



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 07:50 PM GMT

PDB ID : 2O8F
Title : human MutSalpα (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 validation report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

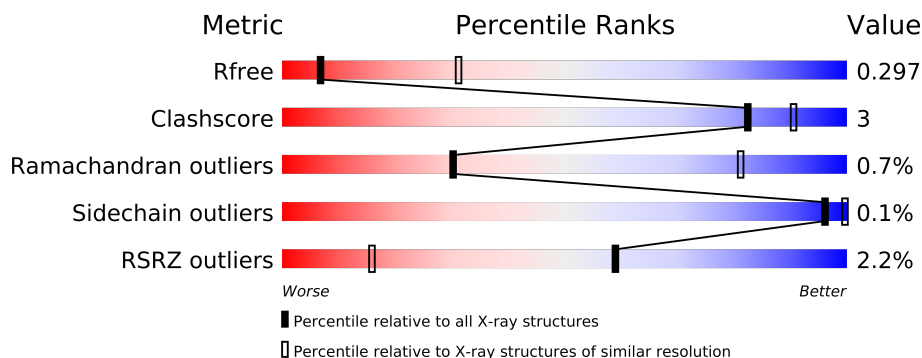
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	17	
2	F	18	
3	A	934	
4	B	1022	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14708 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

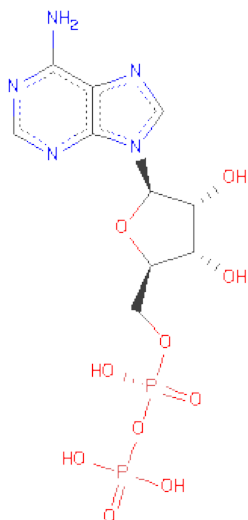
There are 2 discrepancies between the modelled and reference sequences:

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: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is water.

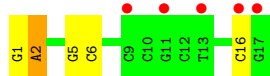
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	17	Total	O	0	0
			17	17		
7	E	1	Total	O	0	0
			1	1		

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.

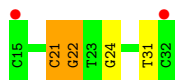
- Molecule 1: 5'-D(*GP*AP*CP*GP*GP*CP*CP*GP*CP*CP*GP*CP*TP*AP*GP*CP*G)-3',

Chain E: 



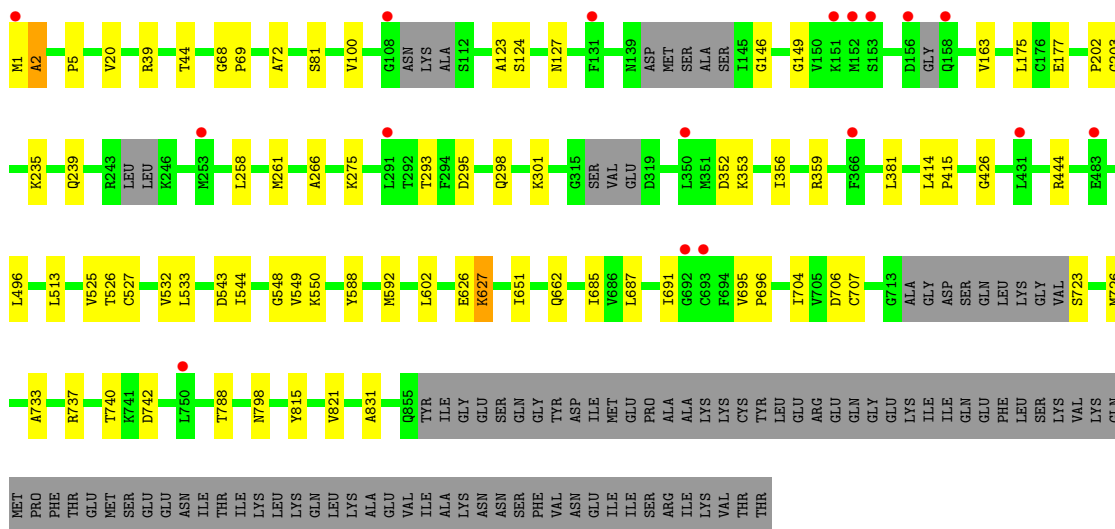
- Molecule 2: 5'-D(*CP*GP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*CP*CP*GP*TP*C)-3'

Chain F: 



- Molecule 3: DNA mismatch repair protein Msh2

Chain A: 



- Molecule 4: DNA mismatch repair protein MSH6

Chain B: 

GLU	CYS	THR	LYS	T757	P531	MET
CYS	GLU	PHE	THR	L758	GLY	GLY
ASP	GLU	PHE	PHE	I795	K543	SER
PRO	GLN	GLY	D1106	E796	S550	ALA
SER	GLN	SER	I1109	L798	GLY	GLN
GLU	THR	PHE	P1110	I805	H552	SER
ILE		THR	I1113	K833	T553	GLU
T1284	F1285		N1124	H837	R554	SER
L1308	P1309	GLY	A1126	P838	V558	GLN
L1332		A1127	P1135	F882	Q572	ALA
E1335		P1135	R1145	L887	D576	HIS
VAL	CYS	R1145	L1149	I891	L585	VAL
LEU	ALA	L1149	M1153	K930	V586	SER
ALA	SER	M1153	V1160	F933	P590	ASP
GLU	ARG	V1160	P1161	ASP	P591	SER
SER	GLU	P1161	V1173	S935	E604	ARG
THR	VAL	V1173	R1176	D936	L613	P362
ASP	ALA	L1177	G1178	L952	L647	P362
ALA	VAL	ALA	ALA	L955	I651	D380
VAL	HIS	SER	SER	E956	GLY	E381
HIS	LYS	ASP	ASP	K957	V653	R384
LEU	LEU	ARG	ARG	Y969	E665	T395
LEU	THR	ILE	ILE	A680	S666	L396
THR	LEU	MET	MET	E699	E865	Y397
THR	LEU	SER	SER	P982	S666	P408
ILE	ILE	GLY	GLY	P991		K412
LYS	GLU	S1188	S1188	GLU	T716	T416
LEU		E1193	E1193	E993	V717	H437
		L1194	L1194	K997	S718	A440
		L1209	L1209	W1007	THR	L447
		L1235	L1235	L1061	ARG	L447
		T1239	T1239	A1064	SER	N456
		R1263	R1263	P1087	GLY	W456
		C1269	C1269	L1091	ALA	A457
		N1270	N1270	S1094	ILE	D471
		VAL	VAL	F746	PHE	S472
		GLU	GLU	L747	THR	L473
		ASN	ASN	T1100		V474
						Q475
						K476
						Y505
						Y524

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.293 0.253 , 0.297	Depositor DCC
R_{free} test set	2382 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 101.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 47211 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	14708	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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	0.61	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 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
3:A:2:ALA:H	4:B:476:LYS:HE2	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	21	74
4	B	913/1022 (89%)	830 (91%)	80 (9%)	3 (0%)	50	92

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1731/1956 (88%)	1553 (90%)	166 (10%)	12 (1%)	30	81

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%)	96	99
All	All	1525/1707 (89%)	1523 (100%)	2 (0%)	96	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 ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	29,29,29	1.06	2 (6%)	45,45,45	1.81	8 (17%)

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	-	0/16/32/32	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	3.29	1.47	1.40
6	A	936	ADP	C4-N9	-2.12	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	936	ADP	N3-C2-N1	-6.18	123.54	128.71
6	A	936	ADP	N3-C4-N9	5.55	135.45	125.43
6	A	936	ADP	C5-C4-N3	-3.37	118.36	125.70
6	A	936	ADP	PA-O3A-PB	-3.29	122.03	131.68
6	A	936	ADP	C4-C5-N7	-3.20	106.78	109.52
6	A	936	ADP	O4'-C1'-N9	2.76	111.00	108.44
6	A	936	ADP	C2-N3-C4	2.49	121.09	114.01
6	A	936	ADP	C3'-C2'-C1'	2.44	104.72	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	17/17 (100%)	1.49	5 (29%) 1 1	105, 113, 127, 132	0
2	F	18/18 (100%)	0.72	2 (11%) 6 2	102, 112, 118, 118	0
3	A	832/934 (89%)	0.42	17 (2%) 62 18	38, 111, 114, 120	0
4	B	933/1022 (91%)	0.46	16 (1%) 67 21	38, 110, 121, 126	0
All	All	1800/1991 (90%)	0.45	40 (2%) 59 16	38, 111, 118, 132	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	17	DG	4.6
4	B	651	ILE	4.0
3	A	152	MET	3.4
3	A	291	LEU	3.1
3	A	1	MET	3.0
3	A	108	GLY	3.0
1	E	16	DC	3.0
4	B	550	SER	2.9
2	F	15	DC	2.9
1	E	9	DC	2.9
3	A	156	ASP	2.7
4	B	1308	LEU	2.6
4	B	1269	CYS	2.6
4	B	1087	PRO	2.5
2	F	32	DC	2.5
4	B	716	THR	2.4
4	B	1285	PHE	2.4
4	B	997	LYS	2.4
3	A	151	LYS	2.4
3	A	153	SER	2.3
1	E	13	DT	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	693	CYS	2.2
3	A	431	LEU	2.2
4	B	717	VAL	2.2
3	A	750	LEU	2.2
3	A	350	LEU	2.2
4	B	1135	PRO	2.2
3	A	158	GLN	2.2
4	B	747	LEU	2.1
3	A	483	GLU	2.1
3	A	253	MET	2.1
3	A	366	PHE	2.1
4	B	1235	LEU	2.1
4	B	1284	THR	2.0
3	A	131	PHE	2.0
4	B	543	LYS	2.0
4	B	1332	LEU	2.0
3	A	692	GLY	2.0
1	E	11	DG	2.0
4	B	1126	LYS	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 ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MG	A	935	1/1	0.32	1.12	92,92,92,92	0
6	ADP	A	936	27/27	0.23	-1.02	110,110,111,111	0

6.5 Other polymers ⓘ

There are no such residues in this entry.