

Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 07:48 PM EST

PDB ID	:	208D
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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	Е	15	80%	13%	7%					
2	F	15	67%	33%						
3	А	934	6%	12%	11%					
4	В	1022	4% 79%	12%	9%					



2O8D

2 Entry composition (i)

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	Е	15	Total 307	C 145	N 62	O 86	Р 14	0	0	0

• 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 302	C 144	N 53	O 91	Р 14	0	0	0

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

Mol	Chain	Residues		Α	toms		ZeroOcc	AltConf	Trace	
3	А	830	Total 6439	C 4085	N 1092	O 1228	S 34	0	0	0

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

Mol	Chain	Residues		Α	toms		ZeroOcc	AltConf	Trace	
4	В	932	Total 7443	C 4721	N 1277	0 1394	${ m S}{51}$	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	339	MET	-	initiating methionine	UNP P52701
В	340	GLY	-	cloning artifact	UNP P52701

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Mg 1 1	0	0
5	В	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	Δ	1	Total	С	Ν	Ο	Р	0	0	
0 A	1	27	10	5	10	2	0	0		
6	D	1	Total	С	Ν	Ο	Р	0	0	
0 B		27	10	5	10	2	0	0		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Е	1	Total O 1 1	0	0
7	F	3	Total O 3 3	0	0
7	А	2	Total O 2 2	0	0
7	В	40	$\begin{array}{cc} \text{Total} & \text{O} \\ 40 & 40 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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'









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants	260.38Å 260.38Å 260.38Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution(A)	50.00 - 3.00	Depositor
Resolution (A)	48.35 - 3.00	EDS
% Data completeness	99.8 (50.00-3.00)	Depositor
(in resolution range)	99.8 (48.35-3.00)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.39 (at 3.01 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
P. P.	0.239 , 0.278	Depositor
n, n_{free}	0.242 , 0.277	DCC
R_{free} test set	3088 reflections $(5.10%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	83.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 106.8	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mal Chain		Bond lengths		ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Е	0.65	0/345	1.39	5/531~(0.9%)
2	F	0.66	0/337	1.39	4/518~(0.8%)
3	А	0.33	0/6539	0.61	0/8828
4	В	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	$Observed(^{o})$	$Ideal(^{o})$
1	Е	4	DC	O4'-C4'-C3'	-9.00	100.60	106.00
1	Ε	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	Ε	4	DC	C4'-C3'-C2'	-6.12	97.59	103.10
1	Е	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	В	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 (i)

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



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

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.

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	Clash
Atom-1	Atom-2	distance (\AA)	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:586:VAL:HG11	4:B:613:LEU:HD11	1.69	0.75
4:B:897:ASN:HB3	4:B:901:ARG:NE	2.02	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
3:A:646:ASP:CG	3:A:647:GLU:H	1.96	0.68
4:B:892:SER:O	4:B:901:ARG:HB3	1.94	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



	a de pagen	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:O	3:A:321:THR:HG23	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:20:VAL:HG21	3:A:68:GLY:HA2	1.87	0.55
3:A:619:TYR:HB3	3:A:694:PHE:HB3	1.88	0.55
3:A:1:MET:O	3:A:2:ALA:HB3	2.07	0.55
3:A:527:CYS:HA	3:A:549:VAL:HG23	1.88	0.54
3:A:740:THR:HG23	3:A:742:ASP:H	1.71	0.54
3:A:488:LEU:O	3:A:492:MET:HG2	2.08	0.54
4:B:404:ASN:OD1	4:B:411:ARG:NH1	2.41	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:585:LEU:HD12	4:B:709:TYR:CE2	2.47	0.50
4:B:993:GLU:HG3	4:B:1005:ARG:HD2	1.93	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
2:F:28:DT:H2"	2:F:29:DT:H5"	1.94	0.49
3:A:672:MET:SD	4:B:1188:SER:N	2.86	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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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:374:GLN:O	3:A:378:GLU:HG2	2.14	0.47
3:A:838:LYS:HG3	3:A:839:HIS:N	2.29	0.47
4:B:970:TRP:HZ3	4:B:997:LYS:HD2	1.79	0.47
3:A:709:LEU:HD12	3:A:739:ALA:HB2	1.97	0.47
4:B:945:ARG:HD2	4:B:1024:ARG:HH12	1.80	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:H	3:A:337:GLN:HG3	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:667:ASP:CG	4:B:668:SER:H	2.19	0.45
4:B:1109:ILE:HA	4:B:1110:PRO:HD3	1.82	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
3:A:520:GLY:HA3	3:A:560:ASN:HD21	1.82	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
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:O	4:B:1155:GLN:HB3	2.18	0.44
4:B:782:LEU:HD13	4:B:787:ALA:HB1	1.99	0.44
3:A:336:PRO:HG2	3:A:386:ASP:HB2	2.00	0.43
3:A:646:ASP:CG	3:A:647:GLU:N	2.67	0.43
3:A:706:ASP:HB2	3:A:742:ASP:HB2	2.00	0.43
4:B:1127:ALA:HB1	4:B:1263:ARG:HD2	1.99	0.43
3:A:29:LYS:HE3	3:A:49:ASP:OD2	2.18	0.43
4:B:990:LEU:HA	4:B:991:PRO:HD3	1.81	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:HA	4:B:926:LEU:HD23	1.76	0.43
3:A:415:PRO:O	3:A:419:GLN:HG2	2.19	0.43
4:B:385:ARG:HD2	4:B:386:PRO:HD2	2.00	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:516:ILE:HB	4:B:694:CYS:HA	2.02	0.42
4:B:1308:LEU:HB3	4:B:1313:ILE:HD11	2.01	0.42
3:A:352:ASP:O	3:A:356:ILE:HG13	2.19	0.42
3:A:463:VAL:C	3:A:465:ASN:H	2.23	0.42
3:A:575:ASP:HA	3:A:578:VAL:HB	2.02	0.42
3:A:492:MET:HE2	3:A:513:LEU:HD21	2.01	0.41
3:A:672:MET:SD	4:B:1188:SER:HB2	2.60	0.41
3:A:29:LYS:HA	3:A:30:PRO:HD3	1.95	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
3:A:687:LEU:O	3:A:691:ILE:HG13	2.19	0.41
4:B:1081:LEU:HA	4:B:1082:PRO:HD3	1.89	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:1136:ASN:O	4:B:1137:MET:CB	2.68	0.41
3:A:300:MET:HG3	3:A:707:CYS:HA	2.02	0.41
4:B:889:GLN:HG2	4:B:901:ARG:NH1	2.35	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:487:GLU:OE1	4:B:495:ARG:NH1	2.54	0.41
4:B:788:ILE:HG21	4:B:1079:ILE:HD12	2.02	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:414:LEU:N	3:A:415:PRO:HD2	2.36	0.40
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:148:VAL:HG12	3:A:165:TYR:HB3	2.03	0.40
3:A:506:ASP:HA	3:A:507:PRO:HD3	1.84	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	Perce	entiles
3	А	816/934~(87%)	732 (90%)	76~(9%)	8 (1%)	15	53
4	В	912/1022~(89%)	836~(92%)	66~(7%)	10 (1%)	14	50
All	All	1728/1956~(88%)	1568 (91%)	142 (8%)	18 (1%)	15	53

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	В	665	GLU
4	В	747	LEU
4	В	1297	SER
3	А	138	ASN
4	В	668	SER
4	В	745	ILE
3	А	120	ALA
3	А	146	GLY
4	В	931	ALA
3	А	115	ASN
4	В	667	ASP
4	В	1296	LYS
3	А	229	LYS
3	А	249	LYS
3	А	527	CYS
4	В	1260	VAL
3	А	426	GLY
4	В	1309	PRO

5.3.2 Protein sidechains (i)

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.



Mol	Chain	Analysed	Rotameric	Outliers	P	erce	entiles	3
3	А	693/808~(86%)	692 (100%)	1 (0%)		93	98	
4	В	819/899~(91%)	817 (100%)	2 (0%)		93	98	
All	All	1512/1707~(89%)	1509 (100%)	3 (0%)		93	98	

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

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

Mol	Chain	\mathbf{Res}	Type
3	А	711	ARG
4	В	937	TYR
4	В	1007	TRP

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

Mol	Chain	Res	Type
3	А	377	GLN
3	А	388	ASN
3	А	560	ASN
4	В	751	ASN
4	В	1124	ASN
4	В	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 monosaccharides 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 Be		Dec	Res Link	Bond lengths			Bond angles			
INIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	ADP	В	202	5	24,29,29	0.99	1 (4%)	29,45,45	1.43	4 (13%)
6	ADP	А	936	5	24,29,29	0.99	1 (4%)	29,45,45	1.40	5 (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	В	202	5	-	2/12/32/32	0/3/3/3
6	ADP	А	936	5	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
6	В	202	ADP	C5-C4	2.62	1.47	1.40
6	А	936	ADP	C5-C4	2.59	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	В	202	ADP	N3-C2-N1	-3.45	123.29	128.68
6	А	936	ADP	N3-C2-N1	-3.29	123.53	128.68
6	В	202	ADP	C3'-C2'-C1'	3.22	105.83	100.98
6	А	936	ADP	PA-O3A-PB	-2.98	122.61	132.83
6	В	202	ADP	PA-O3A-PB	-2.83	123.10	132.83
6	А	936	ADP	C3'-C2'-C1'	2.78	105.17	100.98
6	А	936	ADP	C4-C5-N7	-2.62	106.67	109.40
6	В	202	ADP	C4-C5-N7	-2.50	106.79	109.40
6	А	936	ADP	C2-N1-C6	2.08	122.31	118.75

There are no chirality outliers.

All (2) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
6	В	202	ADP	PA-O3A-PB-O3B
6	В	202	ADP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	Ε	15/15~(100%)	0.52	1 (6%) 17 5	85, 93, 111, 114	0
2	F	14/15~(93%)	0.59	1 (7%) 16 5	86, 92, 123, 126	0
3	А	830/934~(88%)	0.51	59 (7%) 16 5	20, 93, 98, 107	0
4	В	932/1022~(91%)	0.33	44 (4%) 31 11	34, 93, 107, 116	0
All	All	1791/1986~(90%)	0.42	105 (5%) 22 7	20, 93, 103, 126	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	В	550	SER	8.2
3	А	541	THR	7.9
3	А	206	THR	7.3
4	В	954	TYR	6.5
3	А	540	SER	6.2
1	Е	15	DG	6.0
4	В	1010	THR	5.6
3	А	202	PRO	5.1
3	А	467	GLU	5.1
4	В	747	LEU	4.7
3	А	316	SER	4.4
3	А	13	SER	4.3
3	А	428	HIS	4.3
3	А	203	GLY	4.1
4	В	718	SER	4.1
4	В	1119	GLU	4.0
3	А	156	ASP	3.9
3	A	204	GLY	3.9
3	А	426	GLY	3.9
3	A	154	ALA	3.8
4	В	552	HIS	3.8



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Mol	Chain	Res	Type	RSRZ
4	В	549	SER	3.7
4	В	728	LYS	3.6
3	А	468	PHE	3.6
3	А	527	CYS	3.5
3	А	584	ILE	3.5
4	В	1334	ARG	3.4
3	А	458	LEU	3.4
2	F	16	DC	3.2
3	А	478	LEU	3.2
3	А	292	THR	3.1
3	А	587	GLY	3.1
4	В	1308	LEU	3.1
4	В	1137	MET	3.1
4	В	1333	PHE	3.1
3	А	207	ALA	3.1
4	В	752	GLY	3.0
4	В	1218	GLY	3.0
4	В	955	LEU	3.0
3	А	284	SER	3.0
3	А	558	SER	3.0
4	В	1124	ASN	3.0
3	А	238	TYR	2.9
4	В	968	VAL	2.9
3	А	210	MET	2.9
3	А	480	GLU	2.9
3	А	557	THR	2.9
4	В	1118	GLU	2.9
3	А	580	GLU	2.8
3	А	380	LEU	2.8
4	В	1264	LEU	2.8
3	A	569	GLU	2.8
4	В	648	SER	2.8
3	A	425	GLU	2.8
4	В	667	ASP	2.7
4	В	1295	PRO	2.7
3	A	737	ARG	2.7
3	A	754	THR	2.7
3	A	852	GLU	2.7
4	В	668	SER	2.6
4	В	947	ASN	2.6
4	В	1009	LYS	2.6
3	А	785	HIS	2.6



Mol	Chain	Res	Type	RSRZ
3	А	460	MET	2.6
3	А	409	GLN	2.5
4	В	665	GLU	2.5
3	А	394	PHE	2.5
4	В	716	THR	2.5
3	А	692	GLY	2.5
3	А	234	THR	2.4
4	В	946	GLU	2.4
4	В	959	ARG	2.4
3	А	431	LEU	2.4
3	А	254	ASN	2.4
4	В	989	ASN	2.4
4	В	753	SER	2.4
4	В	553	THR	2.3
4	В	1121	GLU	2.3
3	А	570	TYR	2.3
3	А	404	CYS	2.3
4	В	715	ASP	2.3
4	В	651	ILE	2.3
4	В	649	ASP	2.3
3	А	656	TYR	2.3
4	В	666	SER	2.3
3	А	640	ALA	2.3
4	В	548	ASP	2.3
3	А	501	ARG	2.3
4	В	1331	ARG	2.3
4	В	1326	MET	2.2
4	В	1120	GLU	2.2
3	А	263	ASN	2.2
3	А	461	ASP	2.2
3	А	429	GLN	2.2
3	А	853	GLU	2.2
3	А	183	GLN	2.2
4	В	669	ILE	2.1
3	А	472	PRO	2.1
3	А	405	TYR	2.1
4	В	964	CYS	2.1
3	А	250	GLY	2.1
3	А	479	SER	2.0
3	А	565	LYS	2.0
3	А	560	ASN	2.0
3	А	155	VAL	2.0

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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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$B-factors(Å^2)$	Q < 0.9
5	MG	В	102	1/1	0.59	0.36	83,83,83,83	0
5	MG	А	935	1/1	0.82	0.53	92,92,92,92	0
6	ADP	В	202	27/27	0.82	0.16	99,100,101,101	0
6	ADP	А	936	27/27	0.90	0.21	89,89,91,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

