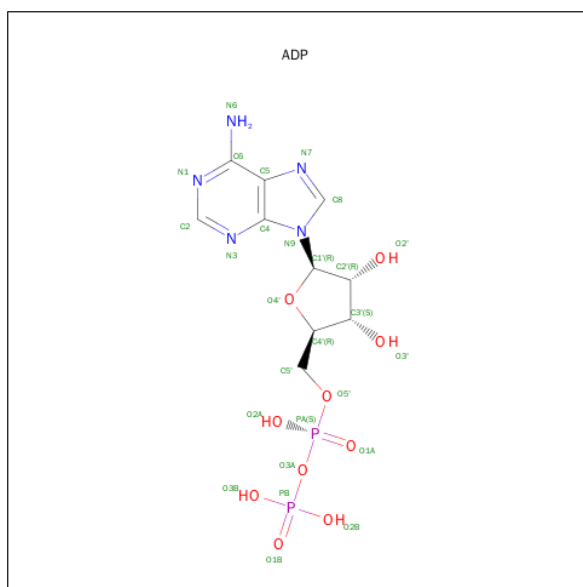
Chain	Residue	Modelled	Actual	Comment	Reference
B	339	MET	-	INITIATING METHIONINE	UNP P52701
B	340	GLY	-	CLONING ARTIFACT	UNP P52701

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 27 10 5 10 2	0	0
6	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 7 is water.

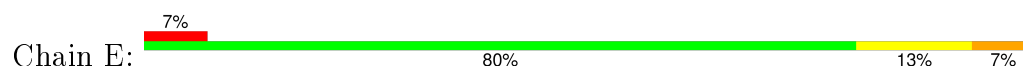
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	B	40	Total O 40 40	0	0
7	E	1	Total O 1 1	0	0
7	F	3	Total O 3 3	0	0



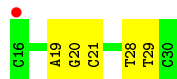
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

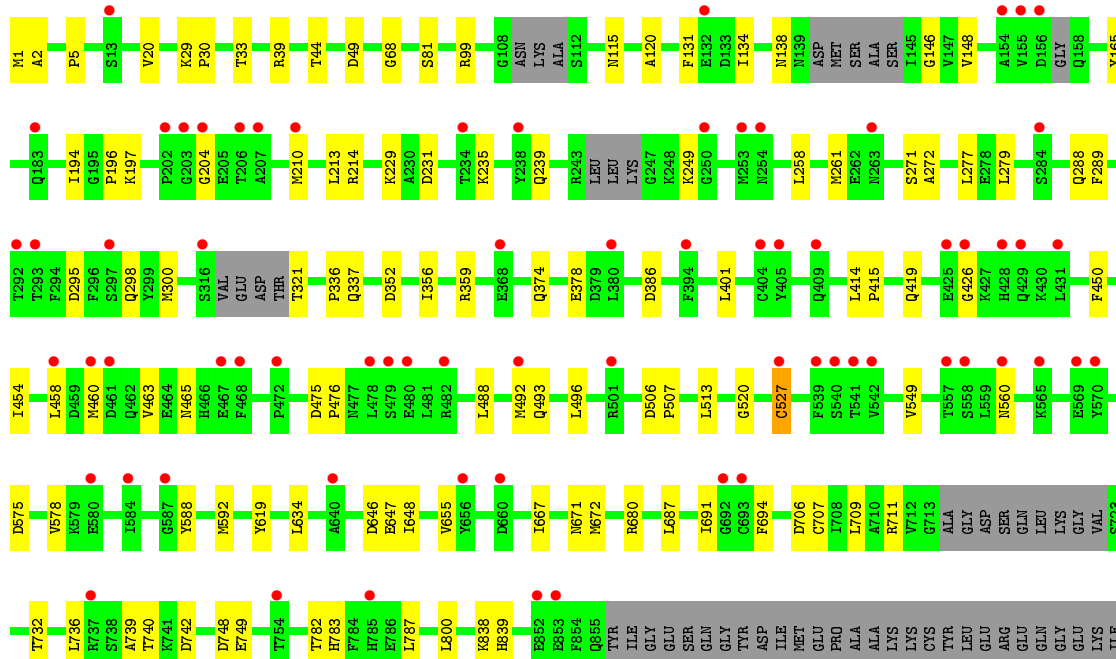
- Molecule 1: 5'-D(\*GP\*AP\*AP\*CP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*TP\*AP\*GP\*G)-3'



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



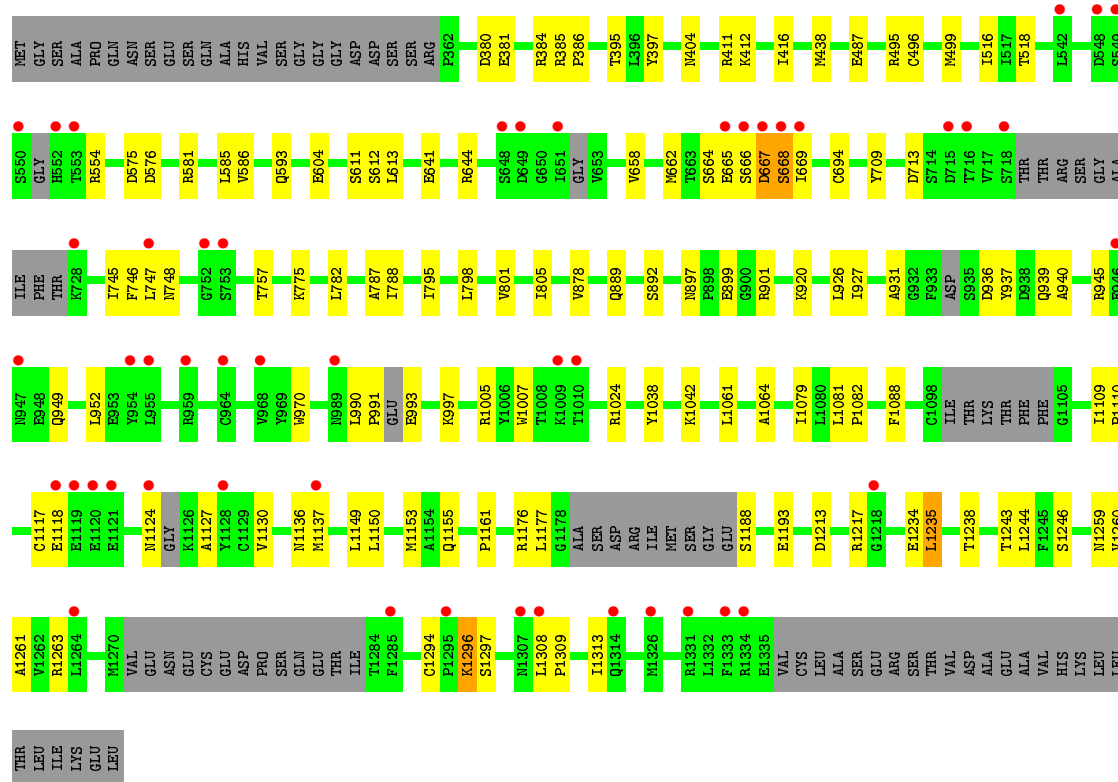
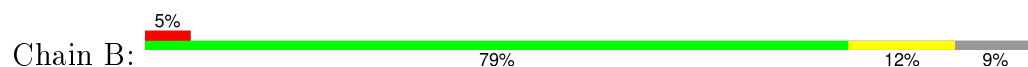
- Molecule 3: DNA mismatch repair protein Msh2





ILE	GLN	GLU	PHE	LEU	SER	LYS	VAL	LYS	GLN	MET	PRO	PHE	THR	GLU	MET	SER	GLY	GLU	ASN	ILE	THR	ILE	LYS	LEU	LYS	GLN	LEU	LYS	ALA	GLU	VAL	ILE	ALA	LYS	ASN	SER	PHE	VAL	ASN	GLU	ILE	ILE	SER	ARG	ILE	LYS	VAL	THR	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• 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, $\alpha$ , $\beta$ , $\gamma$	260.38 Å   260.38 Å   260.38 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 3.00 48.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.00) 99.8 (48.35-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.239   ,   0.278 0.242   ,   0.277	Depositor DCC
$R_{free}$ test set	3088 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 106.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 60518 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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

### 5.1 Standard geometry

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	0.65	0/345	1.39	5/531 (0.9%)
2	F	0.66	0/337	1.39	4/518 (0.8%)
3	A	0.33	0/6539	0.61	0/8828
4	B	0.39	0/7587	0.66	1/10226 (0.0%)
All	All	0.38	0/14808	0.70	10/20103 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	DC	O4'-C4'-C3'	-9.00	100.60	106.00
1	E	4	DC	O4'-C1'-N1	8.03	113.62	108.00
2	F	19	DA	P-O3'-C3'	6.97	128.06	119.70
2	F	20	DG	O4'-C1'-N9	6.77	112.74	108.00
1	E	4	DC	C4'-C3'-C2'	-6.12	97.59	103.10
1	E	14	DG	O4'-C1'-N9	5.70	111.99	108.00
2	F	21	DC	P-O3'-C3'	5.60	126.42	119.70
2	F	21	DC	O4'-C1'-N1	5.42	111.80	108.00
4	B	1235	LEU	CA-CB-CG	5.36	127.64	115.30
1	E	4	DC	P-O3'-C3'	5.15	125.88	119.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	307	0	168	1	0
2	F	302	0	169	1	0
3	A	6439	0	6409	65	0
4	B	7443	0	7414	72	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
7	A	2	0	0	0	0
7	B	40	0	0	0	0
7	E	1	0	0	0	0
7	F	3	0	0	0	0
All	All	14593	0	14184	137	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 5.

All (137) 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)
4:B:897:ASN:HB3	4:B:901:ARG:HE	1.35	0.90
3:A:39:ARG:HE	3:A:44:THR:HG21	1.48	0.77
4:B:897:ASN:HB3	4:B:901:ARG:NE	2.02	0.75
4:B:586:VAL:HG11	4:B:613:LEU:HD11	1.69	0.75
4:B:380:ASP:HB2	4:B:384:ARG:H	1.52	0.74
4:B:899:GLU:O	4:B:901:ARG:NH1	2.26	0.69
4:B:1235:LEU:HD21	4:B:1243:THR:HG21	1.75	0.69
4:B:892:SER:O	4:B:901:ARG:HB3	1.94	0.68
3:A:646:ASP:CG	3:A:647:GLU:H	1.96	0.68
3:A:588:TYR:O	3:A:592:MET:HG2	1.94	0.67
3:A:204:GLY:H	3:A:214:ARG:HH22	1.42	0.65
4:B:380:ASP:O	4:B:397:TYR:HB2	1.96	0.65
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.61	0.64
4:B:1259:ASN:O	4:B:1261:ALA:N	2.28	0.63
4:B:746:PHE:CE1	4:B:775:LYS:HD2	2.34	0.62
3:A:39:ARG:HE	3:A:44:THR:CG2	2.13	0.61
1:E:4:DC:H2'	1:E:5:DC:C6	2.36	0.60
4:B:949:GLN:HA	4:B:952:LEU:HB3	1.83	0.60
3:A:235:LYS:HE2	3:A:271:SER:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:581:ARG:HH21	4:B:713:ASP:HB2	1.67	0.59
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.86	0.58
3:A:321:THR:HG23	3:A:321:THR:O	2.02	0.58
4:B:1088:PHE:HB2	4:B:1117:CYS:H	1.68	0.58
3:A:33:THR:HG22	3:A:99:ARG:HH11	1.68	0.57
4:B:1127:ALA:H	4:B:1261:ALA:HA	1.69	0.56
4:B:1118:GLU:HG2	4:B:1124:ASN:HB2	1.87	0.56
3:A:194:ILE:HG13	3:A:196:PRO:HD3	1.88	0.55
3:A:671:ASN:O	3:A:672:MET:HB2	2.06	0.55
3:A:619:TYR:HB3	3:A:694:PHE:HB3	1.88	0.55
3:A:20:VAL:HG21	3:A:68:GLY:HA2	1.87	0.55
3:A:1:MET:O	3:A:2:ALA:HB3	2.07	0.55
3:A:740:THR:HG23	3:A:742:ASP:H	1.71	0.54
3:A:527:CYS:HA	3:A:549:VAL:HG23	1.88	0.54
4:B:404:ASN:OD1	4:B:411:ARG:NH1	2.41	0.54
3:A:488:LEU:O	3:A:492:MET:HG2	2.08	0.54
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.90	0.54
3:A:359:ARG:NH2	3:A:691:ILE:O	2.35	0.54
3:A:732:THR:O	3:A:736:LEU:HB2	2.08	0.53
3:A:258:LEU:HB2	3:A:261:MET:HG2	1.90	0.53
3:A:204:GLY:H	3:A:214:ARG:NH2	2.06	0.53
3:A:231:ASP:OD1	3:A:272:ALA:HB2	2.09	0.53
4:B:381:GLU:HB2	4:B:395:THR:HB	1.91	0.52
4:B:991:PRO:O	4:B:993:GLU:N	2.42	0.52
3:A:295:ASP:HB3	3:A:298:GLN:HG3	1.92	0.52
4:B:748:ASN:H	4:B:757:THR:HG21	1.75	0.51
3:A:680:ARG:NH2	3:A:748:ASP:OD1	2.44	0.51
3:A:131:PHE:HD1	3:A:134:ILE:HD12	1.75	0.51
4:B:1136:ASN:O	4:B:1137:MET:HB3	2.11	0.51
3:A:838:LYS:HG3	3:A:839:HIS:H	1.76	0.51
3:A:235:LYS:HB2	3:A:239:GLN:HG3	1.94	0.50
4:B:993:GLU:HG3	4:B:1005:ARG:HD2	1.93	0.50
4:B:585:LEU:HD12	4:B:709:TYR:CE2	2.47	0.50
4:B:798:LEU:O	4:B:805:ILE:HD11	2.11	0.50
4:B:936:ASP:O	4:B:940:ALA:N	2.44	0.49
4:B:1234:GLU:HG3	4:B:1238:THR:HB	1.94	0.49
3:A:460:MET:HA	3:A:463:VAL:HB	1.93	0.49
3:A:672:MET:SD	4:B:1188:SER:N	2.86	0.49
2:F:28:DT:H2"	2:F:29:DT:H5"	1.94	0.49
4:B:518:THR:HG21	4:B:593:GLN:NE2	2.29	0.48
4:B:1038:TYR:CE2	4:B:1042:LYS:HE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:MET:HA	3:A:213:LEU:HD12	1.96	0.47
3:A:634:LEU:HB2	3:A:655:VAL:HB	1.96	0.47
3:A:838:LYS:HG3	3:A:839:HIS:N	2.29	0.47
3:A:374:GLN:O	3:A:378:GLU:HG2	2.14	0.47
4:B:970:TRP:HZ3	4:B:997:LYS:HD2	1.79	0.47
4:B:945:ARG:HD2	4:B:1024:ARG:HH12	1.80	0.47
3:A:709:LEU:HD12	3:A:739:ALA:HB2	1.97	0.47
3:A:496:LEU:HD21	3:A:513:LEU:HB2	1.97	0.47
3:A:667:ILE:HA	3:A:800:LEU:O	2.15	0.47
4:B:412:LYS:HE3	4:B:416:ILE:HD11	1.96	0.47
4:B:385:ARG:CD	4:B:386:PRO:HD2	2.45	0.46
4:B:381:GLU:HB2	4:B:395:THR:CB	2.45	0.46
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.97	0.46
3:A:337:GLN:HG3	3:A:337:GLN:H	1.54	0.46
4:B:554:ARG:HH12	4:B:604:GLU:HB2	1.81	0.45
4:B:1177:LEU:O	4:B:1217:ARG:NH2	2.43	0.45
4:B:1109:ILE:HA	4:B:1110:PRO:HD3	1.82	0.45
4:B:667:ASP:CG	4:B:668:SER:H	2.19	0.45
4:B:889:GLN:O	4:B:901:ARG:HA	2.15	0.45
4:B:1213:ASP:HA	4:B:1246:SER:OG	2.17	0.45
4:B:801:VAL:HG21	4:B:878:VAL:HG21	1.98	0.45
4:B:1149:LEU:O	4:B:1153:MET:HG2	2.17	0.45
3:A:520:GLY:HA3	3:A:560:ASN:HD21	1.82	0.45
4:B:575:ASP:OD1	4:B:576:ASP:N	2.41	0.44
3:A:782:THR:HG21	3:A:787:LEU:HD13	1.99	0.44
3:A:277:LEU:C	3:A:279:LEU:H	2.21	0.44
4:B:611:SER:OG	4:B:612:SER:N	2.51	0.44
4:B:658:VAL:O	4:B:662:MET:HG2	2.18	0.44
4:B:782:LEU:HD13	4:B:787:ALA:HB1	1.99	0.44
4:B:782:LEU:O	4:B:1155:GLN:HB3	2.18	0.44
3:A:646:ASP:CG	3:A:647:GLU:N	2.67	0.43
4:B:1127:ALA:HB1	4:B:1263:ARG:HD2	1.99	0.43
3:A:706:ASP:HB2	3:A:742:ASP:HB2	2.00	0.43
3:A:336:PRO:HG2	3:A:386:ASP:HB2	2.00	0.43
4:B:990:LEU:HA	4:B:991:PRO:HD3	1.81	0.43
3:A:29:LYS:HE3	3:A:49:ASP:OD2	2.18	0.43
4:B:1294:CYS:C	4:B:1296:LYS:H	2.22	0.43
4:B:667:ASP:C	4:B:669:ILE:H	2.22	0.43
4:B:926:LEU:HD23	4:B:926:LEU:HA	1.76	0.43
4:B:385:ARG:HD2	4:B:386:PRO:HD2	2.00	0.43
3:A:415:PRO:O	3:A:419:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:641:GLU:HB3	4:B:644:ARG:HG3	2.01	0.42
3:A:450:PHE:CZ	3:A:454:ILE:HD11	2.54	0.42
4:B:438:MET:H	4:B:438:MET:HG2	1.61	0.42
3:A:401:LEU:HD11	3:A:458:LEU:HD11	2.00	0.42
4:B:1308:LEU:HB3	4:B:1313:ILE:HD11	2.01	0.42
4:B:516:ILE:HB	4:B:694:CYS:HA	2.02	0.42
3:A:463:VAL:C	3:A:465:ASN:H	2.23	0.42
3:A:352:ASP:O	3:A:356:ILE:HG13	2.19	0.42
3:A:575:ASP:HA	3:A:578:VAL:HB	2.02	0.42
3:A:672:MET:SD	4:B:1188:SER:HB2	2.60	0.41
3:A:492:MET:HE2	3:A:513:LEU:HD21	2.01	0.41
3:A:687:LEU:O	3:A:691:ILE:HG13	2.19	0.41
3:A:29:LYS:HA	3:A:30:PRO:HD3	1.95	0.41
4:B:1081:LEU:HA	4:B:1082:PRO:HD3	1.89	0.41
3:A:288:GLN:O	3:A:289:PHE:HB2	2.20	0.41
3:A:475:ASP:HA	3:A:476:PRO:HD2	1.88	0.41
4:B:1136:ASN:O	4:B:1137:MET:CB	2.68	0.41
3:A:197:LYS:HB3	3:A:197:LYS:HE2	1.73	0.41
4:B:496:CYS:HA	4:B:499:MET:HG2	2.02	0.41
4:B:889:GLN:HG2	4:B:901:ARG:NH1	2.35	0.41
3:A:300:MET:HG3	3:A:707:CYS:HA	2.02	0.41
3:A:1:MET:O	3:A:2:ALA:CB	2.69	0.41
4:B:664:SER:O	4:B:666:SER:N	2.53	0.41
4:B:1150:LEU:CD2	4:B:1161:PRO:HD2	2.50	0.41
3:A:749:GLU:HG3	3:A:783:HIS:ND1	2.35	0.41
4:B:920:LYS:NZ	4:B:927:ILE:HD12	2.36	0.41
3:A:493:GLN:HA	3:A:496:LEU:HD12	2.03	0.41
4:B:788:ILE:HG21	4:B:1079:ILE:HD12	2.02	0.41
4:B:487:GLU:OE1	4:B:495:ARG:NH1	2.54	0.41
4:B:1130:VAL:HB	4:B:1244:LEU:HD23	2.03	0.41
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.85	0.41
3:A:646:ASP:HB3	3:A:648:ILE:HG13	2.02	0.40
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	2.02	0.40
3:A:414:LEU:N	3:A:415:PRO:HD2	2.36	0.40
3:A:506:ASP:HA	3:A:507:PRO:HD3	1.84	0.40
3:A:148:VAL:HG12	3:A:165:TYR:HB3	2.03	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	816/934 (87%)	732 (90%)	76 (9%)	8 (1%)	19	61
4	B	912/1022 (89%)	836 (92%)	66 (7%)	10 (1%)	17	58
All	All	1728/1956 (88%)	1568 (91%)	142 (8%)	18 (1%)	19	61

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	665	GLU
4	B	747	LEU
4	B	1297	SER
3	A	138	ASN
4	B	668	SER
4	B	745	ILE
3	A	120	ALA
3	A	146	GLY
4	B	931	ALA
3	A	115	ASN
4	B	667	ASP
4	B	1296	LYS
3	A	229	LYS
3	A	249	LYS
3	A	527	CYS
4	B	1260	VAL
3	A	426	GLY
4	B	1309	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	693/808 (86%)	692 (100%)	1 (0%)	95	99
4	B	819/899 (91%)	817 (100%)	2 (0%)	95	99
All	All	1512/1707 (89%)	1509 (100%)	3 (0%)	95	99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	711	ARG
4	B	937	TYR
4	B	1007	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	377	GLN
3	A	388	ASN
3	A	560	ASN
4	B	751	ASN
4	B	1124	ASN
4	B	1327	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1.05	1 (4%)	27,45,45	1.87	4 (14%)
6	ADP	B	202	5	22,29,29	1.04	1 (4%)	27,45,45	1.87	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
6	ADP	B	202	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	C5-C4	3.23	1.47	1.40
6	B	202	ADP	C5-C4	3.27	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	202	ADP	N3-C2-N1	-7.32	123.29	128.89
6	A	936	ADP	N3-C2-N1	-7.01	123.53	128.89
6	A	936	ADP	C4-C5-N7	-3.06	106.67	109.48
6	A	936	ADP	PA-O3A-PB	-3.00	122.61	132.67
6	B	202	ADP	C4-C5-N7	-2.92	106.79	109.48
6	B	202	ADP	PA-O3A-PB	-2.85	123.10	132.67
6	A	936	ADP	C2'-C1'-N9	-2.39	110.64	114.29
6	B	202	ADP	C2'-C1'-N9	-2.14	111.02	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	15/15 (100%)	0.59	1 (6%) 21 7	85, 93, 111, 114	0
2	F	14/15 (93%)	0.68	1 (7%) 19 7	86, 92, 123, 126	0
3	A	830/934 (88%)	0.55	70 (8%) 14 5	20, 93, 98, 107	0
4	B	932/1022 (91%)	0.37	49 (5%) 30 12	34, 93, 107, 116	0
All	All	1791/1986 (90%)	0.46	121 (6%) 20 7	20, 93, 103, 126	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	550	SER	8.5
3	A	541	THR	8.1
3	A	206	THR	7.5
4	B	954	TYR	6.8
3	A	540	SER	6.5
1	E	15	DG	6.3
4	B	1010	THR	5.8
3	A	202	PRO	5.3
3	A	467	GLU	5.2
4	B	747	LEU	4.8
3	A	13	SER	4.5
3	A	316	SER	4.5
3	A	428	HIS	4.4
3	A	203	GLY	4.3
4	B	718	SER	4.2
4	B	1119	GLU	4.1
3	A	156	ASP	4.0
3	A	204	GLY	4.0
3	A	426	GLY	4.0
3	A	154	ALA	3.9
4	B	552	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
4	B	549	SER	3.8
3	A	468	PHE	3.7
4	B	728	LYS	3.7
3	A	527	CYS	3.6
4	B	1334	ARG	3.6
3	A	584	ILE	3.6
3	A	458	LEU	3.5
2	F	16	DC	3.5
3	A	292	THR	3.3
3	A	587	GLY	3.3
3	A	478	LEU	3.2
4	B	1308	LEU	3.2
4	B	1137	MET	3.2
4	B	1333	PHE	3.2
4	B	752	GLY	3.2
4	B	1218	GLY	3.2
3	A	207	ALA	3.1
3	A	284	SER	3.1
3	A	558	SER	3.1
4	B	955	LEU	3.1
3	A	238	TYR	3.1
4	B	1124	ASN	3.1
3	A	210	MET	3.0
4	B	968	VAL	3.0
3	A	557	THR	3.0
3	A	480	GLU	3.0
3	A	580	GLU	3.0
4	B	1118	GLU	2.9
4	B	1264	LEU	2.9
3	A	380	LEU	2.9
3	A	569	GLU	2.9
4	B	648	SER	2.9
3	A	425	GLU	2.9
4	B	667	ASP	2.8
3	A	737	ARG	2.8
3	A	754	THR	2.8
4	B	1295	PRO	2.8
3	A	852	GLU	2.8
4	B	668	SER	2.7
4	B	947	ASN	2.7
4	B	1009	LYS	2.7
3	A	460	MET	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	785	HIS	2.7
3	A	409	GLN	2.6
4	B	716	THR	2.6
3	A	394	PHE	2.6
4	B	665	GLU	2.6
3	A	692	GLY	2.6
3	A	234	THR	2.5
4	B	946	GLU	2.5
4	B	959	ARG	2.5
3	A	570	TYR	2.5
4	B	753	SER	2.5
3	A	404	CYS	2.5
3	A	254	ASN	2.5
4	B	989	ASN	2.5
3	A	431	LEU	2.4
3	A	656	TYR	2.4
4	B	553	THR	2.4
4	B	1121	GLU	2.4
3	A	501	ARG	2.4
4	B	649	ASP	2.4
4	B	715	ASP	2.4
3	A	640	ALA	2.4
4	B	651	ILE	2.4
4	B	1331	ARG	2.4
4	B	1326	MET	2.4
4	B	548	ASP	2.4
4	B	666	SER	2.4
3	A	461	ASP	2.3
3	A	263	ASN	2.3
3	A	853	GLU	2.3
4	B	1120	GLU	2.3
3	A	429	GLN	2.3
3	A	183	GLN	2.3
3	A	405	TYR	2.2
3	A	472	PRO	2.2
4	B	669	ILE	2.2
4	B	964	CYS	2.2
3	A	250	GLY	2.2
3	A	479	SER	2.1
3	A	565	LYS	2.1
3	A	539	PHE	2.1
3	A	132	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	297	SER	2.1
4	B	1285	PHE	2.1
3	A	560	ASN	2.1
3	A	293	THR	2.1
3	A	660	ASP	2.1
3	A	482	ARG	2.1
3	A	155	VAL	2.1
3	A	253	MET	2.0
3	A	492	MET	2.0
4	B	1314	GLN	2.0
4	B	542	LEU	2.0
4	B	1128	TYR	2.0
3	A	542	VAL	2.0
3	A	693	CYS	2.0
3	A	368	GLU	2.0
4	B	1307	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
6	ADP	A	936	27/27	0.90	0.21	-0.87	89,89,91,91	0
6	ADP	B	202	27/27	0.82	0.16	-0.97	99,100,101,101	0
5	MG	B	102	1/1	0.59	0.36	-	83,83,83,83	0
5	MG	A	935	1/1	0.82	0.53	-	92,92,92,92	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.