



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:55 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 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>

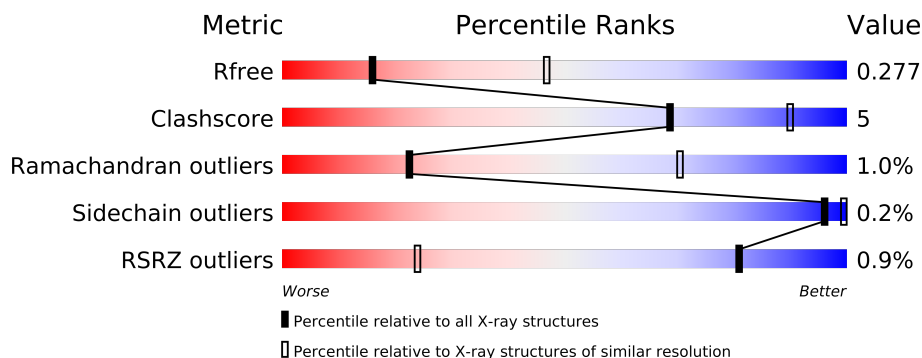
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 ≥ 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	15	
2	F	15	
3	A	934	
4	B	1022	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	MG	A	935	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14593 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*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			

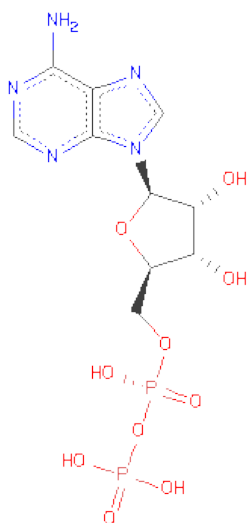
There are 2 discrepancies between the modelled and reference sequences:

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

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

Diagram illustrating a 15-bit bus structure. The bus is composed of 15 multiplexers (G1, C4, C5, G6, C7, G8, C9, G14, G15). Red dots above C7, G8, C9, and G15 indicate they are selected.

Chain F:

```

graph LR
    C16[C16] --- A19[A19]
    C16 --- G20[G20]
    C16 --- C21[C21]
    A19 --- T28[T28]
    A19 --- T29[T29]
    G20 --- T28
    G20 --- T29
    C21 --- T28
    C21 --- T29
    T28 --- C30[C30]
    T29 --- C30
  
```

Chain A:

ILE	THR	T782	V578	R359	G204	M1
ILE	ILE	H783	Y588	Q374	E205	
LEU	LEU	L787	M592	E378	A206	P5
LYS	LYS	L800	Y619	D386	M210	V20
GLN	GLN	K838	L634	L401	L213	K29
ALA	ALA	H839	D646	L414	R214	P30
GLU	GLU	Q855	E947	P415	K229	T33
VAL	VAL	T782	I648	Q419	A230	R39
ILE	ILE	T782	V655	G426	D231	T44
ALA	ALA	ILE	V671	F450	K243	
GLY	GLY	ILE	M672	I454	LEU	D49
ASN	ASN	GLU	V655	G426	LYS	G68
ASN	ASN	SER	I667	F450	LEU	S81
SER	SER	GLN	M671	I454	LEU	R99
PHE	PHE	GLY	M672	I454	LYS	
VAL	VAL	THR	B680	M458	G247	G108
ASN	ASN	GLU	L687	M460	K248	ASN
GLU	GLU	ILE	I691	V463	K249	LYS
ILE	ILE	ILE	F594	M465	L258	ALA
ILE	ILE	ALA	D706	E466	M261	S112
ARG	ARG	ALA	C707	E467	S271	N115
LYS	LYS	LYS	I708	D475	A272	A120
VAL	VAL	THR	L709	P476	L277	F131
THR	THR	THR	R711	L488	E278	I134
THR	THR	GLN	G712	M492	L279	
THR	THR	GLY	G713	Q493	Q288	N138
THR	THR	GLY	GLY	L496	F289	N139
THR	THR	ILE	ASP	L496	D295	ASP
THR	THR	GLN	SER	D506	Q298	MET
THR	THR	GLU	GLN	P507	Y299	SER
THR	THR	PHE	LEU	L513	M300	SER
THR	THR	LEU	GLY	L513	G316	I145
THR	THR	LYS	VAL	G520	VAL	G146
THR	THR	VAL	S723	C527	GLU	V147
THR	THR	LYS	T732	E538	ASP	V148
THR	THR	GLN	L736	M538	THR	D156
THR	THR	PHE	P741	T641	T321	GLY
THR	THR	THR	A739	T641	Q336	Q158
THR	THR	GLU	T740	V549	P337	
THR	THR	MET	K741	V549	Q336	Y165
THR	THR	SER	D742	N560	D352	I194
THR	THR	GLU	D748	N560	D352	G195
THR	THR	ASN	E749	D576	T366	P196
THR	THR	ASN	E749	D576	T366	K207

Chain B:

I1313	R1176	E993	T767	R554	MET
E1335	L1177	K997	K775	D575	GLY
VAL	ALA	R1005	L782	D576	SER
CYS	SER	Y1006	A787	R581	ALA
LEU	ASP	W1007	I788	L585	PRO
ALA	ARG	R1024	I795	V586	GLN
SER	ILE	Y1038	L798	Q593	ASN
GLU	MET	K1042	V801	E604	SER
THR	ARG	L1061	I805	S611	GLN
VAL	SER	A1064	V878	L613	ALA
ASP	GLY	I1079	Q889	E641	HIS
ALA	THR	L1080	S892	R644	VAL
ALA	GLU	P1082	N897	I651	SER
ALA	ILE	F1088	P898	V653	GLY
VAL	THR	C1098	E899	V658	ASP
HIS	LYS	ILE	G900	M662	ASP
LYS	LEU	THR	R901	T663	ASP
LEU	S1246	PHE	K920	S664	SER
LEU	M1259	PHE	L926	E665	ARG
ILE	V1260	G1105	I927	S666	P362
LYS	A1261	I1109	A931	D667	D380
LEU	R1263	P1110	G932	L396	E381
	M1270	C1117	F933	Y397	R384
	VAL	E1118	ASP	N404	R385
	GLU	E1119	S935	C694	P386
	ASN	M1124	D936	Y709	T395
	GLU	M1126	Y937	D713	L396
	CYS	GLY	Q938	S718	Y397
	GLU	K1126	Q939	THR	N404
	ASP	A1127	A940	THR	R411
	PRO	V1130	R945	ARG	K412
	SER	M1136	Q949	SER	I416
	GLN	M1137	L952	GLY	M438
	THR	L1149	E953	ALA	E487
	ILE	L1150	Y954	ILE	R495
	T1284	M1153	V968	THR	C496
	C1294	A1154	Y969	PHE	M499
	P1295	Q1155	W970	K728	I516
	K1296	P1161	L990	I745	I517
	S1297		P991	F746	T518
	L1308		GLU	L747	S550
	P1309			N748	GLY
					H552
					T553

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	260.38Å 260.38Å 260.38Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.239 , 0.278 0.243 , 0.277	Depositor DCC
R_{free} test set	3088 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 86.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 60518 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14593	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.65	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 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	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

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 5.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
4:B:581:ARG:HH21	4:B:713:ASP:HB2	1.67	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	22	70
4	B	912/1022 (89%)	836 (92%)	66 (7%)	10 (1%)	21	67
All	All	1728/1956 (88%)	1568 (91%)	142 (8%)	18 (1%)	22	70

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%)	96	99
4	B	819/899 (91%)	817 (100%)	2 (0%)	96	99
All	All	1512/1707 (89%)	1509 (100%)	3 (0%)	96	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 ⓘ

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 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	29,29,29	1.09	2 (6%)	45,45,45	1.78	8 (17%)
6	ADP	B	202	5	29,29,29	1.05	2 (6%)	45,45,45	1.81	7 (15%)

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
6	ADP	B	202	5	-	0/16/32/32	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	202	ADP	C5-C4	3.27	1.47	1.40
6	A	936	ADP	C5-C4	3.23	1.47	1.40
6	A	936	ADP	C4-N9	-2.63	1.33	1.37
6	B	202	ADP	C4-N9	-2.52	1.34	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	202	ADP	N3-C2-N1	-6.48	123.29	128.71
6	A	936	ADP	N3-C2-N1	-6.19	123.53	128.71
6	B	202	ADP	N3-C4-N9	5.22	134.85	125.43
6	A	936	ADP	N3-C4-N9	5.10	134.65	125.43
6	A	936	ADP	C4-C5-N7	-3.33	106.67	109.52
6	B	202	ADP	C4-C5-N7	-3.19	106.79	109.52
6	B	202	ADP	C3'-C2'-C1'	3.14	105.83	100.91
6	B	202	ADP	C5-C4-N3	-3.12	118.91	125.70
6	A	936	ADP	PA-O3A-PB	-3.09	122.61	131.68
6	A	936	ADP	C5-C4-N3	-3.05	119.06	125.70
6	B	202	ADP	PA-O3A-PB	-2.93	123.10	131.68
6	A	936	ADP	C3'-C2'-C1'	2.72	105.17	100.91
6	B	202	ADP	C2-N3-C4	2.51	121.14	114.01
6	A	936	ADP	O4'-C1'-N9	2.39	110.66	108.44
6	A	936	ADP	C2-N3-C4	2.27	120.48	114.01

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	15/15 (100%)	1.16	4 (26%) 1 1	85, 93, 111, 114	0
2	F	15/15 (100%)	0.28	0 100 100	86, 90, 123, 126	0
3	A	830/934 (88%)	0.21	7 (0%) 83 26	20, 93, 98, 107	0
4	B	932/1022 (91%)	0.24	5 (0%) 88 36	34, 93, 107, 116	0
All	All	1792/1986 (90%)	0.23	16 (0%) 81 24	20, 93, 103, 126	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	15	DG	5.5
4	B	747	LEU	2.6
3	A	467	GLU	2.6
3	A	541	THR	2.6
4	B	954	TYR	2.5
3	A	206	THR	2.5
3	A	207	ALA	2.5
1	E	7	DC	2.4
1	E	8	DG	2.2
4	B	1119	GLU	2.2
4	B	552	HIS	2.1
3	A	466	HIS	2.1
3	A	527	CYS	2.0
1	E	9	DC	2.0
4	B	968	VAL	2.0
3	A	538	ASN	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	0.43	11.92	92,92,92,92	0
5	MG	B	102	1/1	0.28	1.54	83,83,83,83	0
6	ADP	A	936	27/27	0.19	-0.96	89,89,91,91	0
6	ADP	B	202	27/27	0.16	-1.45	99,100,101,101	0

6.5 Other polymers

There are no such residues in this entry.