



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:39 am 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

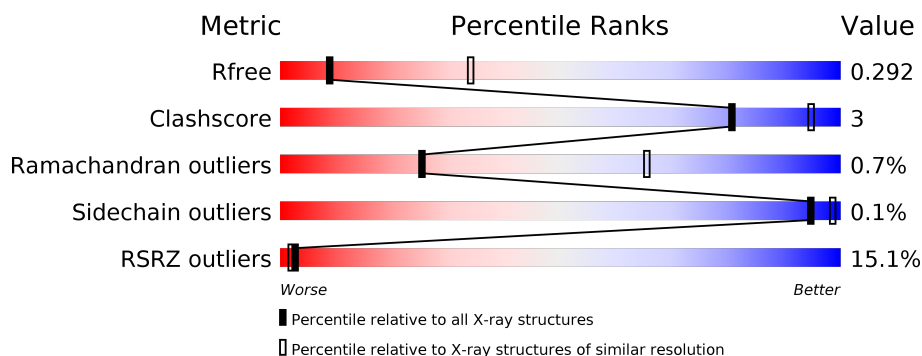
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (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. 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	17	<div> <div>6%</div> <div>71% 24% 6%</div> </div>
2	F	18	<div> <div>17%</div> <div>78% 11% 11%</div> </div>
3	A	934	<div> <div>17%</div> <div>81% 8% 11%</div> </div>
4	B	1022	<div> <div>11%</div> <div>83% 8% 9%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14708 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*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			

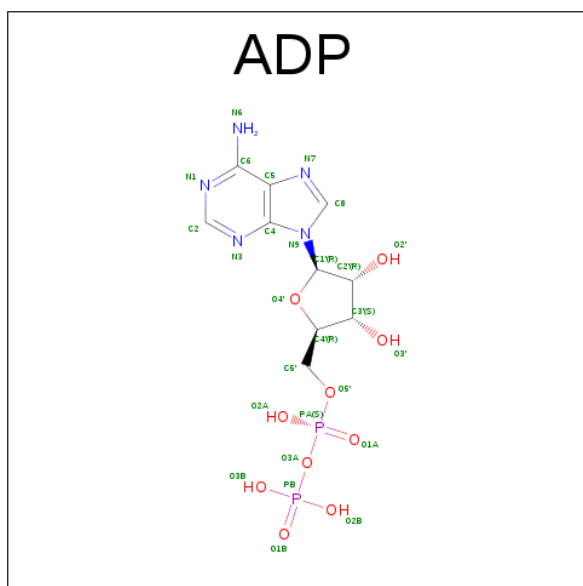
There are 2 discrepancies between the modelled and reference sequences:

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		

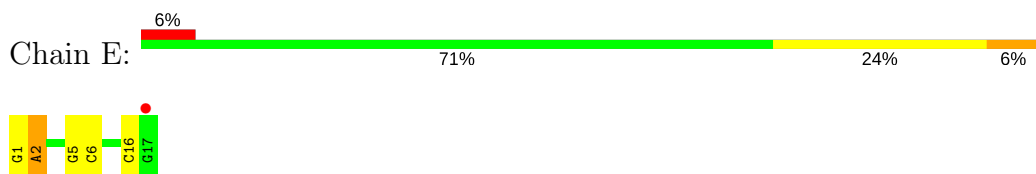
- Molecule 7 is water.

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		

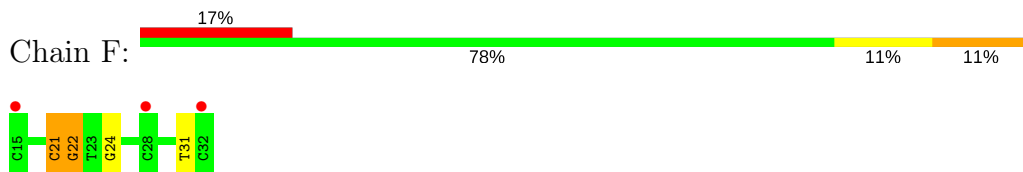
3 Residue-property plots

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

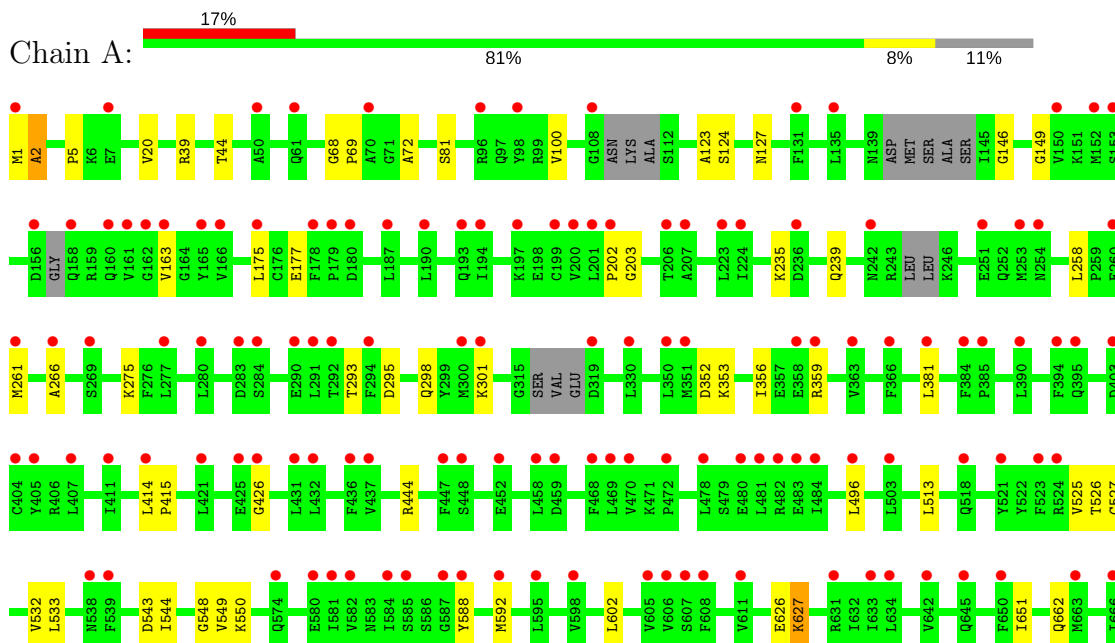
- Molecule 1: 5'-D(*GP*AP*CP*GP*GP*CP*CP*GP*CP*CP*GP*CP*TP*AP*GP*CP*G)-3',

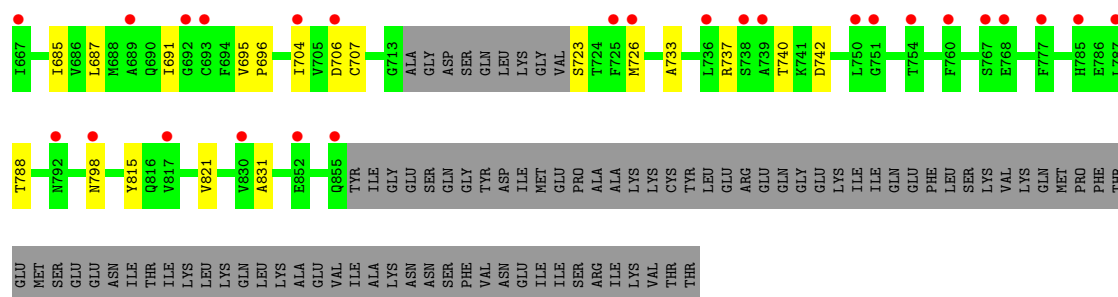


- Molecule 2: 5'-D(*CP*GP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*CP*CP*GP*TP*C)-3'

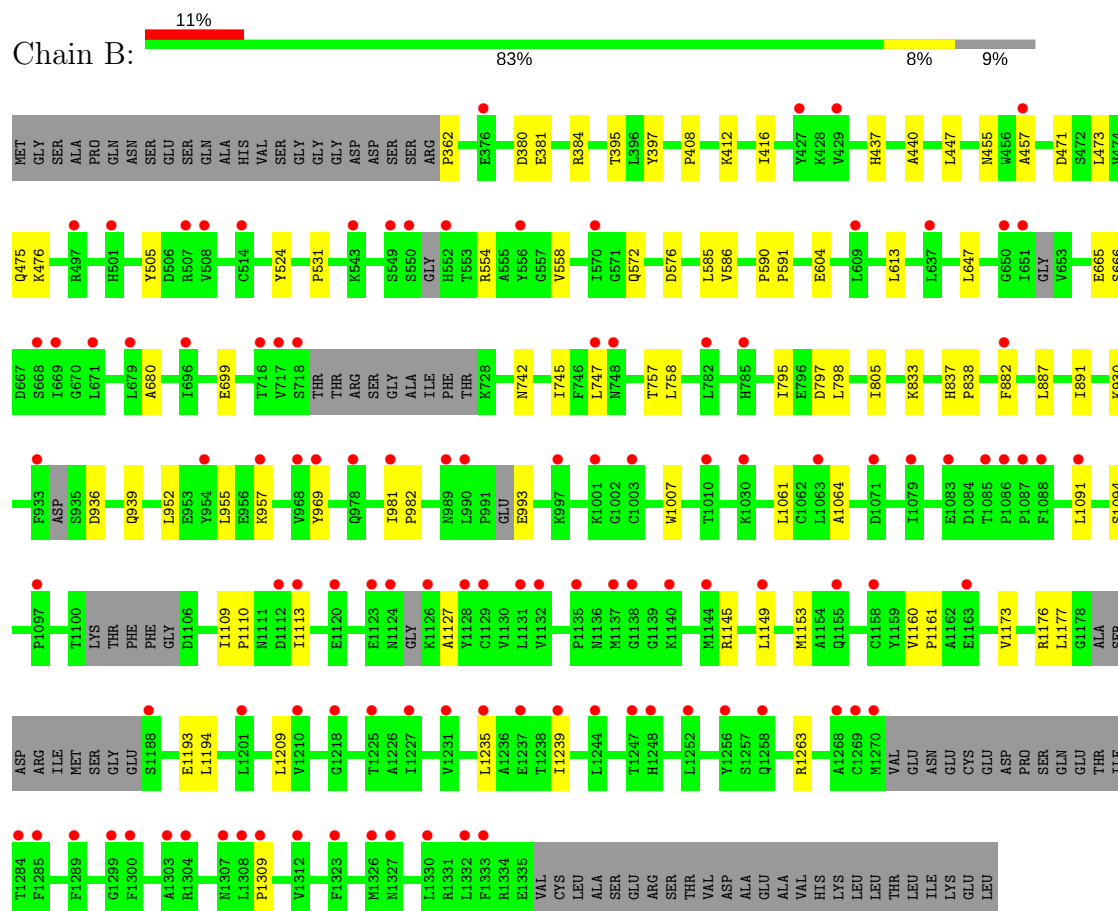


- Molecule 3: DNA mismatch repair protein Msh2





● 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, 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 0.250 , 0.292	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)	0.30 , 136.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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.

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.

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).

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 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

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	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

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 3.

All (90) 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)
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	Interatomic distance (Å)	Clash overlap (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
3:A:258:LEU:H	3:A:261:MET:HB2	1.80	0.47
3:A:295:ASP:HB3	3:A:298:GLN:HG3	1.96	0.47
3:A:544:ILE:HG12	3:A:549:VAL:HG13	1.97	0.47
4:B:957:LYS:HE3	4:B:969:TYR:CD2	2.50	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:175:LEU:N	3:A:293:THR:HG21	2.31	0.44
3:A:39:ARG:HE	3:A:44:THR:CG2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:831:ALA:HA	4:B:1194:LEU:HD13	1.99	0.43
3:A:2:ALA:H	4:B:476:LYS:HE2	1.84	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
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:590:PRO:HA	4:B:591:PRO:HD3	1.81	0.42
3:A:723:SER:HB2	3:A:726:MET:H	1.85	0.42
4:B:887:LEU:O	4:B:891:ILE:HG12	2.18	0.42
3:A:414:LEU:N	3:A:415:PRO:HD2	2.34	0.42
3:A:496:LEU:HB2	3:A:513:LEU:HD12	2.01	0.42
4:B:1091:LEU:HB2	4:B:1113:ILE:HB	2.02	0.42
4:B:572:GLN:HB2	4:B:680:ALA:HB2	2.01	0.42
4:B:742:ASN:O	4:B:1145:ARG:NH1	2.53	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:1109:ILE:HA	4:B:1110:PRO:HD3	1.91	0.41
4:B:554:ARG:NH2	4:B:604:GLU:HG3	2.29	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:685:ILE:HG12	3:A:696:PRO:HD2	2.04	0.40
3:A:706:ASP:HB2	3:A:742:ASP:HB2	2.03	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 [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	818/934 (88%)	723 (88%)	86 (10%)	9 (1%)	17	56
4	B	913/1022 (89%)	830 (91%)	80 (9%)	3 (0%)	44	79
All	All	1731/1956 (88%)	1553 (90%)	166 (10%)	12 (1%)	25	65

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%)	94	98
All	All	1525/1707 (89%)	1523 (100%)	2 (0%)	94	98

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 [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 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	25,29,29	1.06	1 (4%)	24,45,45	1.59	2 (8%)

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

All (1) 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

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	936	ADP	N3-C2-N1	-6.11	123.54	128.86
6	A	936	ADP	C4-C5-N7	-2.72	106.78	109.41

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, 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%)	0.69	1 (5%) 23 17	105, 113, 127, 132	0
2	F	18/18 (100%)	1.05	3 (16%) 2 1	102, 112, 118, 118	0
3	A	832/934 (89%)	1.07	157 (18%) 1 1	38, 111, 114, 120	0
4	B	933/1022 (91%)	0.84	111 (11%) 5 3	38, 110, 121, 126	0
All	All	1800/1991 (90%)	0.94	272 (15%) 3 2	38, 111, 118, 132	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	550	SER	11.0
3	A	153	SER	8.9
3	A	426	GLY	7.1
4	B	1308	LEU	6.8
3	A	366	PHE	6.7
3	A	206	THR	6.2
3	A	152	MET	6.0
4	B	1330	LEU	5.8
4	B	1285	PHE	5.7
3	A	284	SER	5.5
3	A	131	PHE	5.4
4	B	1269	CYS	5.4
3	A	166	VAL	5.3
3	A	291	LEU	5.3
3	A	692	GLY	5.3
3	A	852	GLU	5.1
4	B	651	ILE	5.1
3	A	469	LEU	5.1
1	E	17	DG	4.9
3	A	395	GLN	4.8
3	A	161	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
4	B	954	TYR	4.8
3	A	587	GLY	4.7
4	B	669	ILE	4.7
3	A	421	LEU	4.7
3	A	202	PRO	4.7
4	B	1284	THR	4.6
4	B	716	THR	4.6
3	A	319	ASP	4.6
3	A	693	CYS	4.6
2	F	15	DC	4.5
3	A	292	THR	4.5
3	A	706	ASP	4.5
4	B	717	VAL	4.4
3	A	798	ASN	4.3
3	A	480	GLU	4.3
3	A	236	ASP	4.2
4	B	997	LYS	4.2
3	A	750	LEU	4.1
4	B	1309	PRO	4.1
3	A	242	ASN	4.0
4	B	552	HIS	4.0
4	B	1235	LEU	4.0
4	B	1087	PRO	4.0
3	A	156	ASP	3.9
3	A	726	MET	3.9
3	A	574	GLN	3.9
3	A	478	LEU	3.9
4	B	1085	THR	3.9
3	A	390	LEU	3.8
4	B	1137	MET	3.8
3	A	108	GLY	3.8
3	A	384	PHE	3.8
3	A	330	LEU	3.8
3	A	608	PHE	3.8
3	A	598	VAL	3.8
4	B	1303	ALA	3.7
4	B	1323	PHE	3.7
3	A	767	SER	3.7
4	B	1135	PRO	3.7
4	B	1300	PHE	3.7
3	A	1	MET	3.6
4	B	1131	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	394	PHE	3.5
3	A	585	SER	3.5
4	B	1138	GLY	3.5
4	B	1129	CYS	3.5
4	B	747	LEU	3.5
3	A	436	PHE	3.5
3	A	582	VAL	3.5
3	A	350	LEU	3.5
4	B	989	ASN	3.5
3	A	736	LEU	3.4
3	A	754	THR	3.4
4	B	679	LEU	3.4
4	B	1120	GLU	3.4
4	B	508	VAL	3.4
3	A	197	LYS	3.4
3	A	179	PRO	3.4
3	A	704	ILE	3.4
3	A	404	CYS	3.3
3	A	175	LEU	3.3
4	B	1332	LEU	3.3
4	B	637	LEU	3.3
4	B	1091	LEU	3.3
3	A	224	ILE	3.3
3	A	254	ASN	3.3
3	A	483	GLU	3.3
4	B	556	TYR	3.2
3	A	201	LEU	3.2
3	A	431	LEU	3.2
3	A	458	LEU	3.2
3	A	751	GLY	3.2
4	B	1248	HIS	3.2
3	A	363	VAL	3.2
3	A	830	VAL	3.1
3	A	269	SER	3.1
3	A	452	GLU	3.1
3	A	251	GLU	3.1
3	A	459	ASP	3.1
3	A	414	LEU	3.1
3	A	785	HIS	3.1
4	B	1132	VAL	3.0
3	A	817	VAL	3.0
4	B	543	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	B	1268	ALA	3.0
3	A	777	PHE	3.0
3	A	425	GLU	3.0
3	A	768	GLU	3.0
3	A	738	SER	3.0
3	A	787	LEU	3.0
4	B	1327	ASN	3.0
4	B	507	ARG	3.0
2	F	32	DC	3.0
4	B	1299	GLY	3.0
4	B	981	ILE	3.0
2	F	28	DC	2.9
4	B	1252	LEU	2.9
4	B	1270	MET	2.9
3	A	437	VAL	2.9
3	A	187	LEU	2.9
3	A	180	ASP	2.9
3	A	359	ARG	2.9
4	B	990	LEU	2.9
3	A	158	GLN	2.8
4	B	1128	TYR	2.8
3	A	725	PHE	2.8
4	B	1258	GLN	2.8
3	A	468	PHE	2.8
3	A	689	ALA	2.8
4	B	501	HIS	2.8
3	A	518	GLN	2.8
4	B	1113	ILE	2.8
4	B	1304	ARG	2.8
3	A	150	VAL	2.8
4	B	1086	PRO	2.8
4	B	1001	LYS	2.7
3	A	223	LEU	2.7
4	B	1144	MET	2.7
4	B	1149	LEU	2.7
3	A	667	ILE	2.7
4	B	1231	VAL	2.7
4	B	1312	VAL	2.7
3	A	351	MET	2.7
3	A	163	VAL	2.7
4	B	1003	CYS	2.7
3	A	190	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	B	933	PHE	2.7
3	A	484	ILE	2.7
3	A	470	VAL	2.6
4	B	514	CYS	2.6
4	B	1126	LYS	2.6
3	A	194	ILE	2.6
3	A	482	ARG	2.6
3	A	666	ILE	2.6
3	A	50	ALA	2.6
3	A	588	TYR	2.6
3	A	301	LYS	2.6
4	B	1307	ASN	2.6
3	A	448	SER	2.6
3	A	260	GLU	2.6
3	A	283	ASP	2.6
3	A	381	LEU	2.6
4	B	1289	PHE	2.6
3	A	496	LEU	2.5
3	A	294	PHE	2.5
4	B	1326	MET	2.5
4	B	1333	PHE	2.5
3	A	631	ARG	2.5
3	A	592	MET	2.5
3	A	135	LEU	2.5
4	B	549	SER	2.5
3	A	634	LEU	2.5
3	A	538	ASN	2.5
3	A	405	TYR	2.5
4	B	1158	CYS	2.5
3	A	207	ALA	2.5
3	A	266	ALA	2.5
4	B	1237	GLU	2.5
3	A	253	MET	2.4
3	A	760	PHE	2.4
4	B	978	GLN	2.4
4	B	1227	ILE	2.4
4	B	1155	GLN	2.4
4	B	1218	GLY	2.4
4	B	1247	THR	2.4
3	A	523	PHE	2.4
3	A	200	VAL	2.4
3	A	447	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	358	GLU	2.4
3	A	584	ILE	2.4
3	A	61	GLN	2.4
3	A	411	ILE	2.4
4	B	1079	ILE	2.4
3	A	739	ALA	2.4
3	A	407	LEU	2.4
4	B	1063	LEU	2.4
3	A	300	MET	2.4
4	B	668	SER	2.4
4	B	1140	LYS	2.4
4	B	1010	THR	2.4
3	A	595	LEU	2.3
3	A	642	VAL	2.3
4	B	497	ARG	2.3
4	B	696	ILE	2.3
4	B	957	LYS	2.3
3	A	178	PHE	2.3
3	A	261	MET	2.3
4	B	1239	ILE	2.3
4	B	1256	TYR	2.3
4	B	1225	THR	2.3
3	A	280	LEU	2.3
4	B	609	LEU	2.3
3	A	524	ARG	2.3
4	B	882	PHE	2.3
3	A	580	GLU	2.3
4	B	376	GLU	2.3
3	A	581	ILE	2.3
3	A	199	CYS	2.2
4	B	718	SER	2.2
3	A	472	PRO	2.2
4	B	1244	LEU	2.2
3	A	792	ASN	2.2
4	B	427	TYR	2.2
3	A	162	GLY	2.2
3	A	432	LEU	2.2
3	A	96	ARG	2.2
4	B	650	GLY	2.2
3	A	605	VAL	2.2
4	B	570	ILE	2.2
4	B	1088	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	290	GLU	2.2
3	A	606	VAL	2.2
4	B	1083	GLU	2.2
4	B	1124	ASN	2.2
3	A	403	ASP	2.2
3	A	165	TYR	2.1
3	A	539	PHE	2.1
3	A	607	SER	2.1
3	A	650	PHE	2.1
4	B	1112	ASP	2.1
3	A	503	LEU	2.1
4	B	1188	SER	2.1
3	A	521	TYR	2.1
3	A	633	ILE	2.1
4	B	1210	VAL	2.1
3	A	611	VAL	2.1
3	A	385	PRO	2.1
4	B	785	HIS	2.1
3	A	193	GLN	2.1
4	B	1097	PRO	2.1
4	B	968	VAL	2.1
3	A	663	MET	2.1
3	A	70	ALA	2.1
4	B	1071	ASP	2.1
3	A	855	GLN	2.1
3	A	98	TYR	2.1
4	B	1030	LYS	2.1
4	B	1123	GLU	2.1
4	B	671	LEU	2.1
4	B	969	TYR	2.1
3	A	277	LEU	2.1
3	A	160	GLN	2.0
3	A	645	GLN	2.0
3	A	7	GLU	2.0
4	B	429	VAL	2.0
3	A	481	LEU	2.0
4	B	748	ASN	2.0
4	B	457	ALA	2.0
4	B	782	LEU	2.0
4	B	1163	GLU	2.0
4	B	1201	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ADP	A	936	27/27	0.95	0.22	-0.99	110,110,111,111	0
5	MG	A	935	1/1	0.94	0.24	-	92,92,92,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.