Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 06:20 PM EDT

PDB ID	:	2O8E
Title	:	human MutSalpha (MSH2/MSH6) bound to a G T mispair, with ADP bound to MSH2 only
Authors	:	Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.
Deposited on	:	2006-12-12
Resolution	:	3.30 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 (i)) were used in the production of this report:

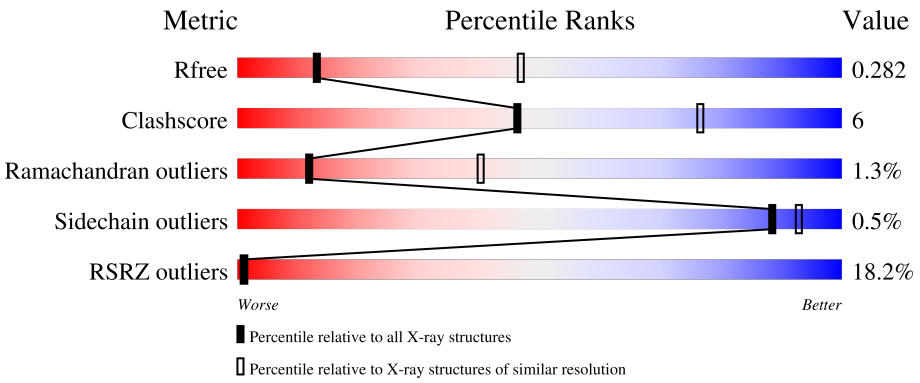
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	E	15	7%; 33%; 60%; 7%
2	F	15	7%; 73%; 20%; 7%
3	A	934	24%; 77%; 11%; 12%
4	B	1022	10%; 73%; 18%; • ; 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14587 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*GP*GP*CP*TP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	15	310	146	64	86	14	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*TP*AP*GP*CP*CP*TP*GP*CP*GP*GP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	15	300	144	51	91	14	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	824	6474	4105	1102	1233	34	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	PHE	engineered mutation	UNP P43246

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	935	7465	4736	1281	1397	51	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	MET	-	initiating methionine	UNP P52701

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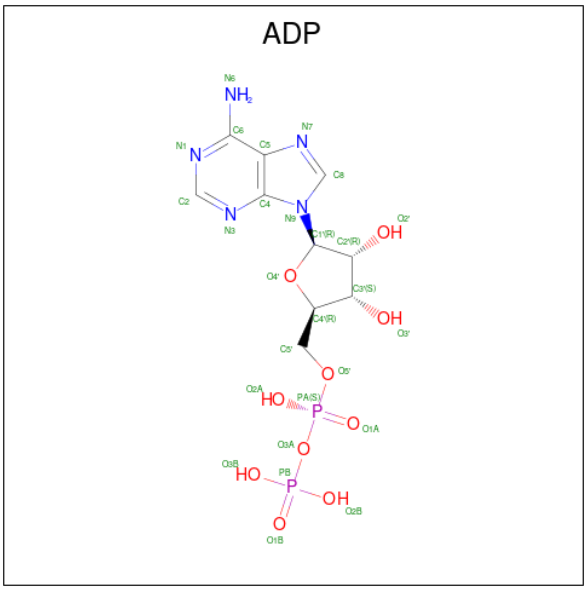
Chain	Residue	Modelled	Actual	Comment	Reference
B	340	GLY	-	cloning artifact	UNP P52701

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

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

- Molecule 7 is water.

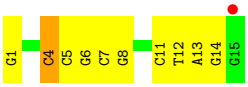
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	10	10	10	0	0

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.

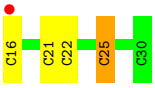
• Molecule 1: 5'-D(*GP*AP*AP*CP*CP*GP*CP*GP*GP*GP*CP*TP*AP*GP*G)-3'

Chain E: 7% 33% 60% 7%



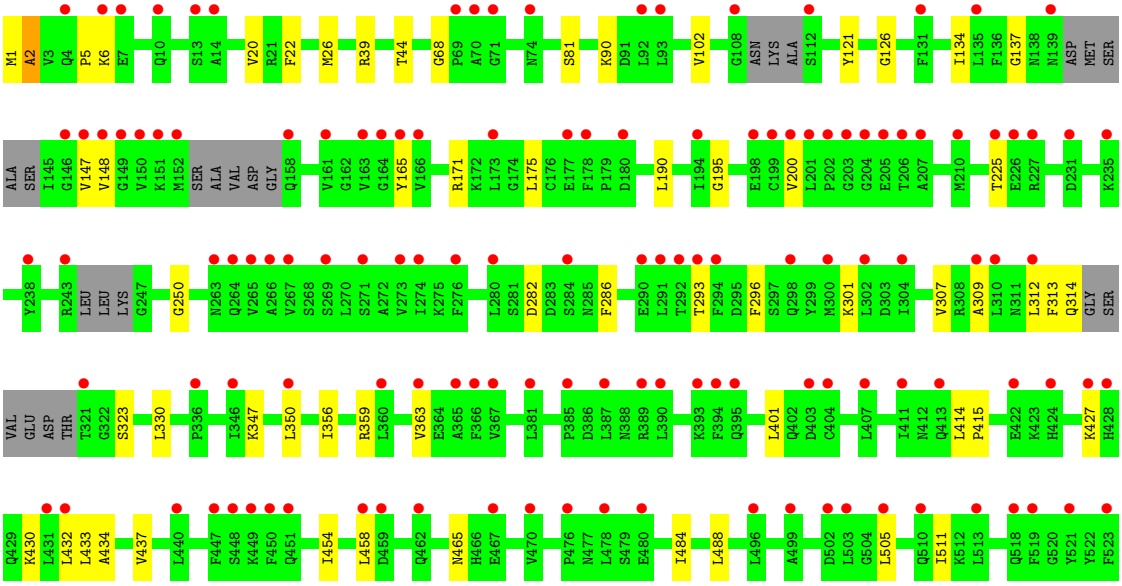
• Molecule 2: 5'-D(*CP*CP*TP*AP*GP*CP*CP*TP*GP*CP*GP*GP*TP*TP*C)-3'

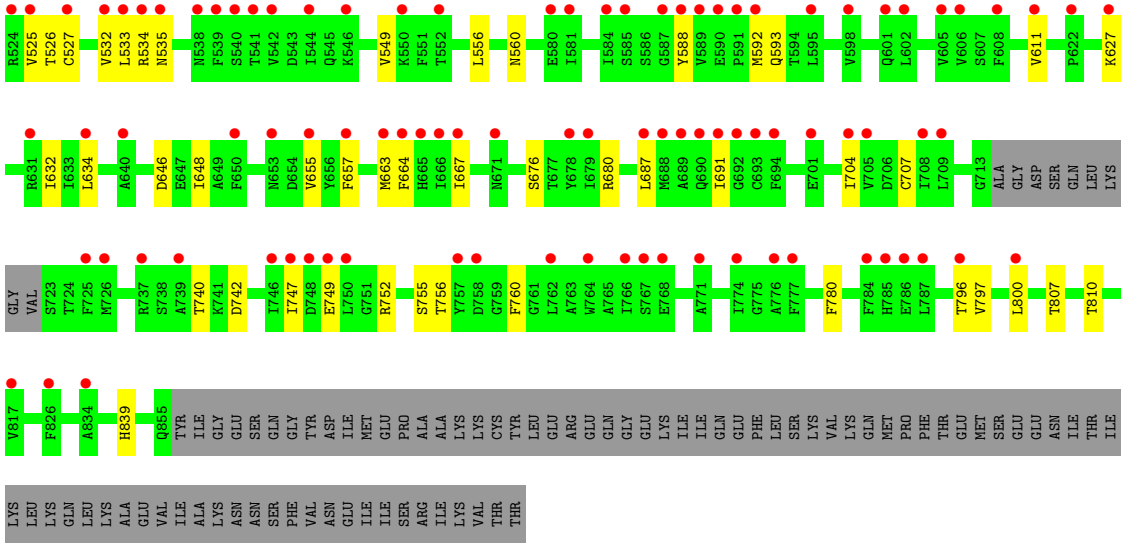
Chain F: 7% 73% 20% 7%



• Molecule 3: DNA mismatch repair protein Msh2

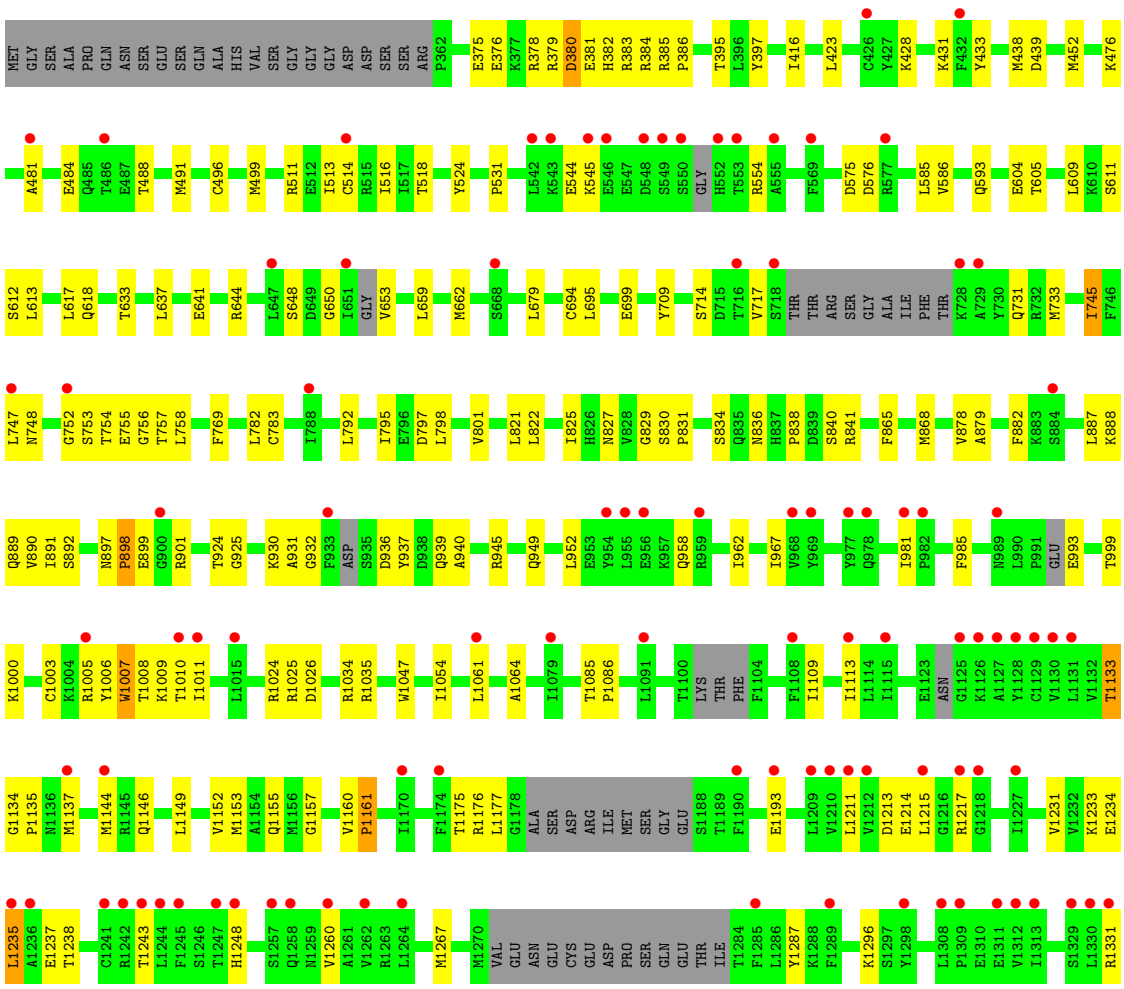
Chain A: 24% 77% 11% 12%

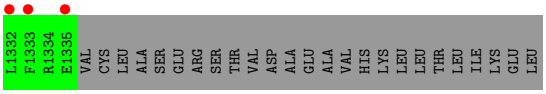




• Molecule 4: DNA mismatch repair protein MSH6

Chain B:




L1332
F1333
R1334
E1335
VAL
CYS
LEU
ALA
SER
GLU
ARG
SER
THR
VAL
ASP
ALA
GLU
ALA
VAL
HIS
LYS
LEU
LEU
THR
LEU
ILE
LYS
GLU
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	257.51Å 257.51Å 257.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 91.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-3.30) 98.4 (91.04-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.253 , 0.291 0.243 , 0.282	Depositor DCC
R_{free} test set	2230 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	91.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 151.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	14587	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP, MG

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	0.75	0/349	1.61	12/538 (2.2%)
2	F	0.65	0/334	1.40	4/513 (0.8%)
3	A	0.32	0/6575	0.58	0/8866
4	B	0.48	1/7609 (0.0%)	0.71	1/10254 (0.0%)
All	All	0.43	1/14867 (0.0%)	0.72	17/20171 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	993	GLU	CD-OE2	6.76	1.33	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	14	DG	O4'-C1'-N9	7.45	113.21	108.00
1	E	1	DG	O4'-C1'-N9	6.80	112.76	108.00
1	E	1	DG	P-O3'-C3'	6.52	127.52	119.70
1	E	4	DC	P-O3'-C3'	6.43	127.42	119.70
4	B	756	GLY	N-CA-C	-6.16	97.70	113.10
1	E	4	DC	O4'-C1'-N1	6.14	112.30	108.00
1	E	14	DG	O4'-C1'-C2'	-5.94	101.15	105.90
1	E	8	DG	O4'-C1'-N9	-5.88	103.89	108.00
1	E	1	DG	C3'-C2'-C1'	-5.72	95.63	102.50
1	E	13	DA	P-O3'-C3'	5.68	126.52	119.70
2	F	21	DC	P-O3'-C3'	5.63	126.46	119.70
2	F	21	DC	O4'-C4'-C3'	-5.63	102.25	104.50
1	E	11	DC	C1'-O4'-C4'	-5.55	104.55	110.10
2	F	16	DC	O4'-C1'-N1	5.38	111.77	108.00
1	E	14	DG	C3'-C2'-C1'	-5.37	96.06	102.50
1	E	12	DT	N3-C4-O4	5.30	123.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	25	DC	O4'-C1'-C2'	-5.05	101.86	105.90

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	310	0	168	4	0
2	F	300	0	171	2	0
3	A	6474	0	6500	62	0
4	B	7465	0	7444	120	0
5	A	1	0	0	0	0
6	A	27	0	12	0	0
7	B	10	0	0	1	0
All	All	14587	0	14295	182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (182) 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)
4:B:1133:THR:HB	4:B:1134:GLY:HA3	1.36	1.07
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.39	0.85
4:B:1133:THR:HB	4:B:1134:GLY:CA	2.06	0.84
4:B:945:ARG:HD2	4:B:1024:ARG:HH12	1.44	0.82
4:B:1133:THR:CB	4:B:1134:GLY:HA3	2.10	0.82
4:B:868:MET:HG2	4:B:1054:ILE:HD12	1.66	0.76
4:B:380:ASP:HB3	4:B:382:HIS:H	1.51	0.75
4:B:897:ASN:HB3	4:B:901:ARG:HH21	1.53	0.73
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.72	0.71
4:B:699:GLU:HB3	4:B:827:ASN:OD1	1.90	0.71
4:B:385:ARG:HD2	4:B:386:PRO:HD2	1.73	0.70
4:B:544:GLU:OE2	4:B:605:THR:OG1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:380:ASP:HB2	4:B:384:ARG:H	1.58	0.68
4:B:897:ASN:HB3	4:B:901:ARG:NH2	2.10	0.66
3:A:525:VAL:HG12	3:A:526:THR:H	1.61	0.66
4:B:930:LYS:H	4:B:930:LYS:HD2	1.61	0.65
4:B:932:GLY:HA2	4:B:936:ASP:H	1.62	0.65
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.78	0.65
4:B:930:LYS:HD2	4:B:930:LYS:N	2.12	0.65
4:B:496:CYS:HA	4:B:499:MET:HG2	1.79	0.65
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.61	0.64
4:B:385:ARG:CD	4:B:386:PRO:HD2	2.28	0.64
3:A:430:LYS:HA	3:A:433:LEU:HB2	1.80	0.64
3:A:359:ARG:NH2	3:A:691:ILE:O	2.32	0.63
4:B:888:LYS:O	4:B:892:SER:OG	2.17	0.63
3:A:350:LEU:HB2	3:A:356:ILE:HG12	1.80	0.61
4:B:641:GLU:HB3	4:B:644:ARG:HG3	1.82	0.61
4:B:381:GLU:HB2	4:B:395:THR:HB	1.82	0.61
3:A:39:ARG:HE	3:A:44:THR:HG21	1.66	0.60
4:B:1153:MET:HB3	4:B:1160:VAL:HG12	1.84	0.60
4:B:1235:LEU:HD21	4:B:1243:THR:HG21	1.84	0.59
1:E:4:DC:H2'	1:E:5:DC:C6	2.38	0.59
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.85	0.58
4:B:1176:ARG:NE	4:B:1193:GLU:HG3	2.18	0.58
4:B:898:PRO:O	4:B:899:GLU:HG3	2.03	0.58
4:B:518:THR:HG21	4:B:593:GLN:NE2	2.19	0.58
4:B:644:ARG:O	4:B:648:SER:HB3	2.04	0.57
4:B:380:ASP:O	4:B:397:TYR:HB2	2.03	0.57
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.87	0.57
4:B:747:LEU:HA	4:B:757:THR:HG21	1.86	0.56
3:A:588:TYR:O	3:A:592:MET:HG2	2.06	0.56
3:A:505:LEU:HD12	3:A:511:ILE:HD11	1.87	0.56
4:B:733:MET:HE1	4:B:1152:VAL:HG22	1.87	0.56
4:B:484:GLU:HB2	4:B:514:CYS:SG	2.46	0.56
3:A:309:ALA:O	3:A:680:ARG:HD2	2.07	0.55
4:B:423:LEU:HD13	4:B:481:ALA:HB2	1.88	0.55
4:B:745:ILE:HD11	4:B:1152:VAL:HG21	1.88	0.55
3:A:430:LYS:C	3:A:432:LEU:H	2.10	0.55
4:B:981:ILE:HD11	4:B:985:PHE:HB2	1.87	0.55
4:B:836:ASN:O	4:B:841:ARG:NH2	2.38	0.55
4:B:1007:TRP:H	4:B:1011:ILE:HD12	1.72	0.55
4:B:585:LEU:HD12	4:B:709:TYR:CE2	2.43	0.54
3:A:414:LEU:N	3:A:415:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:380:ASP:HB2	4:B:384:ARG:N	2.24	0.53
4:B:381:GLU:HB2	4:B:395:THR:CB	2.37	0.53
3:A:634:LEU:HB2	3:A:655:VAL:HB	1.90	0.53
4:B:829:GLY:HA2	4:B:1034:ARG:HG2	1.90	0.53
3:A:664:PHE:HB3	3:A:797:VAL:HG22	1.91	0.53
4:B:868:MET:CG	4:B:1054:ILE:HD12	2.38	0.53
4:B:1025:ARG:HG3	4:B:1026:ASP:N	2.22	0.52
4:B:575:ASP:OD1	4:B:576:ASP:N	2.40	0.52
4:B:496:CYS:HA	4:B:499:MET:CG	2.39	0.52
4:B:887:LEU:O	4:B:891:ILE:HG12	2.10	0.51
4:B:890:VAL:HG23	4:B:891:ILE:HG23	1.92	0.51
4:B:1234:GLU:HG3	4:B:1238:THR:HB	1.92	0.51
1:E:7:DC:H2"	4:B:431:LYS:HD2	1.92	0.51
4:B:782:LEU:O	4:B:1155:GLN:NE2	2.40	0.51
4:B:586:VAL:HG11	4:B:613:LEU:HD11	1.93	0.51
4:B:897:ASN:O	4:B:901:ARG:NE	2.44	0.51
3:A:20:VAL:HG21	3:A:68:GLY:HA2	1.93	0.51
3:A:755:SER:HA	4:B:1248:HIS:HB3	1.92	0.51
4:B:899:GLU:O	4:B:901:ARG:NH1	2.44	0.51
4:B:1175:THR:HG22	4:B:1211:LEU:HD12	1.93	0.51
4:B:609:LEU:HB3	4:B:618:GLN:HE21	1.76	0.50
4:B:889:GLN:HA	4:B:901:ARG:HD3	1.92	0.50
4:B:633:THR:O	4:B:637:LEU:HG	2.12	0.50
4:B:488:THR:OG1	4:B:491:MET:HG3	2.12	0.50
4:B:545:LYS:HE3	4:B:679:LEU:HD21	1.93	0.50
4:B:516:ILE:HB	4:B:694:CYS:HA	1.92	0.50
4:B:1085:THR:HB	4:B:1086:PRO:HD2	1.93	0.49
4:B:949:GLN:HA	4:B:952:LEU:HB3	1.94	0.49
3:A:687:LEU:O	3:A:691:ILE:HG13	2.12	0.49
3:A:90:LYS:NZ	3:A:134:ILE:O	2.45	0.49
4:B:1109:ILE:HD12	4:B:1287:TYR:HB2	1.93	0.49
3:A:330:LEU:HA	3:A:611:VAL:HG21	1.93	0.49
3:A:511:ILE:HG12	3:A:525:VAL:HG22	1.95	0.48
2:F:22:DC:H2"	4:B:452:MET:HE3	1.95	0.48
3:A:359:ARG:O	3:A:363:VAL:HG23	2.14	0.48
3:A:740:THR:HG23	3:A:742:ASP:H	1.78	0.48
4:B:428:LYS:HD2	4:B:484:GLU:OE2	2.14	0.48
3:A:454:ILE:HG23	3:A:458:LEU:HD13	1.96	0.48
4:B:585:LEU:C	4:B:585:LEU:HD23	2.34	0.48
3:A:307:VAL:HG22	3:A:312:LEU:HD12	1.97	0.47
4:B:958:GLN:O	4:B:962:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1215:LEU:HD21	4:B:1231:VAL:HG21	1.96	0.47
3:A:646:ASP:HB3	3:A:648:ILE:HG13	1.97	0.47
4:B:644:ARG:HG2	4:B:653:VAL:HG11	1.96	0.47
4:B:801:VAL:HG21	4:B:878:VAL:HG21	1.97	0.47
3:A:401:LEU:HD11	3:A:458:LEU:HD11	1.95	0.47
3:A:839:HIS:NE2	4:B:1234:GLU:OE1	2.47	0.47
4:B:1137:MET:SD	4:B:1267:MET:HG2	2.54	0.47
4:B:1176:ARG:O	4:B:1176:ARG:HG3	2.14	0.47
4:B:1233:LYS:O	4:B:1237:GLU:HB3	2.14	0.47
1:E:5:DC:H2'	1:E:6:DG:C8	2.50	0.46
3:A:126:GLY:HA3	3:A:147:VAL:HG23	1.98	0.46
3:A:756:THR:O	3:A:760:PHE:HB3	2.15	0.46
4:B:524:TYR:CE1	4:B:531:PRO:HA	2.50	0.46
3:A:556:LEU:HD23	3:A:560:ASN:HB2	1.98	0.46
4:B:792:LEU:HG	4:B:1157:GLY:HA2	1.96	0.46
4:B:1175:THR:HB	4:B:1177:LEU:HG	1.98	0.46
4:B:611:SER:OG	4:B:612:SER:N	2.45	0.46
4:B:797:ASP:HB3	4:B:882:PHE:CD1	2.51	0.46
3:A:200:VAL:HA	3:A:225:THR:O	2.16	0.46
3:A:667:ILE:HG12	3:A:800:LEU:HB2	1.97	0.45
4:B:1113:ILE:HD11	4:B:1146:GLN:HE21	1.80	0.45
4:B:754:THR:C	4:B:755:GLU:HG3	2.36	0.45
3:A:313:PHE:HZ	3:A:347:LYS:HG3	1.82	0.45
4:B:1214:GLU:OE1	4:B:1217:ARG:HD3	2.16	0.45
3:A:307:VAL:HG13	3:A:312:LEU:HB2	1.99	0.45
4:B:936:ASP:O	4:B:940:ALA:N	2.44	0.45
4:B:830:SER:HA	4:B:831:PRO:HD3	1.83	0.45
4:B:930:LYS:H	4:B:930:LYS:CD	2.27	0.44
4:B:484:GLU:O	4:B:511:ARG:HA	2.17	0.44
3:A:22:PHE:O	3:A:26:MET:HG3	2.18	0.44
3:A:663:MET:HB2	3:A:796:THR:HB	2.00	0.44
3:A:632:ILE:HB	3:A:657:PHE:HB2	1.99	0.44
3:A:175:LEU:H	3:A:293:THR:HG21	1.83	0.44
4:B:967:ILE:HG12	4:B:981:ILE:HB	1.99	0.43
3:A:532:VAL:O	3:A:533:LEU:HB2	2.18	0.43
3:A:484:ILE:O	3:A:488:LEU:HG	2.18	0.43
3:A:1:MET:O	3:A:2:ALA:HB3	2.19	0.43
3:A:301:LYS:HB2	3:A:707:CYS:HB3	2.01	0.43
3:A:427:LYS:HA	3:A:430:LYS:HB2	2.00	0.43
3:A:807:THR:HB	3:A:810:THR:HB	2.01	0.43
4:B:659:LEU:HD23	4:B:662:MET:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:39:ARG:HE	3:A:44:THR:CG2	2.30	0.43
4:B:822:LEU:HD23	4:B:822:LEU:HA	1.88	0.43
4:B:838:PRO:C	4:B:840:SER:H	2.22	0.43
3:A:313:PHE:CZ	3:A:347:LYS:HG3	2.54	0.43
4:B:865:PHE:CZ	4:B:1047:TRP:HB3	2.54	0.43
3:A:434:ALA:HA	3:A:437:VAL:HB	1.99	0.43
4:B:375:GLU:HG2	4:B:378:ARG:CZ	2.49	0.43
4:B:924:THR:HB	4:B:925:GLY:H	1.59	0.43
4:B:379:ARG:HD3	4:B:383:ARG:O	2.18	0.42
4:B:748:ASN:H	4:B:757:THR:HG21	1.84	0.42
4:B:879:ALA:HA	4:B:882:PHE:CD2	2.54	0.42
4:B:999:THR:OG1	4:B:1000:LYS:N	2.51	0.42
4:B:376:GLU:H	4:B:376:GLU:HG3	1.59	0.42
4:B:438:MET:CG	4:B:439:ASP:H	2.33	0.42
4:B:731:GLN:HB2	4:B:783:CYS:SG	2.59	0.42
4:B:758:LEU:HD22	4:B:1149:LEU:HD22	2.02	0.42
4:B:897:ASN:O	4:B:901:ARG:CZ	2.68	0.42
3:A:747:ILE:HB	3:A:780:PHE:HD1	1.83	0.42
4:B:882:PHE:CE2	4:B:891:ILE:HD11	2.54	0.42
3:A:556:LEU:O	3:A:560:ASN:N	2.50	0.42
4:B:769:PHE:HE1	4:B:1054:ILE:HG22	1.84	0.42
3:A:148:VAL:HG12	3:A:165:TYR:HB3	2.02	0.42
3:A:313:PHE:O	3:A:314:GLN:HG3	2.19	0.42
4:B:695:LEU:HA	4:B:695:LEU:HD23	1.73	0.42
3:A:190:LEU:HD11	3:A:296:PHE:HB2	2.01	0.42
4:B:416:ILE:HG23	4:B:513:ILE:HD11	2.01	0.42
3:A:282:ASP:HB2	3:A:286:PHE:CE2	2.54	0.41
4:B:1177:LEU:HA	4:B:1213:ASP:HB3	2.02	0.41
3:A:102:VAL:HB	3:A:121:TYR:HB2	2.02	0.41
4:B:694:CYS:O	4:B:695:LEU:HB2	2.21	0.41
4:B:378:ARG:HD3	7:B:47:HOH:O	2.19	0.41
4:B:428:LYS:HE3	4:B:433:TYR:CZ	2.55	0.41
3:A:430:LYS:HG2	3:A:433:LEU:HB2	2.02	0.41
3:A:527:CYS:HA	3:A:549:VAL:HG23	2.02	0.41
4:B:1003:CYS:SG	4:B:1005:ARG:NH1	2.93	0.41
4:B:1144:MET:O	4:B:1211:LEU:HD13	2.21	0.41
3:A:1:MET:H2	4:B:476:LYS:HG3	1.85	0.41
4:B:821:LEU:O	4:B:825:ILE:HG13	2.21	0.41
4:B:1008:THR:O	4:B:1010:THR:N	2.54	0.41
3:A:627:LYS:HA	3:A:704:ILE:HB	2.03	0.41
3:A:534:ARG:HG3	3:A:535:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:430:LYS:C	3:A:432:LEU:N	2.74	0.40
4:B:593:GLN:HG3	4:B:617:LEU:HB2	2.02	0.40
1:E:5:DC:C2'	1:E:6:DG:C8	3.04	0.40
2:F:25:DC:O5'	3:A:6:LYS:HD3	2.20	0.40
3:A:171:ARG:HE	3:A:593:GLN:HE22	1.68	0.40
3:A:676:SER:O	3:A:680:ARG:HG3	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	810/934 (87%)	725 (90%)	78 (10%)	7 (1%)	17 48
4	B	915/1022 (90%)	813 (89%)	86 (9%)	16 (2%)	9 35
All	All	1725/1956 (88%)	1538 (89%)	164 (10%)	23 (1%)	12 40

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	753	SER
3	A	749	GLU
4	B	650	GLY
4	B	834	SER
4	B	931	ALA
4	B	1009	LYS
4	B	1161	PRO
4	B	714	SER
4	B	752	GLY
4	B	1296	LYS
3	A	137	GLY
4	B	745	ILE

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Mol	Chain	Res	Type
3	A	2	ALA
3	A	465	ASN
4	B	898	PRO
4	B	1133	THR
3	A	323	SER
4	B	1135	PRO
4	B	1331	ARG
3	A	250	GLY
4	B	717	VAL
4	B	1260	VAL
3	A	195	GLY

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.

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	707/807 (88%)	706 (100%)	1 (0%)	93 97
4	B	821/899 (91%)	814 (99%)	7 (1%)	78 87
All	All	1528/1706 (90%)	1520 (100%)	8 (0%)	88 93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	752	ARG
4	B	380	ASP
4	B	937	TYR
4	B	1006	TYR
4	B	1007	TRP
4	B	1035	ARG
4	B	1161	PRO
4	B	1235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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	24,29,29	0.97	1 (4%)	29,45,45	1.50	4 (13%)

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	-	4/12/32/32	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	2.44	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	936	ADP	PA-O3A-PB	-3.44	121.04	132.83
6	A	936	ADP	N3-C2-N1	-3.41	123.35	128.68
6	A	936	ADP	C3'-C2'-C1'	3.27	105.89	100.98
6	A	936	ADP	C4-C5-N7	-2.70	106.58	109.40

There are no chirality outliers.

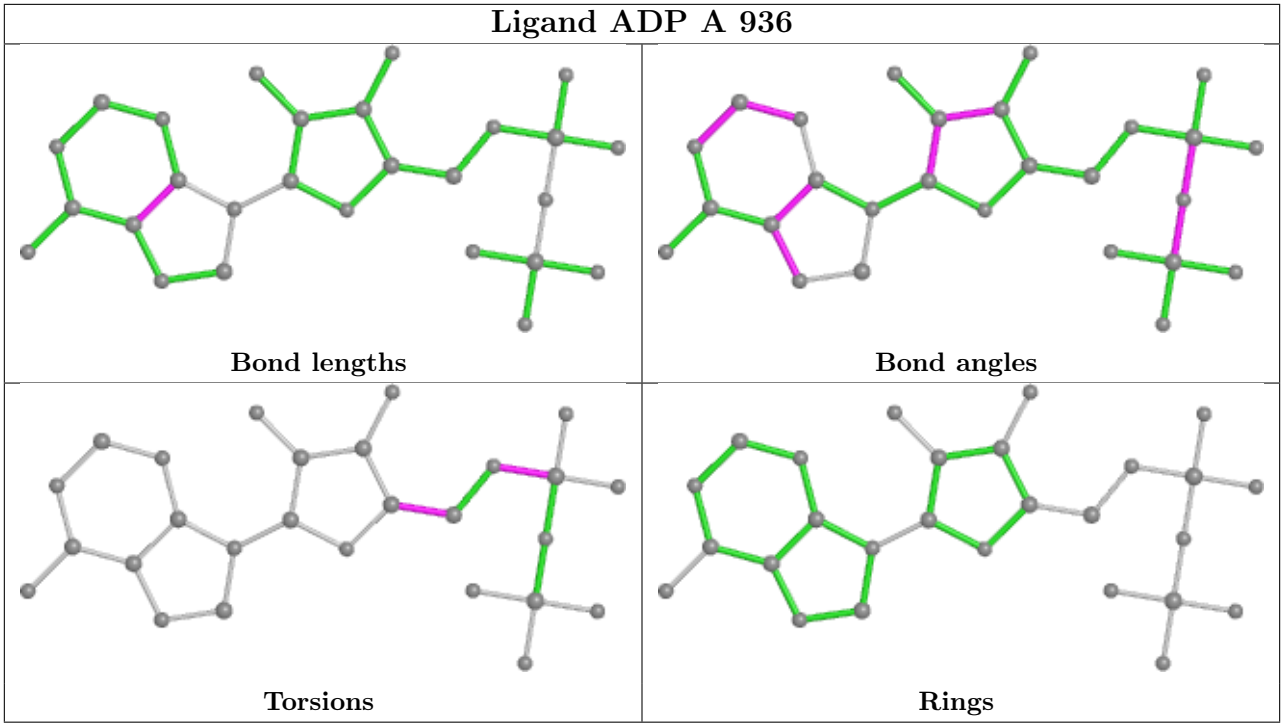
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	936	ADP	C5'-O5'-PA-O1A
6	A	936	ADP	C5'-O5'-PA-O3A
6	A	936	ADP	O4'-C4'-C5'-O5'
6	A	936	ADP	C3'-C4'-C5'-O5'

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, 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%)	0.42	1 (6%)	17	17	93, 101, 115, 116	0
2	F	15/15 (100%)	0.63	1 (6%)	17	17	90, 100, 119, 123	0
3	A	824/934 (88%)	1.34	223 (27%)	0	0	95, 103, 108, 113	0
4	B	935/1022 (91%)	0.80	100 (10%)	6	5	37, 102, 116, 122	0
All	All	1789/1986 (90%)	1.05	325 (18%)	1	1	37, 103, 114, 123	0

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	206	THR	15.0
3	A	541	THR	12.8
3	A	207	ALA	11.0
3	A	202	PRO	8.9
4	B	549	SER	8.9
3	A	693	CYS	8.4
3	A	776	ALA	7.5
3	A	692	GLY	7.4
3	A	588	TYR	7.3
3	A	534	ARG	7.1
4	B	1128	TYR	6.9
4	B	550	SER	6.9
3	A	231	ASP	6.4
3	A	708	ILE	6.3
3	A	166	VAL	6.3
3	A	292	THR	6.1
4	B	1335	GLU	6.0
3	A	108	GLY	5.9
3	A	538	ASN	5.9
3	A	165	TYR	5.8
3	A	533	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
3	A	585	SER	5.7
3	A	150	VAL	5.7
3	A	394	PHE	5.6
3	A	750	LEU	5.3
3	A	210	MET	5.3
4	B	1298	TYR	5.3
3	A	540	SER	5.3
3	A	200	VAL	5.3
3	A	395	GLN	5.2
3	A	587	GLY	5.2
3	A	432	LEU	5.1
3	A	467	GLU	5.1
3	A	664	PHE	5.0
3	A	273	VAL	4.9
4	B	1126	LYS	4.9
3	A	201	LEU	4.8
3	A	404	CYS	4.8
3	A	363	VAL	4.8
3	A	480	GLU	4.8
3	A	746	ILE	4.7
3	A	590	GLU	4.7
3	A	263	ASN	4.7
3	A	605	VAL	4.7
3	A	584	ILE	4.6
3	A	694	PHE	4.6
3	A	350	LEU	4.6
3	A	447	PHE	4.5
3	A	267	VAL	4.5
3	A	535	ASN	4.5
4	B	552	HIS	4.4
3	A	666	ILE	4.3
4	B	982	PRO	4.3
3	A	462	GLN	4.3
3	A	304	ILE	4.3
3	A	294	PHE	4.3
3	A	7	GLU	4.2
4	B	954	TYR	4.2
4	B	747	LEU	4.2
3	A	151	LYS	4.2
4	B	1308	LEU	4.2
3	A	542	VAL	4.2
3	A	269	SER	4.1

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Mol	Chain	Res	Type	RSRZ
3	A	678	TYR	4.0
4	B	1313	ILE	4.0
4	B	577	ARG	4.0
3	A	496	LEU	3.9
4	B	1174	PHE	3.9
4	B	1218	GLY	3.9
3	A	608	PHE	3.9
3	A	390	LEU	3.9
3	A	527	CYS	3.9
3	A	739	ALA	3.8
3	A	178	PHE	3.8
3	A	163	VAL	3.8
3	A	591	PRO	3.8
3	A	152	MET	3.8
3	A	284	SER	3.8
4	B	1332	LEU	3.8
3	A	785	HIS	3.7
3	A	737	ARG	3.7
3	A	458	LEU	3.7
4	B	981	ILE	3.7
4	B	729	ALA	3.7
3	A	667	ILE	3.7
4	B	1010	THR	3.6
3	A	4	GLN	3.6
4	B	1312	VAL	3.6
3	A	365	ALA	3.6
4	B	1115	ILE	3.6
3	A	225	THR	3.6
3	A	450	PHE	3.5
3	A	459	ASP	3.5
4	B	1210	VAL	3.5
4	B	1129	CYS	3.5
3	A	592	MET	3.5
3	A	173	LEU	3.5
4	B	989	ASN	3.5
3	A	726	MET	3.5
4	B	542	LEU	3.5
4	B	1127	ALA	3.5
3	A	147	VAL	3.4
4	B	1130	VAL	3.4
3	A	595	LEU	3.4
3	A	768	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	521	TYR	3.4
3	A	70	ALA	3.4
3	A	293	THR	3.4
3	A	238	TYR	3.4
3	A	235	LYS	3.4
3	A	663	MET	3.4
3	A	650	PHE	3.3
3	A	199	CYS	3.3
3	A	149	GLY	3.3
3	A	449	LYS	3.3
4	B	1131	LEU	3.3
3	A	148	VAL	3.3
4	B	716	THR	3.3
3	A	158	GLN	3.3
4	B	1311	GLU	3.3
3	A	539	PHE	3.3
3	A	276	PHE	3.2
3	A	524	ARG	3.2
3	A	387	LEU	3.2
3	A	478	LEU	3.2
3	A	411	ILE	3.2
3	A	787	LEU	3.2
3	A	194	ILE	3.2
3	A	393	LYS	3.2
3	A	226	GLU	3.2
3	A	366	PHE	3.2
3	A	519	PHE	3.2
3	A	689	ALA	3.2
3	A	431	LEU	3.2
3	A	139	ASN	3.1
3	A	671	ASN	3.1
3	A	164	GLY	3.1
3	A	440	LEU	3.1
4	B	1309	PRO	3.1
4	B	1212	VAL	3.1
3	A	291	LEU	3.1
4	B	1257	SER	3.1
4	B	546	GLU	3.0
3	A	767	SER	3.0
3	A	13	SER	3.0
3	A	704	ILE	3.0
4	B	651	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
4	B	553	THR	3.0
4	B	718	SER	2.9
3	A	525	VAL	2.9
3	A	227	ARG	2.9
4	B	959	ARG	2.9
4	B	1243	THR	2.9
3	A	6	LYS	2.9
4	B	933	PHE	2.9
3	A	266	ALA	2.9
3	A	784	PHE	2.9
3	A	640	ALA	2.9
3	A	205	GLU	2.9
3	A	204	GLY	2.8
3	A	428	HIS	2.8
3	A	290	GLU	2.8
3	A	346	ILE	2.8
3	A	550	LYS	2.8
3	A	601	GLN	2.8
3	A	131	PHE	2.8
3	A	589	VAL	2.8
4	B	956	GLU	2.8
4	B	1331	ARG	2.8
3	A	321	THR	2.8
4	B	1005	ARG	2.8
3	A	470	VAL	2.8
3	A	552	THR	2.8
4	B	1329	SER	2.8
3	A	360	LEU	2.8
4	B	1015	LEU	2.8
3	A	71	GLY	2.8
4	B	1170	ILE	2.8
3	A	631	ARG	2.8
3	A	665	HIS	2.8
3	A	764	TRP	2.7
4	B	1244	LEU	2.7
3	A	826	PHE	2.7
4	B	1245	PHE	2.7
4	B	543	LYS	2.7
3	A	762	LEU	2.7
4	B	788	ILE	2.7
4	B	978	GLN	2.7
4	B	1247	THR	2.7

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Mol	Chain	Res	Type	RSRZ
4	B	1227	ILE	2.7
3	A	687	LEU	2.7
4	B	548	ASP	2.7
3	A	657	PHE	2.7
3	A	424	HIS	2.7
4	B	1285	PHE	2.7
3	A	203	GLY	2.7
3	A	427	LYS	2.6
4	B	481	ALA	2.6
4	B	1091	LEU	2.6
3	A	10	GLN	2.6
3	A	518	GLN	2.6
3	A	606	VAL	2.6
3	A	381	LEU	2.6
4	B	1235	LEU	2.6
3	A	622	PRO	2.6
4	B	1209	LEU	2.6
3	A	777	PHE	2.6
3	A	280	LEU	2.6
3	A	93	LEU	2.6
3	A	774	ILE	2.6
3	A	523	PHE	2.6
3	A	611	VAL	2.6
3	A	92	LEU	2.6
3	A	407	LEU	2.6
4	B	426	CYS	2.6
3	A	688	MET	2.5
4	B	969	TYR	2.5
3	A	602	LEU	2.5
3	A	448	SER	2.5
3	A	385	PRO	2.5
3	A	771	ALA	2.5
4	B	1125	GLY	2.5
3	A	403	ASP	2.5
3	A	598	VAL	2.5
3	A	817	VAL	2.5
3	A	310	LEU	2.5
3	A	634	LEU	2.5
4	B	1248	HIS	2.5
3	A	264	GLN	2.5
3	A	180	ASP	2.5
4	B	1108	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	265	VAL	2.5
3	A	367	VAL	2.5
4	B	1079	ILE	2.5
3	A	758	ASP	2.4
3	A	505	LEU	2.4
4	B	968	VAL	2.4
4	B	555	ALA	2.4
3	A	422	GLU	2.4
3	A	544	ILE	2.4
4	B	1211	LEU	2.4
3	A	796	THR	2.4
3	A	503	LEU	2.4
4	B	1330	LEU	2.4
3	A	513	LEU	2.4
4	B	647	LEU	2.4
4	B	1289	PHE	2.4
3	A	302	LEU	2.4
4	B	955	LEU	2.4
3	A	580	GLU	2.3
3	A	766	ILE	2.3
3	A	476	PRO	2.3
3	A	725	PHE	2.3
4	B	1011	ILE	2.3
3	A	112	SER	2.3
4	B	432	PHE	2.3
3	A	747	ILE	2.3
3	A	627	LYS	2.3
3	A	499	ALA	2.3
4	B	977	TYR	2.3
3	A	135	LEU	2.3
3	A	298	GLN	2.3
3	A	748	ASP	2.3
4	B	1113	ILE	2.3
3	A	69	PRO	2.3
3	A	274	ILE	2.3
4	B	752	GLY	2.2
4	B	1262	VAL	2.2
3	A	413	GLN	2.2
4	B	668	SER	2.2
4	B	545	LYS	2.2
3	A	800	LEU	2.2
4	B	1190	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
4	B	1193	GLU	2.2
3	A	309	ALA	2.2
3	A	161	VAL	2.2
4	B	514	CYS	2.2
2	F	16	DC	2.2
3	A	300	MET	2.2
4	B	884	SER	2.2
4	B	728	LYS	2.2
4	B	1333	PHE	2.2
4	B	1264	LEU	2.2
4	B	1144	MET	2.2
3	A	389	ARG	2.2
4	B	900	GLY	2.2
4	B	1061	LEU	2.1
4	B	1137	MET	2.1
1	E	15	DG	2.1
3	A	271	SER	2.1
3	A	679	ILE	2.1
4	B	1241	CYS	2.1
4	B	1215	LEU	2.1
4	B	1217	ARG	2.1
3	A	834	ALA	2.1
4	B	1236	ALA	2.1
3	A	691	ILE	2.1
3	A	146	GLY	2.1
4	B	1258	GLN	2.1
3	A	502	ASP	2.1
3	A	336	PRO	2.1
3	A	655	VAL	2.1
3	A	198	GLU	2.1
3	A	749	GLU	2.1
4	B	1242	ARG	2.1
4	B	1260	VAL	2.1
3	A	581	ILE	2.1
3	A	690	GLN	2.1
3	A	546	LYS	2.1
3	A	705	VAL	2.1
4	B	569	PHE	2.0
3	A	243	ARG	2.0
3	A	14	ALA	2.0
3	A	510	GLN	2.0
3	A	757	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	653	ASN	2.0
3	A	786	GLU	2.0
3	A	532	VAL	2.0
3	A	709	LEU	2.0
3	A	74	ASN	2.0
4	B	486	THR	2.0
3	A	701	GLU	2.0
3	A	177	GLU	2.0
3	A	312	LEU	2.0
3	A	451	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

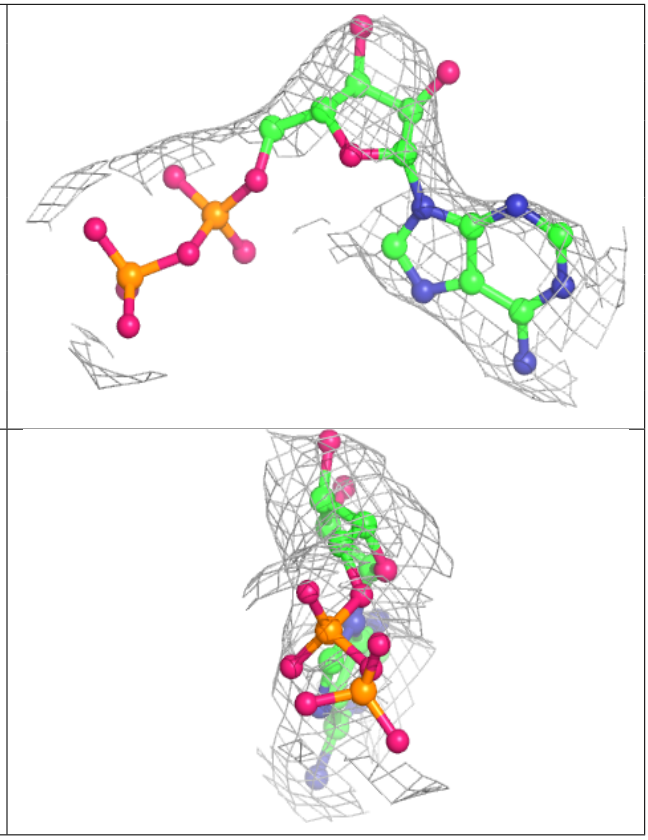
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	935	1/1	0.92	0.29	79,79,79,79	0
6	ADP	A	936	27/27	0.93	0.20	97,98,100,100	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.

Electron density around ADP A 936:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.