



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 AM GMT

PDB ID : 2O8B  
Title : human MutSalpha (MSH2/MSH6) bound to ADP and a G T mispair  
Authors : Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.  
Deposited on : 2006-12-12  
Resolution : 2.75 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

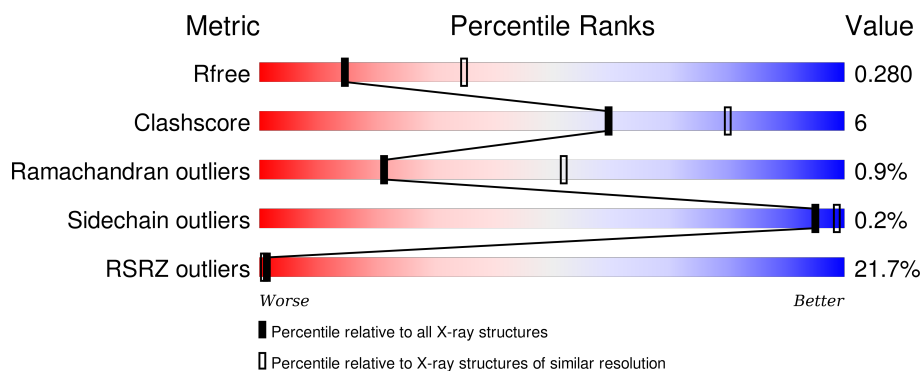
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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>33%</div> <div>53%</div> <div>13%</div> </div>
2	F	15	<div> <div>47%</div> <div>27%</div> <div>20%</div> <div>7%</div> </div>
3	A	934	<div> <div>27%</div> <div>76%</div> <div>13%</div> <div>11%</div> </div>
4	B	1022	<div> <div>13%</div> <div>77%</div> <div>13%</div> <div>9%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14692 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\*TP\*GP\*CP\*GP\*G  
P\*TP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			303	145	53	91	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	831	Total	C	N	O	S	0	0	0
			6536	4144	1113	1245	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	930	Total	C	N	O	S	0	0	0
			7447	4725	1279	1392	51			

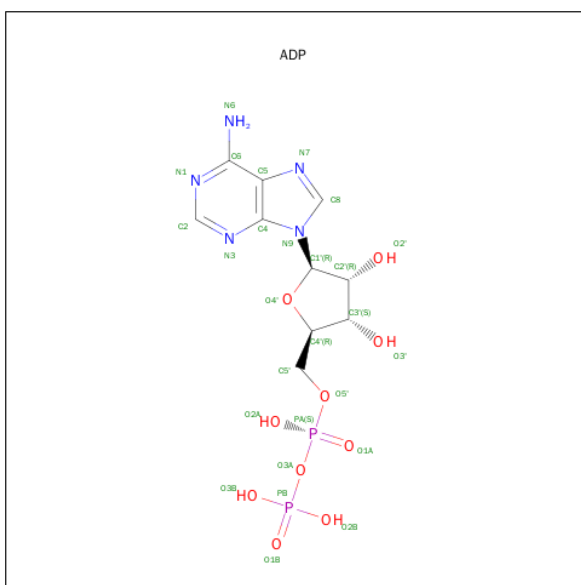
There are 2 discrepancies between the modelled and reference sequences:

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:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

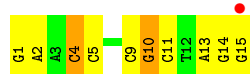
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	B	39	Total O 39 39	0	0
7	E	2	Total O 2 2	0	0
7	F	1	Total O 1 1	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.

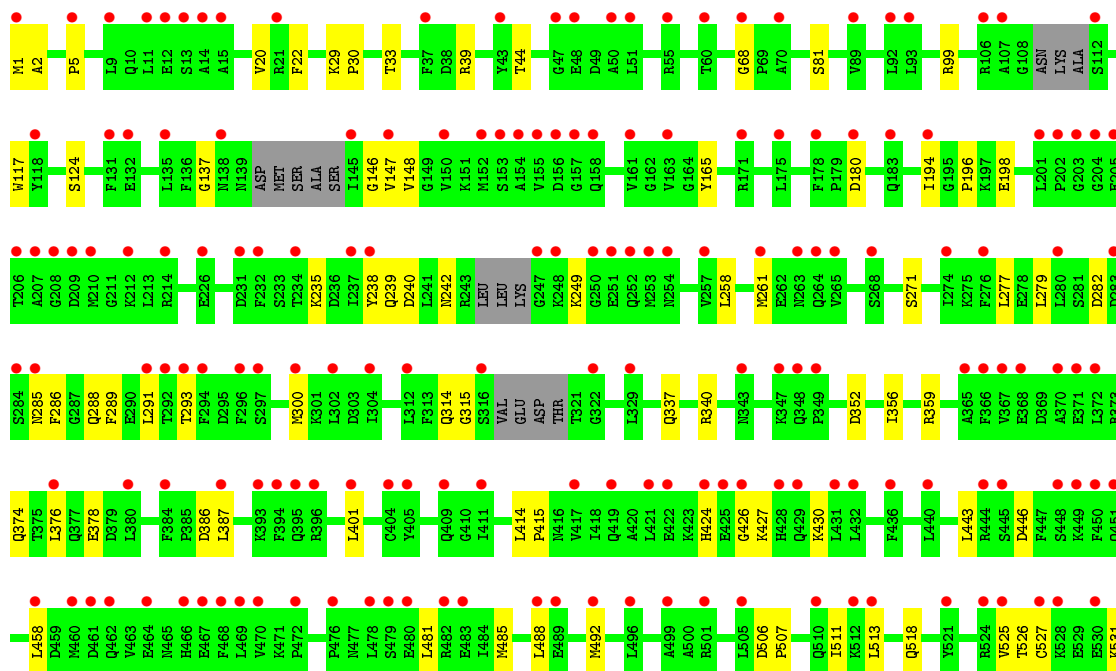
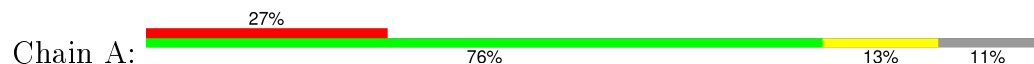
- Molecule 1: 5'-D(\*GP\*AP\*AP\*CP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*TP\*AP\*GP\*G)-3'

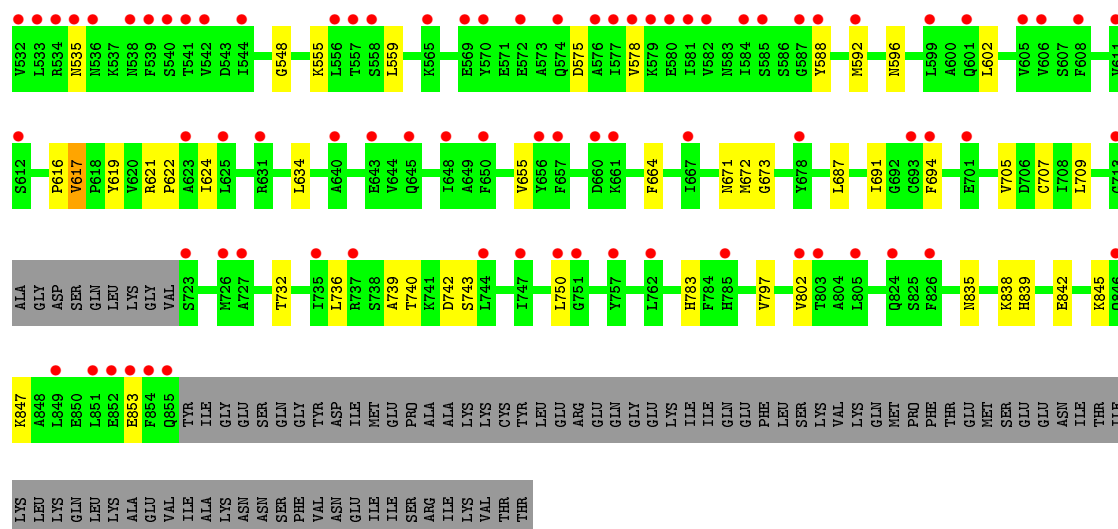


- Molecule 2: 5'-D(\*CP\*CP\*TP\*AP\*GP\*CP\*GP\*TP\*GP\*CP\*GP\*GP\*TP\*TP\*C)-3'

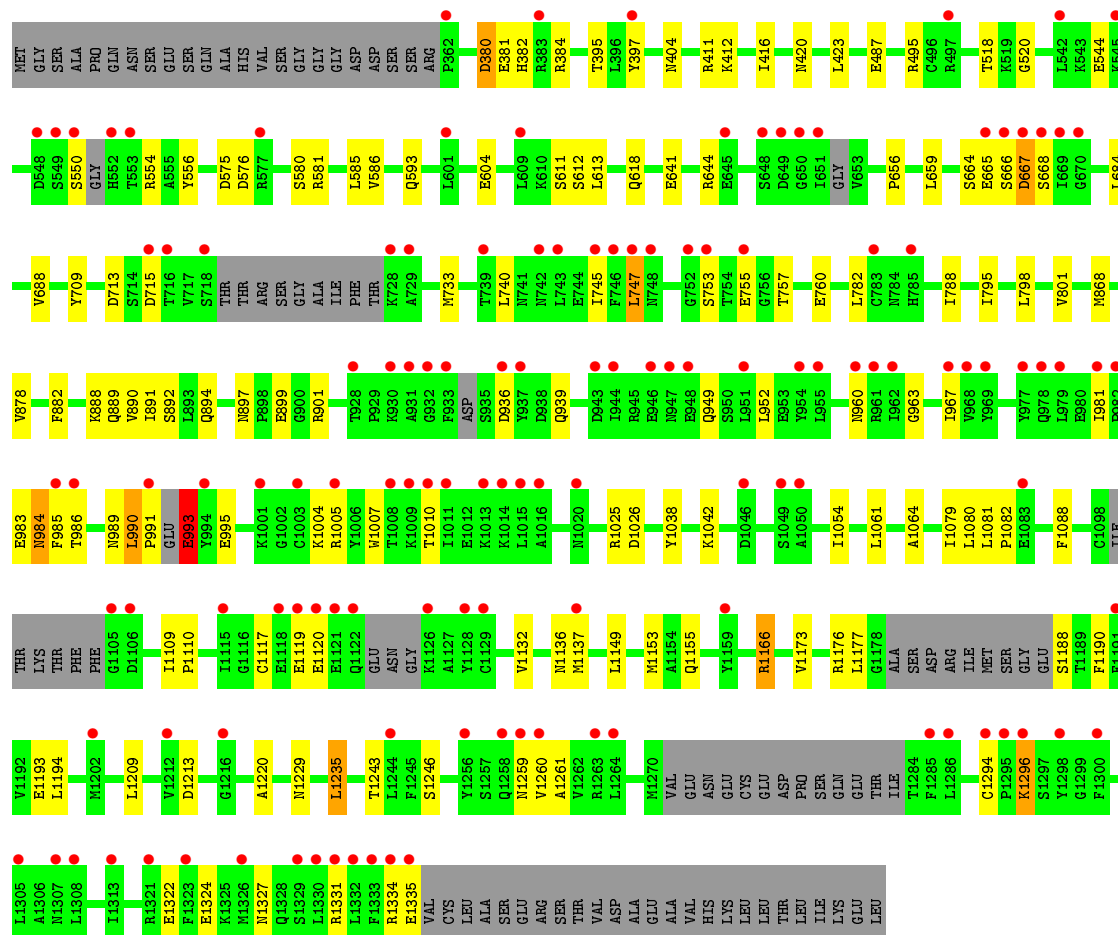


- Molecule 3: DNA mismatch repair protein Msh2





• 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, $\alpha$ , $\beta$ , $\gamma$	258.74Å 258.74Å 258.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 48.05 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.75) 99.8 (48.05-2.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.243 , 0.281 0.242 , 0.280	Depositor DCC
$R_{free}$ test set	3873 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 104.1	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 76711 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14692	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 2.84% 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	1.71	6/345 (1.7%)	1.73	9/531 (1.7%)
2	F	5.11	17/338 (5.0%)	3.26	24/520 (4.6%)
3	A	0.39	2/6640 (0.0%)	0.63	0/8953
4	B	0.68	12/7591 (0.2%)	0.74	8/10228 (0.1%)
All	All	0.98	37/14914 (0.2%)	0.90	41/20232 (0.2%)

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
2	F	0	1
4	B	0	2
All	All	0	3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	30	DC	N1-C6	80.97	1.85	1.37
2	F	30	DC	C4-C5	19.80	1.58	1.43
2	F	30	DC	N3-C4	19.45	1.47	1.33
4	B	1322	GLU	CD-OE2	19.43	1.47	1.25
4	B	1119	GLU	CD-OE1	16.43	1.43	1.25
4	B	1166	ARG	CZ-NH1	16.34	1.54	1.33
4	B	1322	GLU	CD-OE1	15.13	1.42	1.25
1	E	1	DG	C6-N1	12.60	1.48	1.39
1	E	1	DG	N3-C4	12.35	1.44	1.35
4	B	993	GLU	CG-CD	11.59	1.69	1.51
1	E	1	DG	N7-C5	11.02	1.45	1.39
2	F	29	DT	C5-C6	-10.99	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	30	DC	C5-C6	10.74	1.43	1.34
2	F	29	DT	N1-C6	10.46	1.45	1.38
2	F	30	DC	C2'-C1'	10.44	1.62	1.52
4	B	550	SER	C-O	9.55	1.41	1.23
2	F	28	DT	N1-C2	9.42	1.45	1.38
1	E	15	DG	C6-O6	9.30	1.32	1.24
2	F	30	DC	C4-N4	9.26	1.42	1.33
4	B	1335	GLU	C-O	8.85	1.40	1.23
4	B	984	ASN	CG-OD1	8.44	1.42	1.24
2	F	29	DT	C5-C7	8.39	1.55	1.50
4	B	963	GLY	C-O	8.32	1.36	1.23
3	A	853	GLU	CD-OE1	8.30	1.34	1.25
2	F	28	DT	C4-C5	7.99	1.52	1.45
4	B	1119	GLU	CD-OE2	7.96	1.34	1.25
2	F	30	DC	C1'-N1	7.48	1.58	1.49
4	B	993	GLU	CD-OE1	7.29	1.33	1.25
2	F	30	DC	C2-O2	7.24	1.30	1.24
3	A	853	GLU	CD-OE2	6.96	1.33	1.25
2	F	30	DC	C4'-O4'	6.63	1.51	1.45
2	F	30	DC	O4'-C1'	6.61	1.50	1.42
1	E	1	DG	N9-C8	6.38	1.42	1.37
2	F	30	DC	C2-N3	-6.11	1.30	1.35
4	B	990	LEU	CG-CD1	6.08	1.74	1.51
1	E	2	DA	N9-C4	6.01	1.41	1.37
2	F	30	DC	C4'-C3'	5.18	1.58	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	30	DC	C5-C6-N1	-40.48	100.76	121.00
2	F	30	DC	C6-N1-C2	34.16	133.96	120.30
4	B	1166	ARG	NE-CZ-NH2	-16.12	112.24	120.30
2	F	30	DC	C6-N1-C1'	-15.97	101.63	120.80
2	F	30	DC	N1-C2-N3	-15.90	108.07	119.20
2	F	30	DC	C2-N3-C4	14.96	127.38	119.90
1	E	14	DG	O4'-C1'-N9	12.31	116.62	108.00
2	F	30	DC	O4'-C1'-C2'	9.50	113.50	105.90
2	F	30	DC	O4'-C4'-C3'	9.44	111.67	106.00
4	B	993	GLU	CG-CD-OE1	-9.02	100.26	118.30
2	F	23	DT	O4'-C1'-N1	-8.98	101.71	108.00
2	F	30	DC	N1-C2-O2	8.55	124.03	118.90
4	B	984	ASN	CB-CG-OD1	-8.36	104.87	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	30	DC	N3-C2-O2	8.26	127.68	121.90
2	F	30	DC	C4-C5-C6	8.23	121.51	117.40
2	F	29	DT	N1-C2-N3	-7.43	110.14	114.60
4	B	990	LEU	CB-CG-CD2	-7.23	98.71	111.00
2	F	28	DT	C4-C5-C7	7.00	123.20	119.00
2	F	29	DT	C4-C5-C7	6.92	123.16	119.00
4	B	1235	LEU	CA-CB-CG	6.83	131.00	115.30
2	F	29	DT	C6-N1-C2	6.74	124.67	121.30
2	F	30	DC	C1'-O4'-C4'	-6.66	103.44	110.10
1	E	14	DG	C3'-C2'-C1'	-6.62	94.56	102.50
1	E	14	DG	C1'-O4'-C4'	-6.60	103.50	110.10
1	E	11	DC	O4'-C1'-N1	6.55	112.58	108.00
2	F	28	DT	N3-C4-C5	6.24	118.94	115.20
1	E	11	DC	C1'-O4'-C4'	-6.16	103.94	110.10
1	E	4	DC	O4'-C1'-N1	5.93	112.15	108.00
2	F	21	DC	P-O3'-C3'	5.75	126.60	119.70
2	F	28	DT	C5-C4-O4	-5.74	120.89	124.90
4	B	1166	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	F	21	DC	O4'-C1'-N1	5.70	111.99	108.00
1	E	13	DA	P-O3'-C3'	5.52	126.33	119.70
2	F	29	DT	N1-C2-O2	5.47	127.48	123.10
1	E	10	DG	O4'-C1'-N9	5.36	111.75	108.00
4	B	984	ASN	OD1-CG-ND2	5.35	134.21	121.90
2	F	28	DT	C6-N1-C2	5.35	123.97	121.30
2	F	28	DT	N3-C2-O2	-5.15	119.21	122.30
1	E	1	DG	N1-C2-N3	-5.14	120.82	123.90
4	B	990	LEU	CD1-CG-CD2	5.07	125.72	110.50
2	F	28	DT	C2-N3-C4	-5.05	124.17	127.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	984	ASN	Sidechain
4	B	993	GLU	Sidechain
2	F	30	DC	Sidechain

## 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	2	0
2	F	303	0	171	8	0
3	A	6536	0	6562	72	0
4	B	7447	0	7444	87	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	1	0	0	0	0
7	B	39	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
All	All	14692	0	14369	164	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 (164) 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)
2:F:30:DC:C6	2:F:30:DC:N1	1.85	1.43
4:B:897:ASN:HB3	4:B:901:ARG:HE	1.32	0.92
3:A:39:ARG:HE	3:A:44:THR:HG21	1.42	0.84
2:F:29:DT:H2'	2:F:30:DC:C6	2.13	0.83
4:B:897:ASN:HB3	4:B:901:ARG:NE	1.93	0.82
4:B:892:SER:O	4:B:901:ARG:HB3	1.83	0.78
2:F:30:DC:C1'	2:F:30:DC:C6	2.67	0.77
4:B:1007:TRP:HE1	4:B:1010:THR:HB	1.50	0.76
3:A:359:ARG:NH2	3:A:691:ILE:O	2.19	0.75
2:F:28:DT:H2''	2:F:29:DT:H5''	1.69	0.74
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.70	0.71
4:B:380:ASP:HB2	4:B:384:ARG:H	1.56	0.70
3:A:588:TYR:O	3:A:592:MET:HG2	1.91	0.70
4:B:518:THR:HG22	4:B:520:GLY:H	1.55	0.70
4:B:1235:LEU:HD21	4:B:1243:THR:HG21	1.74	0.69
4:B:981:ILE:HD11	4:B:985:PHE:HB2	1.76	0.68
2:F:30:DC:C6	2:F:30:DC:O4'	2.47	0.68
4:B:518:THR:HG21	4:B:593:GLN:OE1	1.94	0.67
4:B:1080:LEU:HD11	4:B:1166:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:380:ASP:O	4:B:397:TYR:HB2	1.96	0.65
3:A:838:LYS:HG3	3:A:839:HIS:H	1.61	0.65
3:A:235:LYS:HE2	3:A:271:SER:HB2	1.77	0.64
4:B:993:GLU:OE2	4:B:1005:ARG:NH2	2.30	0.64
4:B:1007:TRP:NE1	4:B:1010:THR:HB	2.12	0.63
3:A:258:LEU:HB2	3:A:261:MET:HG2	1.80	0.62
3:A:340:ARG:NH2	3:A:386:ASP:OD2	2.32	0.62
4:B:788:ILE:HG21	4:B:1079:ILE:HD12	1.82	0.62
4:B:949:GLN:HA	4:B:952:LEU:HB3	1.82	0.62
4:B:1136:ASN:O	4:B:1137:MET:HB3	2.01	0.61
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.66	0.61
4:B:889:GLN:O	4:B:901:ARG:HA	2.01	0.60
4:B:899:GLU:O	4:B:901:ARG:NH1	2.35	0.59
2:F:29:DT:OP1	4:B:1004:LYS:NZ	2.36	0.59
4:B:404:ASN:OD1	4:B:411:ARG:NH1	2.34	0.59
4:B:1294:CYS:C	4:B:1296:LYS:H	2.06	0.58
3:A:39:ARG:HE	3:A:44:THR:CG2	2.14	0.58
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.70	0.57
3:A:282:ASP:HB2	3:A:286:PHE:HE2	1.70	0.56
3:A:300:MET:HG3	3:A:707:CYS:HA	1.88	0.56
3:A:488:LEU:O	3:A:492:MET:HG2	2.06	0.55
3:A:427:LYS:HD3	3:A:430:LYS:HD3	1.86	0.55
4:B:576:ASP:OD2	4:B:580:SER:OG	2.24	0.55
3:A:1:MET:O	3:A:2:ALA:HB3	2.05	0.55
4:B:960:ASN:O	4:B:967:ILE:HD12	2.07	0.55
1:E:4:DC:H2'	1:E:5:DC:C6	2.43	0.54
3:A:847:LYS:HG3	4:B:1229:ASN:HD22	1.72	0.54
3:A:671:ASN:O	3:A:672:MET:HB2	2.08	0.54
4:B:1259:ASN:C	4:B:1261:ALA:H	2.10	0.54
4:B:380:ASP:HB3	4:B:382:HIS:H	1.72	0.53
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.89	0.53
3:A:282:ASP:HB2	3:A:286:PHE:CE2	2.43	0.53
4:B:487:GLU:OE1	4:B:495:ARG:NH1	2.41	0.53
4:B:518:THR:HG21	4:B:593:GLN:CD	2.29	0.53
4:B:1038:TYR:CE2	4:B:1042:LYS:HE3	2.43	0.53
4:B:991:PRO:O	4:B:993:GLU:N	2.42	0.52
3:A:732:THR:O	3:A:736:LEU:HB2	2.09	0.52
3:A:194:ILE:HG13	3:A:196:PRO:HD3	1.92	0.52
3:A:672:MET:SD	4:B:1188:SER:HB2	2.51	0.51
4:B:733:MET:CE	4:B:1173:VAL:HG23	2.40	0.51
4:B:801:VAL:HG21	4:B:878:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.92	0.51
4:B:1213:ASP:OD1	4:B:1246:SER:OG	2.27	0.51
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.92	0.51
3:A:619:TYR:HB3	3:A:694:PHE:HB3	1.93	0.51
3:A:555:LYS:O	3:A:559:LEU:HB2	2.11	0.51
3:A:288:GLN:O	3:A:289:PHE:HB2	2.11	0.51
4:B:1331:ARG:HA	4:B:1334:ARG:HD2	1.92	0.51
3:A:443:LEU:HA	3:A:446:ASP:HB2	1.93	0.50
3:A:740:THR:HG23	3:A:742:ASP:H	1.76	0.50
4:B:1025:ARG:HG3	4:B:1026:ASP:N	2.27	0.49
4:B:1149:LEU:O	4:B:1153:MET:HG2	2.12	0.49
4:B:380:ASP:OD2	4:B:384:ARG:NE	2.38	0.48
4:B:1324:GLU:HA	4:B:1327:ASN:HB2	1.95	0.48
3:A:616:PRO:O	3:A:617:VAL:HB	2.13	0.48
3:A:842:GLU:HG2	3:A:845:LYS:HD2	1.95	0.48
4:B:990:LEU:O	4:B:993:GLU:HG2	2.12	0.48
3:A:838:LYS:HG3	3:A:839:HIS:N	2.27	0.48
4:B:894:GLN:N	4:B:894:GLN:OE1	2.45	0.48
3:A:687:LEU:O	3:A:691:ILE:HG13	2.14	0.48
3:A:282:ASP:HB3	3:A:285:ASN:HB2	1.96	0.48
3:A:352:ASP:O	3:A:356:ILE:HG13	2.14	0.47
3:A:147:VAL:HG22	3:A:198:GLU:HB3	1.96	0.47
2:F:20:DG:H2"	2:F:21:DC:H5"	1.96	0.47
4:B:747:LEU:HA	4:B:757:THR:HG21	1.97	0.47
3:A:401:LEU:HD11	3:A:458:LEU:HD11	1.96	0.47
2:F:17:DC:H2"	2:F:18:DT:H5'	1.95	0.46
4:B:782:LEU:O	4:B:1155:GLN:HB3	2.15	0.46
4:B:381:GLU:HB2	4:B:395:THR:HB	1.97	0.46
4:B:755:GLU:HB2	4:B:760:GLU:OE1	2.16	0.46
4:B:611:SER:OG	4:B:612:SER:N	2.43	0.46
3:A:575:ASP:HA	3:A:578:VAL:HB	1.98	0.46
3:A:337:GLN:HG3	3:A:337:GLN:H	1.47	0.45
4:B:890:VAL:HG23	4:B:891:ILE:HG23	1.98	0.45
3:A:492:MET:HE2	3:A:513:LEU:HD21	1.98	0.45
3:A:22:PHE:CZ	3:A:117:TRP:HB2	2.52	0.45
4:B:420:ASN:HB3	4:B:423:LEU:HG	1.98	0.45
3:A:732:THR:HG21	3:A:750:LEU:HD11	1.97	0.45
4:B:656:PRO:HD2	4:B:659:LEU:HD12	1.99	0.45
3:A:664:PHE:HB3	3:A:797:VAL:HG22	1.99	0.45
4:B:882:PHE:O	4:B:888:LYS:HE2	2.17	0.45
4:B:993:GLU:OE2	4:B:1005:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1213:ASP:HA	4:B:1246:SER:OG	2.17	0.44
4:B:889:GLN:HG2	4:B:901:ARG:NH1	2.32	0.44
4:B:995:GLU:HA	4:B:1005:ARG:HA	2.00	0.44
4:B:575:ASP:OD1	4:B:576:ASP:N	2.49	0.44
3:A:374:GLN:O	3:A:378:GLU:HG2	2.17	0.44
4:B:667:ASP:CG	4:B:668:SER:H	2.19	0.44
3:A:33:THR:HG22	3:A:99:ARG:CG	2.48	0.44
4:B:641:GLU:HB3	4:B:644:ARG:HG3	2.00	0.44
3:A:531:LYS:HA	3:A:535:ASN:HB2	2.00	0.43
3:A:29:LYS:HA	3:A:30:PRO:HD3	1.91	0.43
3:A:481:LEU:O	3:A:485:MET:HG2	2.19	0.43
3:A:518:GLN:HE21	3:A:518:GLN:HB3	1.65	0.43
4:B:740:LEU:HA	4:B:740:LEU:HD12	1.90	0.43
3:A:240:ASP:C	3:A:242:ASN:H	2.21	0.43
4:B:733:MET:HE3	4:B:1173:VAL:HG23	2.00	0.43
4:B:1109:ILE:HA	4:B:1110:PRO:HD3	1.83	0.43
4:B:1173:VAL:HG22	4:B:1209:LEU:HB3	1.99	0.43
3:A:525:VAL:HG12	3:A:526:THR:H	1.84	0.43
3:A:235:LYS:HB3	3:A:238:TYR:HB2	2.01	0.43
4:B:1038:TYR:CZ	4:B:1042:LYS:HE3	2.54	0.43
3:A:356:ILE:CG2	3:A:624:ILE:HD13	2.48	0.43
3:A:124:SER:HB3	3:A:198:GLU:OE1	2.19	0.43
3:A:1:MET:O	3:A:2:ALA:CB	2.66	0.43
3:A:673:GLY:O	3:A:802:VAL:HG11	2.19	0.42
4:B:1294:CYS:C	4:B:1296:LYS:N	2.72	0.42
3:A:291:LEU:O	3:A:293:THR:HG23	2.19	0.42
3:A:414:LEU:N	3:A:415:PRO:HD2	2.34	0.42
4:B:1081:LEU:HA	4:B:1082:PRO:HD3	1.85	0.42
3:A:705:VAL:HG13	3:A:743:SER:HA	2.01	0.42
3:A:20:VAL:HG21	3:A:68:GLY:HA2	2.02	0.42
3:A:277:LEU:C	3:A:279:LEU:H	2.23	0.42
4:B:581:ARG:HH21	4:B:713:ASP:HB3	1.85	0.42
3:A:506:ASP:HA	3:A:507:PRO:HD3	1.86	0.42
4:B:868:MET:HG2	4:B:1054:ILE:HD12	2.01	0.42
4:B:664:SER:O	4:B:666:SER:N	2.53	0.42
3:A:527:CYS:HB2	3:A:548:GLY:HA2	2.01	0.42
3:A:634:LEU:HB2	3:A:655:VAL:HB	2.01	0.42
4:B:1190:PHE:CE2	4:B:1194:LEU:HD11	2.55	0.42
4:B:1088:PHE:HB2	4:B:1117:CYS:H	1.85	0.42
3:A:387:LEU:HB2	3:A:596:ASN:HB2	2.02	0.42
3:A:424:HIS:HB2	3:A:427:LYS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:33:THR:CG2	3:A:99:ARG:HH11	2.33	0.42
3:A:783:HIS:HB2	4:B:1220:ALA:HA	2.01	0.41
4:B:585:LEU:HD12	4:B:709:TYR:CE2	2.55	0.41
3:A:314:GLN:HB3	3:A:315:GLY:H	1.60	0.41
4:B:412:LYS:O	4:B:416:ILE:HG12	2.19	0.41
3:A:847:LYS:HG3	4:B:1229:ASN:ND2	2.33	0.41
3:A:511:ILE:HG12	3:A:525:VAL:HG22	2.01	0.41
4:B:684:LEU:O	4:B:688:VAL:HG23	2.20	0.41
4:B:733:MET:CE	4:B:1173:VAL:CG2	2.98	0.41
4:B:983:GLU:HG3	4:B:986:THR:HG21	2.02	0.41
4:B:586:VAL:CG1	4:B:613:LEU:HD11	2.51	0.41
3:A:235:LYS:HB2	3:A:239:GLN:HG3	2.03	0.41
3:A:709:LEU:HD12	3:A:739:ALA:HB2	2.02	0.41
4:B:544:GLU:HG2	4:B:556:TYR:CE1	2.55	0.41
4:B:1177:LEU:HD23	4:B:1213:ASP:HB2	2.02	0.41
3:A:621:ARG:HA	3:A:622:PRO:HD3	1.89	0.41
4:B:788:ILE:HD13	4:B:1079:ILE:HD12	2.02	0.40
4:B:1176:ARG:HA	4:B:1176:ARG:HD2	1.77	0.40
4:B:1132:VAL:O	4:B:1246:SER:HA	2.22	0.40
3:A:376:LEU:HD13	3:A:602:LEU:HD21	2.02	0.40
3:A:148:VAL:HG12	3:A:165:TYR:HB3	2.02	0.40
1:E:9:DC:H2'	1:E:10:DG:C8	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	819/934 (88%)	726 (89%)	87 (11%)	6 (1%)	26	59
4	B	910/1022 (89%)	834 (92%)	66 (7%)	10 (1%)	17	46
All	All	1729/1956 (88%)	1560 (90%)	153 (9%)	16 (1%)	21	52

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	665	GLU
4	B	1120	GLU
4	B	1296	LYS
3	A	137	GLY
4	B	667	ASP
4	B	747	LEU
4	B	989	ASN
3	A	249	LYS
3	A	146	GLY
3	A	617	VAL
4	B	753	SER
4	B	1260	VAL
3	A	835	ASN
4	B	380	ASP
4	B	745	ILE
3	A	426	GLY

### 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	715/808 (88%)	714 (100%)	1 (0%)	95	99
4	B	822/899 (91%)	820 (100%)	2 (0%)	95	99
All	All	1537/1707 (90%)	1534 (100%)	3 (0%)	95	99

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

Mol	Chain	Res	Type
3	A	180	ASP
4	B	618	GLN
4	B	715	ASP

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	451	GLN

### 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	1.06	1 (4%)	27,45,45	1.86	5 (18%)
6	ADP	B	202	5	22,29,29	1.07	2 (9%)	27,45,45	1.90	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	202	ADP	O4'-C1'	2.11	1.43	1.41
6	B	202	ADP	C5-C4	3.24	1.47	1.40
6	A	936	ADP	C5-C4	3.26	1.47	1.40

All (9) 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	-7.17	123.41	128.89
6	B	202	ADP	C2'-C1'-N9	-3.41	109.08	114.29
6	A	936	ADP	C2'-C1'-N9	-3.38	109.13	114.29
6	B	202	ADP	PA-O3A-PB	-2.77	123.37	132.67
6	B	202	ADP	C4-C5-N7	-2.73	106.97	109.48
6	A	936	ADP	C4-C5-N7	-2.58	107.11	109.48
6	A	936	ADP	PA-O3A-PB	-2.43	124.53	132.67
6	A	936	ADP	C2-N1-C6	2.00	122.35	118.77

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	15/15 (100%)	0.53	1 (6%) 21 15	76, 81, 106, 113	0
2	F	15/15 (100%)	0.79	0 100 100	76, 80, 91, 92	0
3	A	831/934 (88%)	1.66	254 (30%) 1 0	32, 83, 92, 106	0
4	B	930/1022 (90%)	1.18	133 (14%) 4 2	65, 82, 97, 109	0
All	All	1791/1986 (90%)	1.40	388 (21%) 1 1	32, 83, 94, 113	0

All (388) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	541	THR	15.0
3	A	723	SER	13.5
4	B	1010	THR	12.6
4	B	550	SER	12.1
3	A	284	SER	10.8
3	A	206	THR	10.7
3	A	154	ALA	10.6
4	B	1333	PHE	9.4
4	B	1121	GLU	8.8
4	B	753	SER	8.8
4	B	954	TYR	8.7
4	B	968	VAL	8.6
4	B	1334	ARG	8.5
4	B	752	GLY	8.4
4	B	1326	MET	8.4
3	A	540	SER	7.6
3	A	569	GLU	7.6
4	B	552	HIS	7.3
3	A	155	VAL	7.2
4	B	1330	LEU	7.1
4	B	549	SER	6.9

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Mol	Chain	Res	Type	RSRZ
3	A	558	SER	6.8
3	A	426	GLY	6.8
3	A	570	TYR	6.7
3	A	587	GLY	6.7
4	B	747	LEU	6.7
3	A	424	HIS	6.7
3	A	533	LEU	6.7
4	B	1009	LYS	6.5
4	B	718	SER	6.5
3	A	203	GLY	6.5
4	B	715	ASP	6.4
4	B	1307	ASN	6.4
3	A	467	GLU	6.3
3	A	204	GLY	6.2
3	A	13	SER	6.2
3	A	640	ALA	6.2
4	B	1332	LEU	6.1
3	A	202	PRO	6.1
3	A	469	LEU	5.9
3	A	238	TYR	5.8
4	B	1258	GLN	5.7
3	A	428	HIS	5.7
4	B	1008	THR	5.6
4	B	716	THR	5.6
4	B	1126	LYS	5.6
3	A	107	ALA	5.6
3	A	727	ALA	5.5
3	A	263	ASN	5.5
4	B	1321	ARG	5.4
3	A	660	ASP	5.4
3	A	757	TYR	5.4
4	B	728	LYS	5.4
4	B	937	TYR	5.4
3	A	210	MET	5.3
3	A	535	ASN	5.3
3	A	538	ASN	5.3
3	A	280	LEU	5.3
3	A	207	ALA	5.3
3	A	404	CYS	5.2
4	B	1308	LEU	5.1
3	A	557	THR	5.1
3	A	584	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
4	B	948	GLU	5.1
3	A	292	THR	5.1
3	A	656	TYR	5.1
4	B	1120	GLU	5.1
4	B	1298	TYR	5.1
4	B	1295	PRO	5.1
3	A	158	GLN	5.0
3	A	253	MET	5.0
4	B	1285	PHE	5.0
3	A	431	LEU	5.0
3	A	468	PHE	4.9
4	B	669	ILE	4.9
3	A	425	GLU	4.9
3	A	112	SER	4.9
3	A	14	ALA	4.8
3	A	482	ARG	4.7
3	A	156	ASP	4.7
3	A	496	LEU	4.7
3	A	606	VAL	4.7
4	B	553	THR	4.7
3	A	852	GLU	4.7
3	A	201	LEU	4.6
3	A	366	PHE	4.6
4	B	1003	CYS	4.6
3	A	152	MET	4.6
4	B	1137	MET	4.6
3	A	157	GLY	4.6
4	B	1105	GLY	4.5
3	A	585	SER	4.5
4	B	977	TYR	4.5
4	B	1119	GLU	4.5
3	A	479	SER	4.5
3	A	380	LEU	4.4
3	A	648	ILE	4.4
3	A	265	VAL	4.4
3	A	458	LEU	4.4
3	A	539	PHE	4.3
3	A	851	LEU	4.3
3	A	826	PHE	4.3
3	A	785	HIS	4.3
3	A	480	GLU	4.3
3	A	393	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
3	A	661	LYS	4.2
3	A	528	LYS	4.2
3	A	254	ASN	4.2
3	A	283	ASP	4.2
3	A	510	GLN	4.2
4	B	1331	ARG	4.2
4	B	969	TYR	4.1
4	B	967	ILE	4.1
3	A	367	VAL	4.0
4	B	1016	ALA	4.0
3	A	478	LEU	4.0
3	A	417	VAL	4.0
3	A	432	LEU	4.0
3	A	371	GLU	3.9
4	B	982	PRO	3.9
4	B	542	LEU	3.9
3	A	737	ARG	3.9
3	A	472	PRO	3.9
4	B	994	TYR	3.9
3	A	387	LEU	3.8
3	A	276	PHE	3.8
3	A	492	MET	3.7
3	A	384	PHE	3.7
4	B	548	ASP	3.7
3	A	505	LEU	3.7
3	A	461	ASP	3.7
4	B	955	LEU	3.6
4	B	383	ARG	3.6
4	B	1129	CYS	3.6
3	A	530	GLU	3.6
3	A	532	VAL	3.6
3	A	466	HIS	3.6
3	A	611	VAL	3.6
4	B	981	ILE	3.5
3	A	9	LEU	3.5
3	A	55	ARG	3.5
3	A	460	MET	3.5
3	A	234	THR	3.5
4	B	1015	LEU	3.5
3	A	161	VAL	3.5
3	A	693	CYS	3.5
3	A	304	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
3	A	499	ALA	3.5
4	B	665	GLU	3.5
3	A	208	GLY	3.4
3	A	132	GLU	3.4
4	B	1323	PHE	3.4
3	A	153	SER	3.4
3	A	744	LEU	3.4
3	A	631	ARG	3.4
3	A	257	VAL	3.4
3	A	657	PHE	3.4
3	A	436	PHE	3.4
3	A	247	GLY	3.4
3	A	316	SER	3.3
3	A	297	SER	3.3
3	A	422	GLU	3.3
4	B	577	ARG	3.3
3	A	248	LYS	3.3
3	A	232	PHE	3.3
4	B	1005	ARG	3.3
4	B	1128	TYR	3.3
4	B	947	ASN	3.3
3	A	524	ARG	3.3
4	B	666	SER	3.3
3	A	394	PHE	3.3
4	B	1001	LYS	3.2
3	A	368	GLU	3.2
3	A	849	LEU	3.2
4	B	931	ALA	3.2
4	B	1122	GLN	3.2
4	B	649	ASP	3.2
3	A	343	ASN	3.2
4	B	545	LYS	3.2
4	B	1013	LYS	3.2
3	A	1	MET	3.2
3	A	501	ARG	3.1
3	A	605	VAL	3.1
3	A	565	LYS	3.1
3	A	625	LEU	3.1
3	A	409	GLN	3.1
4	B	1335	GLU	3.1
3	A	12	GLU	3.1
3	A	293	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	268	SER	3.1
4	B	1296	LYS	3.0
4	B	1313	ILE	3.0
4	B	1329	SER	3.0
3	A	419	GLN	3.0
3	A	175	LEU	3.0
3	A	106	ARG	3.0
3	A	421	LEU	3.0
3	A	429	GLN	3.0
4	B	944	ILE	3.0
3	A	138	ASN	3.0
3	A	580	GLU	3.0
4	B	1014	LYS	3.0
3	A	542	VAL	3.0
3	A	726	MET	2.9
3	A	396	ARG	2.9
3	A	405	TYR	2.9
3	A	462	GLN	2.9
4	B	962	ILE	2.9
3	A	525	VAL	2.9
3	A	577	ILE	2.9
3	A	43	TYR	2.9
3	A	264	GLN	2.9
3	A	450	PHE	2.9
3	A	11	LEU	2.8
3	A	376	LEU	2.8
3	A	444	ARG	2.8
3	A	171	ARG	2.8
3	A	853	GLU	2.8
3	A	180	ASP	2.8
4	B	1264	LEU	2.8
4	B	667	ASP	2.8
4	B	986	THR	2.8
3	A	574	GLN	2.8
4	B	1083	GLU	2.8
3	A	285	ASN	2.8
4	B	951	LEU	2.8
3	A	608	PHE	2.8
4	B	1260	VAL	2.8
3	A	534	ARG	2.7
3	A	147	VAL	2.7
3	A	449	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
4	B	1300	PHE	2.7
3	A	92	LEU	2.7
3	A	802	VAL	2.7
3	A	296	PHE	2.7
3	A	578	VAL	2.7
3	A	582	VAL	2.7
3	A	667	ILE	2.7
3	A	521	TYR	2.7
3	A	214	ARG	2.6
3	A	470	VAL	2.6
4	B	933	PHE	2.6
3	A	135	LEU	2.6
4	B	651	ILE	2.6
3	A	854	PHE	2.6
4	B	1159	TYR	2.6
3	A	512	LYS	2.6
3	A	579	LYS	2.6
3	A	395	GLN	2.6
3	A	855	GLN	2.6
3	A	131	PHE	2.6
4	B	1263	ARG	2.6
4	B	946	GLU	2.6
3	A	145	ILE	2.6
4	B	1049	SER	2.6
1	E	15	DG	2.6
3	A	701	GLU	2.6
3	A	645	GLN	2.6
3	A	205	GLU	2.6
3	A	150	VAL	2.6
4	B	650	GLY	2.5
3	A	588	TYR	2.5
3	A	451	GLN	2.5
3	A	556	LEU	2.5
4	B	928	THR	2.5
3	A	612	SER	2.5
3	A	231	ASP	2.5
4	B	1011	ILE	2.5
3	A	527	CYS	2.5
3	A	250	GLY	2.5
3	A	252	GLN	2.5
3	A	713	GLY	2.5
3	A	209	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	401	LEU	2.5
3	A	513	LEU	2.5
3	A	226	GLU	2.5
3	A	291	LEU	2.4
3	A	15	ALA	2.4
3	A	370	ALA	2.4
4	B	668	SER	2.4
4	B	1294	CYS	2.4
3	A	750	LEU	2.4
4	B	943	ASP	2.4
4	B	1106	ASP	2.4
4	B	1118	GLU	2.4
4	B	978	GLN	2.4
3	A	60	THR	2.4
3	A	751	GLY	2.4
3	A	194	ILE	2.4
3	A	483	GLU	2.4
4	B	930	LYS	2.4
3	A	183	GLN	2.4
4	B	1286	LEU	2.4
4	B	936	ASP	2.4
4	B	362	PRO	2.3
3	A	163	VAL	2.3
4	B	1046	ASP	2.3
4	B	1191	PHE	2.3
3	A	623	ALA	2.3
4	B	1256	TYR	2.3
3	A	322	GLY	2.3
3	A	347	LYS	2.3
4	B	645	GLU	2.3
4	B	648	SER	2.3
3	A	237	ILE	2.3
3	A	47	GLY	2.3
3	A	372	LEU	2.3
3	A	762	LEU	2.3
3	A	5	PRO	2.3
3	A	349	PRO	2.3
3	A	348	GLN	2.3
4	B	785	HIS	2.3
4	B	961	ARG	2.3
3	A	51	LEU	2.3
3	A	312	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	B	985	PHE	2.3
3	A	89	VAL	2.3
4	B	1212	VAL	2.3
3	A	544	ILE	2.3
4	B	601	LEU	2.3
4	B	979	LEU	2.3
3	A	694	PHE	2.3
3	A	261	MET	2.3
3	A	536	ASN	2.3
4	B	670	GLY	2.3
4	B	783	CYS	2.3
3	A	48	GLU	2.2
3	A	643	GLU	2.2
3	A	50	ALA	2.2
3	A	576	ALA	2.2
4	B	960	ASN	2.2
3	A	824	GLN	2.2
4	B	739	THR	2.2
3	A	300	MET	2.2
3	A	274	ILE	2.2
3	A	489	GLU	2.2
3	A	118	TYR	2.2
3	A	21	ARG	2.2
4	B	748	ASN	2.2
3	A	93	LEU	2.2
3	A	448	SER	2.2
3	A	678	TYR	2.2
3	A	440	LEU	2.2
3	A	488	LEU	2.2
4	B	1115	ILE	2.2
4	B	1020	ASN	2.2
4	B	755	GLU	2.2
4	B	745	ILE	2.1
4	B	1305	LEU	2.1
4	B	742	ASN	2.1
4	B	729	ALA	2.1
4	B	1202	MET	2.1
4	B	746	PHE	2.1
3	A	251	GLU	2.1
4	B	1050	ALA	2.1
4	B	991	PRO	2.1
3	A	68	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	609	LEU	2.1
4	B	932	GLY	2.1
3	A	464	GLU	2.1
3	A	846	GLN	2.1
3	A	599	LEU	2.1
3	A	37	PHE	2.1
3	A	650	PHE	2.1
3	A	302	LEU	2.1
3	A	805	LEU	2.1
3	A	803	THR	2.1
3	A	411	ILE	2.1
3	A	735	ILE	2.1
4	B	497	ARG	2.1
3	A	70	ALA	2.1
3	A	329	LEU	2.1
3	A	445	SER	2.1
3	A	601	GLN	2.1
3	A	178	PHE	2.1
4	B	397	TYR	2.1
4	B	1244	LEU	2.0
3	A	747	ILE	2.0
3	A	572	GLU	2.0
4	B	1216	GLY	2.0
4	B	743	LEU	2.0
3	A	294	PHE	2.0
3	A	476	PRO	2.0
3	A	581	ILE	2.0
3	A	212	LYS	2.0
4	B	1259	ASN	2.0
3	A	592	MET	2.0
3	A	365	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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	B	202	27/27	0.92	0.24	-0.24	79,80,81,81	0
6	ADP	A	936	27/27	0.90	0.20	-0.68	70,71,73,73	0
5	MG	A	935	1/1	0.95	0.43	-	100,100,100,100	0
5	MG	B	102	1/1	0.92	0.20	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.