



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 AM UTC

PDB ID : 2O8B / pdb_00002o8b
Title : human MutSalpha (MSH2/MSH6) bound to ADP and a G T mispair
Authors : Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.
Deposited on : 2006-12-12
Resolution : 2.75 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

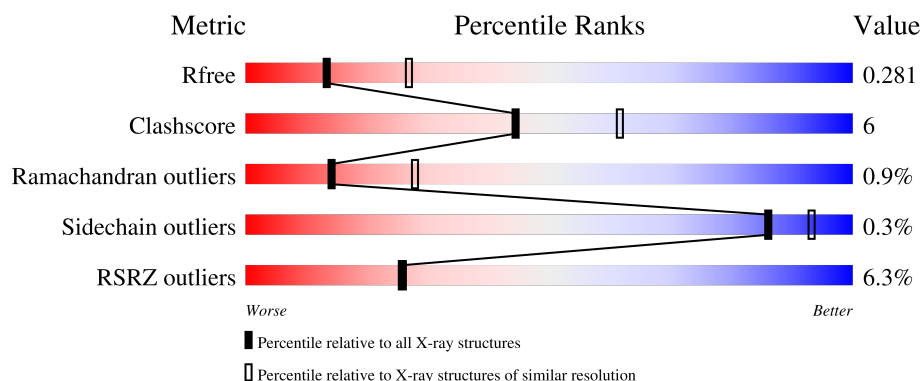
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	15	13% 67% 33%
2	F	15	7% 53% 40% 7%
3	A	934	4% 74% 14% 11%
4	B	1022	7% 76% 14% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14692 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	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*TP*GP*CP*GP*G
P*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			303	145	53	91	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	831	Total	C	N	O	S	0	0	0
			6536	4144	1113	1245	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	930	Total	C	N	O	S	0	0	0
			7447	4725	1279	1392	51			

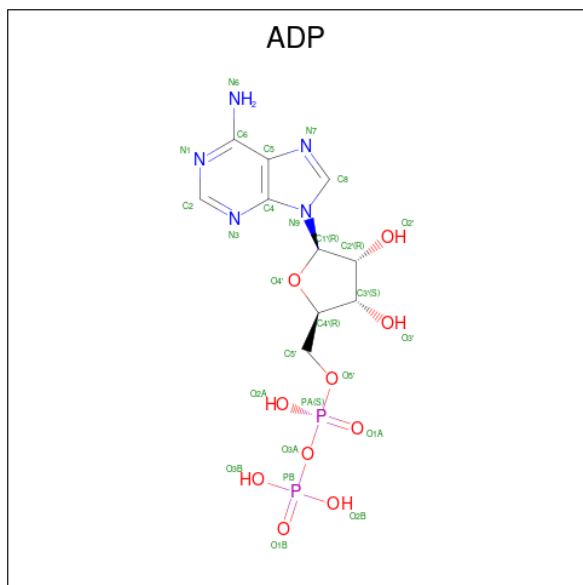
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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

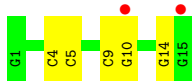
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	2	Total O 2 2	0	0
7	F	1	Total O 1 1	0	0
7	A	1	Total O 1 1	0	0
7	B	39	Total O 39 39	0	0

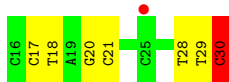
3 Residue-property plots

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.

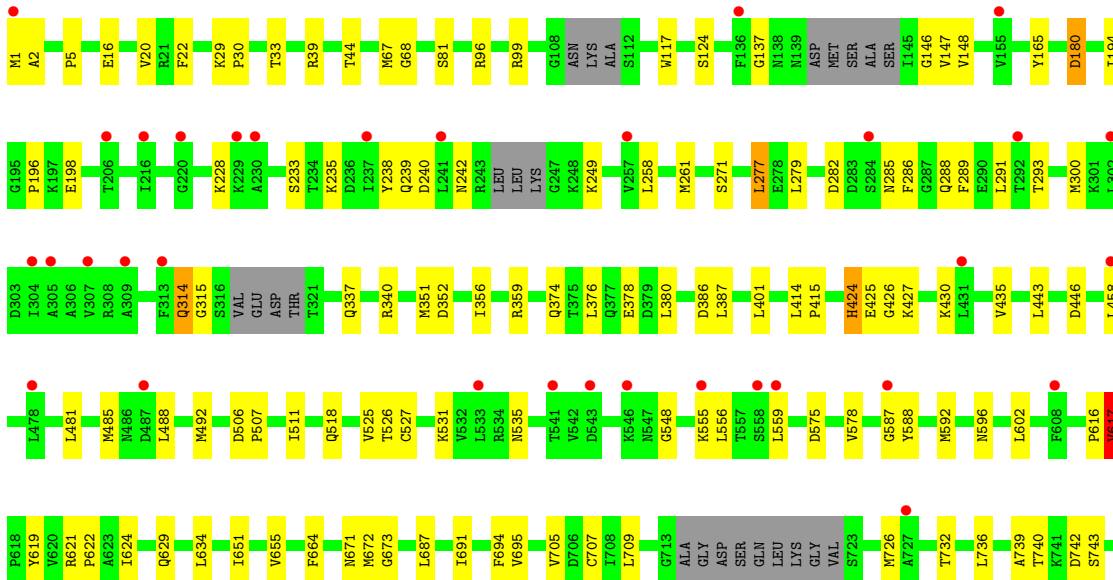
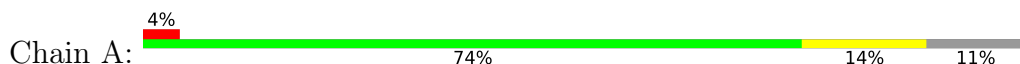
- Molecule 1: 5'-D(*GP*AP*AP*CP*CP*GP*CP*GP*CP*GP*CP*TP*AP*GP*G)-3'

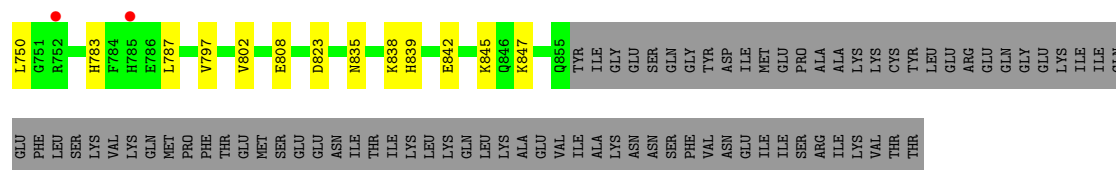


- Molecule 2: 5'-D(*CP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*TP*TP*C)-3'

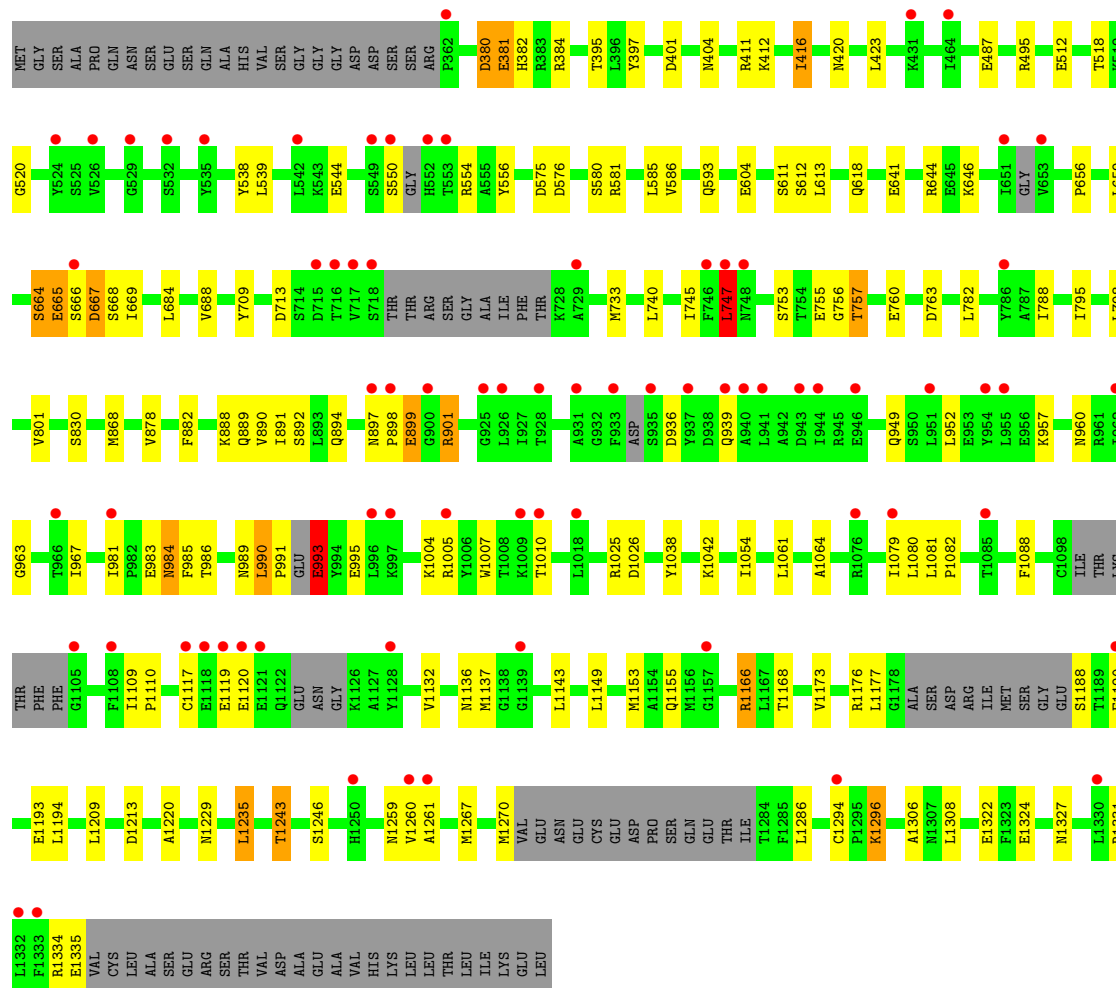
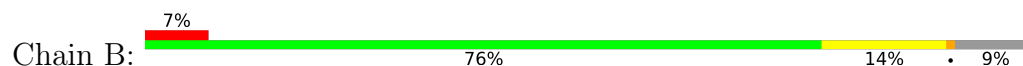


- Molecule 3: DNA mismatch repair protein Msh2





• 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	258.74Å 258.74Å 258.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.75) 99.5 (20.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.281 0.243 , 0.281	Depositor DCC
R_{free} test set	3886 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 96.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14692	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

5.1 Standard geometry

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	0.65	0/345	1.08	1/531 (0.2%)
2	F	1.71	3/338 (0.9%)	1.52	4/520 (0.8%)
3	A	0.48	0/6640	1.00	20/8953 (0.2%)
4	B	0.69	11/7591 (0.1%)	1.06	27/10228 (0.3%)
All	All	0.65	14/14914 (0.1%)	1.05	52/20232 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
4	B	0	2
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	30	DC	N1-C6	24.44	1.85	1.36
4	B	1166	ARG	CZ-NH1	15.39	1.54	1.32
4	B	1322	GLU	CD-OE2	11.41	1.47	1.25
4	B	984	ASN	CG-OD1	9.98	1.42	1.23
4	B	1119	GLU	CD-OE1	9.67	1.43	1.25
4	B	963	GLY	C-O	9.66	1.36	1.23
4	B	550	SER	C-O	8.97	1.41	1.23
4	B	1322	GLU	CD-OE1	8.92	1.42	1.25
4	B	1335	GLU	C-O	8.31	1.40	1.23
2	F	30	DC	C4-C5	7.87	1.58	1.43
4	B	993	GLU	CG-CD	6.92	1.69	1.52
2	F	30	DC	N3-C4	6.86	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	990	LEU	CG-CD1	6.61	1.74	1.52
4	B	963	GLY	C-N	5.32	1.41	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	30	DC	C5-C6-N1	-13.49	100.76	121.00
2	F	30	DC	C6-N1-C1'	-12.05	101.63	119.70
4	B	984	ASN	OD1-CG-ND2	11.61	134.21	122.60
3	A	787	LEU	N-CA-C	-10.03	101.17	113.50
2	F	30	DC	C6-N1-C2	8.91	133.96	120.60
3	A	435	VAL	N-CA-C	-8.13	105.10	112.90
4	B	984	ASN	CB-CG-OD1	-7.96	104.87	120.80
4	B	993	GLU	CG-CD-OE1	-7.89	100.26	118.40
4	B	957	LYS	N-CA-C	-7.88	103.88	113.97
4	B	1166	ARG	NE-CZ-NH2	-7.73	112.24	119.20
4	B	990	LEU	CA-C-N	7.26	128.92	119.84
4	B	990	LEU	C-N-CA	7.26	128.92	119.84
3	A	425	GLU	N-CA-C	-7.26	104.28	113.43
2	F	30	DC	N1-C2-N3	-7.22	108.07	118.90
4	B	830	SER	CA-C-N	7.18	126.68	118.85
4	B	830	SER	C-N-CA	7.18	126.68	118.85
3	A	180	ASP	N-CA-C	7.08	121.03	109.85
4	B	990	LEU	CD1-CG-CD2	6.78	125.72	110.80
3	A	96	ARG	N-CA-C	6.71	121.32	113.20
3	A	424	HIS	CB-CA-C	-6.40	108.52	117.23
4	B	757	THR	N-CA-C	6.33	118.20	110.41
4	B	899	GLU	N-CA-C	6.32	119.00	108.13
4	B	901	ARG	N-CA-C	6.30	119.24	109.60
4	B	665	GLU	N-CA-C	6.24	124.08	110.80
4	B	1168	THR	N-CA-C	-6.19	102.29	110.40
4	B	381	GLU	N-CA-C	-6.01	104.84	111.82
3	A	228	LYS	N-CA-C	5.77	118.07	108.20
4	B	416	ILE	CB-CA-C	-5.66	104.72	111.97
3	A	808	GLU	N-CA-C	-5.63	107.66	114.75
4	B	763	ASP	N-CA-C	5.52	117.70	109.59
1	E	14	DG	O4'-C1'-N9	5.48	116.62	108.40
3	A	651	ILE	CA-C-N	5.47	125.77	119.92
3	A	651	ILE	C-N-CA	5.47	125.77	119.92
3	A	277	LEU	N-CA-C	-5.34	101.76	110.20
3	A	617	VAL	CA-C-N	5.33	126.50	119.84
3	A	617	VAL	C-N-CA	5.33	126.50	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	587	GLY	N-CA-C	-5.32	107.36	115.66
4	B	538	TYR	N-CA-C	5.29	118.33	110.14
4	B	1308	LEU	CA-C-N	5.26	126.41	119.84
4	B	1308	LEU	C-N-CA	5.26	126.41	119.84
4	B	646	LYS	N-CA-C	-5.21	101.45	109.52
3	A	823	ASP	N-CA-C	5.19	116.74	111.14
3	A	233	SER	N-CA-C	5.17	119.46	113.20
4	B	664	SER	N-CA-C	5.13	114.91	108.45
3	A	380	LEU	N-CA-C	5.11	119.72	112.93
4	B	898	PRO	N-CA-C	5.04	122.84	112.47
3	A	695	VAL	N-CA-C	5.03	113.60	107.61
4	B	539	LEU	N-CA-C	-5.02	100.33	108.52
3	A	314	GLN	N-CA-C	5.02	114.99	108.07
4	B	1243	THR	N-CA-C	5.02	117.51	108.48
4	B	756	GLY	N-CA-C	-5.01	101.30	113.18
3	A	629	GLN	N-CA-C	-5.01	107.02	113.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	984	ASN	Sidechain
4	B	993	GLU	Sidechain
2	F	30	DC	Sidechain

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	307	0	168	2	0
2	F	303	0	171	8	0
3	A	6536	0	6562	76	0
4	B	7447	0	7444	94	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	B	39	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
All	All	14692	0	14369	174	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 (174) 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)
2:F:30:DC:C6	2:F:30:DC:N1	1.85	1.43
4:B:897:ASN:HB3	4:B:901:ARG:HE	1.32	0.92
3:A:39:ARG:HE	3:A:44:THR:HG21	1.42	0.84
2:F:29:DT:H2'	2:F:30:DC:C6	2.13	0.83
4:B:897:ASN:HB3	4:B:901:ARG:NE	1.93	0.82
4:B:892:SER:O	4:B:901:ARG:HB3	1.83	0.78
2:F:30:DC:C6	2:F:30:DC:C1'	2.67	0.77
4:B:1007:TRP:HE1	4:B:1010:THR:HB	1.50	0.76
3:A:359:ARG:NH2	3:A:691:ILE:O	2.19	0.75
2:F:28:DT:H2''	2:F:29:DT:H5''	1.69	0.74
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.70	0.71
4:B:380:ASP:HB2	4:B:384:ARG:H	1.56	0.70
3:A:588:TYR:O	3:A:592:MET:HG2	1.91	0.70
4:B:518:THR:HG22	4:B:520:GLY:H	1.55	0.70
4:B:1235:LEU:HD21	4:B:1243:THR:HG21	1.74	0.69
4:B:981:ILE:HD11	4:B:985:PHE:HB2	1.76	0.68
2:F:30:DC:C6	2:F:30:DC:O4'	2.47	0.68
4:B:518:THR:HG21	4:B:593:GLN:OE1	1.94	0.67
4:B:1080:LEU:HD11	4:B:1166:ARG:NH2	2.11	0.66
4:B:380:ASP:O	4:B:397:TYR:HB2	1.96	0.65
3:A:838:LYS:HG3	3:A:839:HIS:H	1.61	0.65
3:A:235:LYS:HE2	3:A:271:SER:HB2	1.77	0.64
4:B:993:GLU:OE2	4:B:1005:ARG:NH2	2.30	0.64
4:B:733:MET:HE3	4:B:1173:VAL:HG23	1.80	0.64
4:B:1007:TRP:NE1	4:B:1010:THR:HB	2.12	0.63
4:B:1294:CYS:C	4:B:1296:LYS:H	2.06	0.63
3:A:258:LEU:HB2	3:A:261:MET:HG2	1.80	0.62
3:A:340:ARG:NH2	3:A:386:ASP:OD2	2.32	0.62
4:B:788:ILE:HG21	4:B:1079:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:949:GLN:HA	4:B:952:LEU:HB3	1.82	0.62
4:B:1136:ASN:O	4:B:1137:MET:HB3	2.01	0.61
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.66	0.61
4:B:889:GLN:O	4:B:901:ARG:HA	2.01	0.60
4:B:1259:ASN:C	4:B:1261:ALA:H	2.10	0.59
4:B:899:GLU:O	4:B:901:ARG:NH1	2.35	0.59
2:F:29:DT:OP1	4:B:1004:LYS:NZ	2.36	0.59
4:B:404:ASN:OD1	4:B:411:ARG:NH1	2.34	0.59
3:A:39:ARG:HE	3:A:44:THR:CG2	2.14	0.58
4:B:518:THR:HG21	4:B:593:GLN:CD	2.29	0.57
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.70	0.57
3:A:282:ASP:HB2	3:A:286:PHE:HE2	1.70	0.56
3:A:300:MET:HG3	3:A:707:CYS:HA	1.88	0.56
3:A:427:LYS:HD3	3:A:430:LYS:HD3	1.86	0.55
3:A:488:LEU:O	3:A:492:MET:HG2	2.06	0.55
3:A:1:MET:O	3:A:2:ALA:HB3	2.05	0.55
4:B:576:ASP:OD2	4:B:580:SER:OG	2.24	0.55
4:B:960:ASN:O	4:B:967:ILE:HD12	2.07	0.55
1:E:4:DC:H2'	1:E:5:DC:C6	2.43	0.54
3:A:847:LYS:HG3	4:B:1229:ASN:HD22	1.72	0.54
3:A:671:ASN:O	3:A:672:MET:HB2	2.08	0.54
4:B:380:ASP:HB3	4:B:382:HIS:H	1.72	0.53
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.89	0.53
3:A:282:ASP:HB2	3:A:286:PHE:CE2	2.43	0.53
4:B:487:GLU:OE1	4:B:495:ARG:NH1	2.41	0.53
4:B:1038:TYR:CE2	4:B:1042:LYS:HE3	2.43	0.53
3:A:300:MET:HA	3:A:351:MET:HE2	1.90	0.52
4:B:991:PRO:O	4:B:993:GLU:N	2.42	0.52
4:B:1213:ASP:OD1	4:B:1246:SER:OG	2.27	0.52
3:A:194:ILE:HG13	3:A:196:PRO:HD3	1.92	0.52
3:A:732:THR:O	3:A:736:LEU:HB2	2.09	0.52
3:A:672:MET:SD	4:B:1188:SER:HB2	2.51	0.51
4:B:801:VAL:HG21	4:B:878:VAL:HG21	1.92	0.51
4:B:733:MET:CE	4:B:1173:VAL:HG23	2.40	0.51
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.92	0.51
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.92	0.51
3:A:16:GLU:HG3	3:A:67:MET:HE3	1.93	0.51
3:A:288:GLN:O	3:A:289:PHE:HB2	2.11	0.51
3:A:555:LYS:O	3:A:559:LEU:HB2	2.11	0.51
3:A:619:TYR:HB3	3:A:694:PHE:HB3	1.93	0.51
4:B:1331:ARG:HA	4:B:1334:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:443:LEU:HA	3:A:446:ASP:HB2	1.93	0.50
3:A:740:THR:HG23	3:A:742:ASP:H	1.76	0.50
4:B:1143:LEU:HD22	4:B:1267:MET:HE1	1.94	0.50
4:B:1025:ARG:HG3	4:B:1026:ASP:N	2.27	0.49
4:B:1149:LEU:O	4:B:1153:MET:HG2	2.12	0.49
3:A:616:PRO:O	3:A:617:VAL:HB	2.13	0.48
3:A:842:GLU:HG2	3:A:845:LYS:HD2	1.95	0.48
4:B:380:ASP:OD2	4:B:384:ARG:NE	2.38	0.48
4:B:1324:GLU:HA	4:B:1327:ASN:HB2	1.95	0.48
4:B:667:ASP:CG	4:B:668:SER:H	2.19	0.48
4:B:990:LEU:O	4:B:993:GLU:HG2	2.12	0.48
3:A:838:LYS:HG3	3:A:839:HIS:N	2.27	0.48
3:A:240:ASP:C	3:A:242:ASN:H	2.21	0.48
4:B:894:GLN:OE1	4:B:894:GLN:N	2.45	0.48
3:A:687:LEU:O	3:A:691:ILE:HG13	2.14	0.48
3:A:282:ASP:HB3	3:A:285:ASN:HB2	1.96	0.48
3:A:352:ASP:O	3:A:356:ILE:HG13	2.14	0.47
4:B:1294:CYS:C	4:B:1296:LYS:N	2.72	0.47
3:A:147:VAL:HG22	3:A:198:GLU:HB3	1.96	0.47
3:A:277:LEU:C	3:A:279:LEU:H	2.23	0.47
2:F:20:DG:H2''	2:F:21:DC:H5''	1.96	0.47
4:B:747:LEU:HA	4:B:757:THR:HG21	1.97	0.47
3:A:401:LEU:HD11	3:A:458:LEU:HD11	1.96	0.47
2:F:17:DC:H2''	2:F:18:DT:H5'	1.95	0.46
4:B:782:LEU:O	4:B:1155:GLN:HB3	2.15	0.46
4:B:381:GLU:HB2	4:B:395:THR:HB	1.97	0.46
4:B:755:GLU:HB2	4:B:760:GLU:OE1	2.16	0.46
3:A:575:ASP:HA	3:A:578:VAL:HB	1.98	0.46
4:B:611:SER:OG	4:B:612:SER:N	2.43	0.45
3:A:337:GLN:H	3:A:337:GLN:HG3	1.47	0.45
4:B:890:VAL:HG23	4:B:891:ILE:HG23	1.98	0.45
3:A:22:PHE:CZ	3:A:117:TRP:HB2	2.52	0.45
4:B:420:ASN:HB3	4:B:423:LEU:HG	1.98	0.45
3:A:732:THR:HG21	3:A:750:LEU:HD11	1.97	0.45
4:B:656:PRO:HD2	4:B:659:LEU:HD12	1.99	0.45
3:A:664:PHE:HB3	3:A:797:VAL:HG22	1.99	0.45
4:B:882:PHE:O	4:B:888:LYS:HE2	2.17	0.45
4:B:993:GLU:OE2	4:B:1005:ARG:NE	2.49	0.45
3:A:726:MET:HE1	4:B:1306:ALA:HB2	2.00	0.44
4:B:1213:ASP:HA	4:B:1246:SER:OG	2.17	0.44
4:B:575:ASP:OD1	4:B:576:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:889:GLN:HG2	4:B:901:ARG:NH1	2.32	0.44
4:B:995:GLU:HA	4:B:1005:ARG:HA	2.00	0.44
3:A:374:GLN:O	3:A:378:GLU:HG2	2.17	0.44
3:A:672:MET:HE2	3:A:672:MET:HB3	1.87	0.44
3:A:33:THR:HG22	3:A:99:ARG:CG	2.48	0.44
3:A:556:LEU:C	3:A:556:LEU:HD23	2.43	0.44
4:B:641:GLU:HB3	4:B:644:ARG:HG3	2.00	0.44
3:A:531:LYS:HA	3:A:535:ASN:HB2	2.00	0.43
3:A:29:LYS:HA	3:A:30:PRO:HD3	1.91	0.43
3:A:481:LEU:O	3:A:485:MET:HG2	2.19	0.43
3:A:518:GLN:HE21	3:A:518:GLN:HB3	1.65	0.43
4:B:740:LEU:HD12	4:B:740:LEU:HA	1.90	0.43
4:B:1270:MET:HE2	4:B:1286:LEU:HD21	2.00	0.43
4:B:1109:ILE:HA	4:B:1110:PRO:HD3	1.83	0.43
4:B:1173:VAL:HG22	4:B:1209:LEU:HB3	1.99	0.43
3:A:525:VAL:HG12	3:A:526:THR:H	1.84	0.43
3:A:235:LYS:HB3	3:A:238:TYR:HB2	2.01	0.43
3:A:356:ILE:CG2	3:A:624:ILE:HD13	2.48	0.43
4:B:1038:TYR:CZ	4:B:1042:LYS:HE3	2.54	0.43
3:A:124:SER:HB3	3:A:198:GLU:OE1	2.19	0.43
3:A:1:MET:O	3:A:2:ALA:CB	2.66	0.43
3:A:673:GLY:O	3:A:802:VAL:HG11	2.19	0.42
3:A:291:LEU:O	3:A:293:THR:HG23	2.19	0.42
3:A:414:LEU:N	3:A:415:PRO:HD2	2.34	0.42
3:A:705:VAL:HG13	3:A:743:SER:HA	2.01	0.42
4:B:1081:LEU:HA	4:B:1082:PRO:HD3	1.85	0.42
3:A:20:VAL:HG21	3:A:68:GLY:HA2	2.02	0.42
3:A:506:ASP:HA	3:A:507:PRO:HD3	1.86	0.42
4:B:581:ARG:HH21	4:B:713:ASP:HB3	1.85	0.42
4:B:868:MET:HG2	4:B:1054:ILE:HD12	2.01	0.42
4:B:664:SER:O	4:B:666:SER:N	2.53	0.42
3:A:527:CYS:HB2	3:A:548:GLY:HA2	2.01	0.42
3:A:634:LEU:HB2	3:A:655:VAL:HB	2.01	0.42
4:B:1088:PHE:HB2	4:B:1117:CYS:H	1.85	0.42
4:B:1190:PHE:CE2	4:B:1194:LEU:HD11	2.55	0.42
3:A:387:LEU:HB2	3:A:596:ASN:HB2	2.02	0.42
4:B:1259:ASN:C	4:B:1261:ALA:N	2.77	0.42
3:A:33:THR:CG2	3:A:99:ARG:HH11	2.33	0.42
3:A:424:HIS:HB2	3:A:427:LYS:H	1.85	0.42
4:B:585:LEU:C	4:B:585:LEU:HD23	2.45	0.42
3:A:783:HIS:HB2	4:B:1220:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:585:LEU:HD12	4:B:709:TYR:CE2	2.55	0.41
3:A:314:GLN:HB3	3:A:315:GLY:H	1.60	0.41
4:B:412:LYS:O	4:B:416:ILE:HG12	2.19	0.41
3:A:511:ILE:HG12	3:A:525:VAL:HG22	2.01	0.41
3:A:847:LYS:HG3	4:B:1229:ASN:ND2	2.33	0.41
4:B:401:ASP:C	4:B:401:ASP:OD1	2.63	0.41
4:B:684:LEU:O	4:B:688:VAL:HG23	2.20	0.41
4:B:586:VAL:CG1	4:B:613:LEU:HD11	2.51	0.41
4:B:733:MET:CE	4:B:1173:VAL:CG2	2.98	0.41
4:B:983:GLU:HG3	4:B:986:THR:HG21	2.02	0.41
3:A:235:LYS:HB2	3:A:239:GLN:HG3	2.03	0.41
3:A:709:LEU:HD12	3:A:739:ALA:HB2	2.02	0.41
4:B:544:GLU:HG2	4:B:556:TYR:CE1	2.55	0.41
4:B:1177:LEU:HD23	4:B:1213:ASP:HB2	2.02	0.41
3:A:621:ARG:HA	3:A:622:PRO:HD3	1.89	0.41
4:B:788:ILE:HD13	4:B:1079:ILE:HD12	2.02	0.40
3:A:376:LEU:HD13	3:A:602:LEU:HD21	2.02	0.40
4:B:1132:VAL:O	4:B:1246:SER:HA	2.22	0.40
4:B:1176:ARG:HD2	4:B:1176:ARG:HA	1.77	0.40
3:A:148:VAL:HG12	3:A:165:TYR:HB3	2.02	0.40
1:E:9:DC:H2'	1:E:10:DG:C8	2.57	0.40
4:B:667:ASP:C	4:B:669:ILE:H	2.29	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	819/934 (88%)	726 (89%)	87 (11%)	6 (1%)	18	34
4	B	910/1022 (89%)	834 (92%)	66 (7%)	10 (1%)	11	22
All	All	1729/1956 (88%)	1560 (90%)	153 (9%)	16 (1%)	14	28

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	665	GLU
4	B	1120	GLU
4	B	1296	LYS
3	A	137	GLY
4	B	667	ASP
4	B	747	LEU
4	B	989	ASN
3	A	249	LYS
3	A	146	GLY
3	A	617	VAL
4	B	753	SER
4	B	1260	VAL
3	A	835	ASN
4	B	380	ASP
4	B	745	ILE
3	A	426	GLY

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	715/808 (88%)	714 (100%)	1 (0%)	88	95
4	B	822/899 (91%)	818 (100%)	4 (0%)	81	89
All	All	1537/1707 (90%)	1532 (100%)	5 (0%)	86	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	180	ASP
4	B	512	GLU
4	B	618	GLN
4	B	747	LEU
4	B	1235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
3	A	24	GLN
3	A	61	GLN
3	A	288	GLN
3	A	377	GLN
3	A	610	HIS
3	A	629	GLN
3	A	801	HIS
4	B	367	HIS
4	B	415	GLN
4	B	1048	GLN
4	B	1229	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 oligosaccharides 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ADP	A	936	5	28,29,29	1.53	5 (17%)	43,45,45	1.76	8 (18%)
6	ADP	B	202	5	28,29,29	1.45	5 (17%)	43,45,45	1.80	9 (20%)

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	-	1/16/32/32	0/3/3/3
6	ADP	B	202	5	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	4.92	1.47	1.39
6	B	202	ADP	C5-C4	4.89	1.47	1.39
6	A	936	ADP	PA-O3A	3.09	1.62	1.59
6	B	202	ADP	C5-C6	2.80	1.48	1.41
6	A	936	ADP	C5-C6	2.55	1.48	1.41
6	A	936	ADP	C5-N7	-2.40	1.34	1.39
6	A	936	ADP	C8-N7	2.38	1.36	1.31
6	B	202	ADP	C8-N7	2.37	1.36	1.31
6	B	202	ADP	C5-N7	-2.04	1.35	1.39
6	B	202	ADP	PA-O3A	2.02	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	202	ADP	C5-C4-N3	-5.77	118.77	126.72
6	A	936	ADP	C5-C4-N3	-5.54	119.08	126.72
6	A	936	ADP	N3-C4-N9	4.63	135.04	127.17
6	B	202	ADP	N3-C4-N9	4.61	135.00	127.17
6	B	202	ADP	C2-N3-C4	3.82	121.16	111.83
6	A	936	ADP	C2-N3-C4	3.52	120.44	111.83
6	B	202	ADP	N3-C2-N1	-3.50	123.29	128.58
6	A	936	ADP	N3-C2-N1	-3.42	123.41	128.58
6	B	202	ADP	C4-C5-N7	-3.16	106.97	110.58
6	A	936	ADP	C4-C5-N7	-3.04	107.11	110.58
6	A	936	ADP	C4-N9-C8	2.66	108.53	105.74
6	B	202	ADP	C4-N9-C8	2.46	108.32	105.74
6	A	936	ADP	C5-N7-C8	2.34	107.13	103.45
6	B	202	ADP	C5-N7-C8	2.21	106.93	103.45
6	A	936	ADP	C2-N1-C6	2.20	122.35	118.73
6	B	202	ADP	C3'-C2'-C1'	2.11	105.45	101.46
6	B	202	ADP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

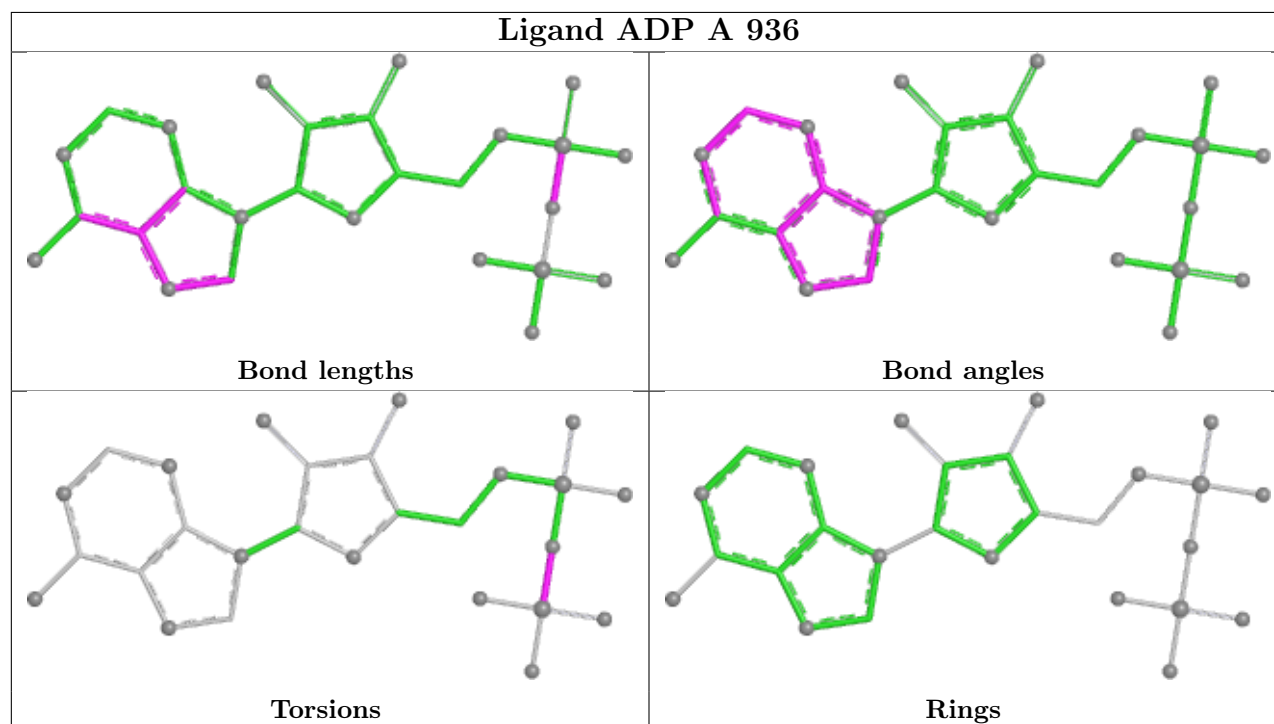
All (3) torsion outliers are listed below:

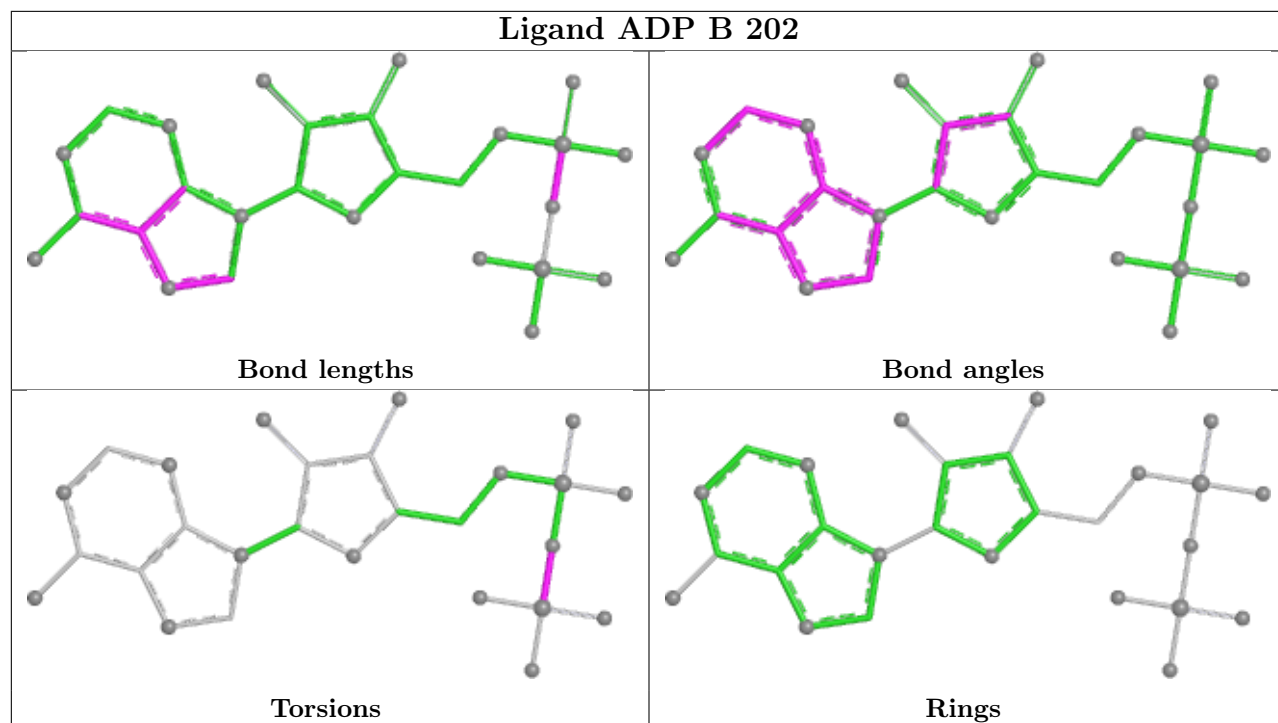
Mol	Chain	Res	Type	Atoms
6	B	202	ADP	PA-O3A-PB-O3B
6	A	936	ADP	PA-O3A-PB-O3B
6	B	202	ADP	PA-O3A-PB-O2B

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 than 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

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%)	1.05	2 (13%) 7 6	76, 81, 106, 113	0
2	F	15/15 (100%)	0.89	1 (6%) 24 23	76, 80, 91, 92	0
3	A	831/934 (88%)	0.63	35 (4%) 40 39	32, 83, 92, 106	0
4	B	930/1022 (90%)	0.63	74 (7%) 18 18	65, 82, 97, 109	0
All	All	1791/1986 (90%)	0.63	112 (6%) 26 26	32, 83, 94, 113	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	946	GLU	5.1
4	B	747	LEU	5.0
3	A	1	MET	4.9
4	B	717	VAL	4.8
4	B	716	THR	4.3
4	B	939	GLN	4.2
4	B	715	ASP	4.1
4	B	900	GLY	4.1
3	A	257	VAL	4.0
3	A	237	ILE	3.8
4	B	933	PHE	3.6
4	B	935	SER	3.6
4	B	362	PRO	3.5
4	B	552	HIS	3.5
4	B	718	SER	3.5
4	B	1118	GLU	3.4
3	A	230	ALA	3.4
4	B	937	TYR	3.4
4	B	1010	THR	3.4
4	B	1005	ARG	3.4
4	B	941	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	458	LEU	3.3
4	B	553	THR	3.2
3	A	533	LEU	3.2
4	B	955	LEU	3.2
3	A	284	SER	3.2
4	B	1261	ALA	3.2
4	B	1009	LYS	3.1
3	A	752	ARG	3.1
4	B	940	ALA	3.0
4	B	1121	GLU	3.0
4	B	997	LYS	3.0
3	A	541	THR	3.0
3	A	727	ALA	3.0
4	B	931	ALA	3.0
4	B	1260	VAL	3.0
4	B	549	SER	2.9
4	B	981	ILE	2.9
4	B	1119	GLU	2.8
4	B	926	LEU	2.8
4	B	996	LEU	2.8
3	A	478	LEU	2.8
4	B	928	THR	2.8
4	B	550	SER	2.8
3	A	543	ASP	2.8
1	E	15	DG	2.8
3	A	304	ILE	2.8
3	A	302	LEU	2.7
3	A	558	SER	2.7
3	A	313	PHE	2.7
3	A	216	ILE	2.7
3	A	546	LYS	2.6
4	B	1333	PHE	2.6
4	B	431	LYS	2.5
3	A	155	VAL	2.5
3	A	307	VAL	2.5
4	B	746	PHE	2.5
4	B	666	SER	2.4
4	B	925	GLY	2.4
3	A	587	GLY	2.4
3	A	229	LYS	2.4
3	A	206	THR	2.4
4	B	748	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	220	GLY	2.4
3	A	309	ALA	2.4
4	B	1120	GLU	2.4
4	B	1128	TYR	2.3
3	A	292	THR	2.3
4	B	1018	LEU	2.3
4	B	786	TYR	2.3
3	A	555	LYS	2.3
2	F	25	DC	2.3
4	B	529	GLY	2.3
4	B	1139	GLY	2.3
4	B	1117	CYS	2.3
4	B	1330	LEU	2.3
4	B	464	ILE	2.3
4	B	651	ILE	2.3
4	B	898	PRO	2.3
4	B	1105	GLY	2.3
4	B	1076	ARG	2.2
4	B	1294	CYS	2.2
3	A	241	LEU	2.2
3	A	305	ALA	2.2
4	B	966	THR	2.2
4	B	954	TYR	2.2
4	B	542	LEU	2.2
4	B	951	LEU	2.2
4	B	1157	GLY	2.2
4	B	943	ASP	2.2
4	B	526	VAL	2.2
4	B	524	TYR	2.1
3	A	487	ASP	2.1
4	B	962	ILE	2.1
3	A	559	LEU	2.1
4	B	535	TYR	2.1
4	B	944	ILE	2.1
4	B	1332	LEU	2.1
4	B	897	ASN	2.1
3	A	785	HIS	2.1
4	B	1108	PHE	2.1
4	B	1190	PHE	2.1
4	B	532	SER	2.1
4	B	729	ALA	2.1
4	B	1079	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	10	DG	2.0
4	B	1250	HIS	2.0
3	A	136	PHE	2.0
3	A	608	PHE	2.0
4	B	1085	THR	2.0
3	A	431	LEU	2.0
4	B	653	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

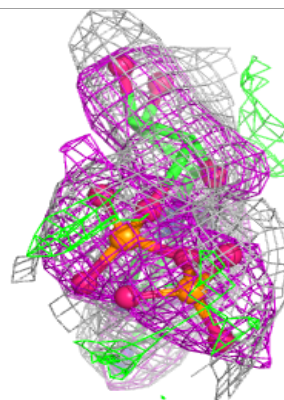
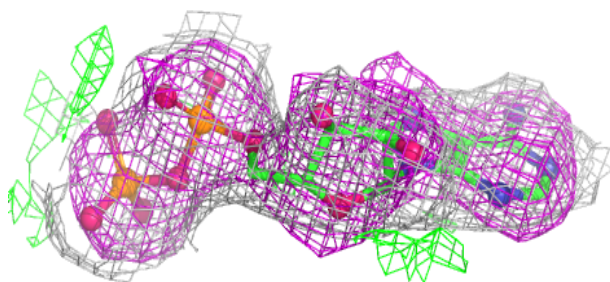
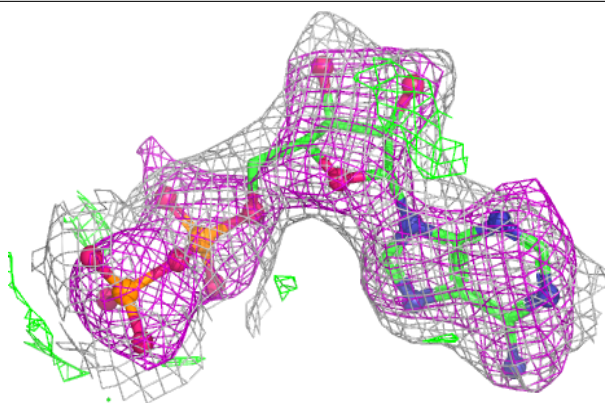
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ADP	B	202	27/27	0.77	0.15	79,80,81,81	0
5	MG	A	935	1/1	0.92	0.14	100,100,100,100	0
6	ADP	A	936	27/27	0.94	0.08	70,71,73,73	0
5	MG	B	102	1/1	0.95	0.07	76,76,76,76	0

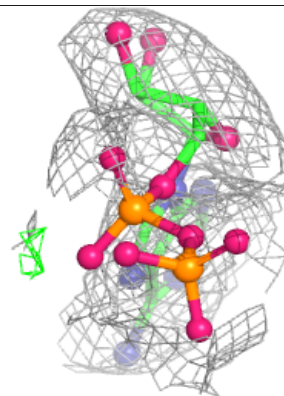
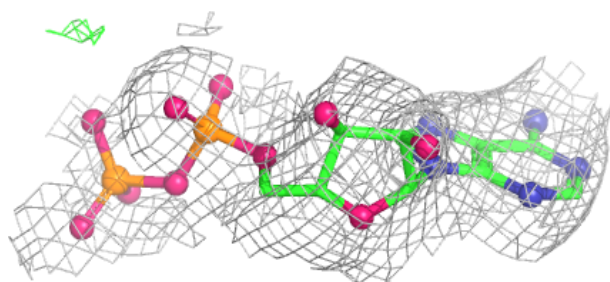
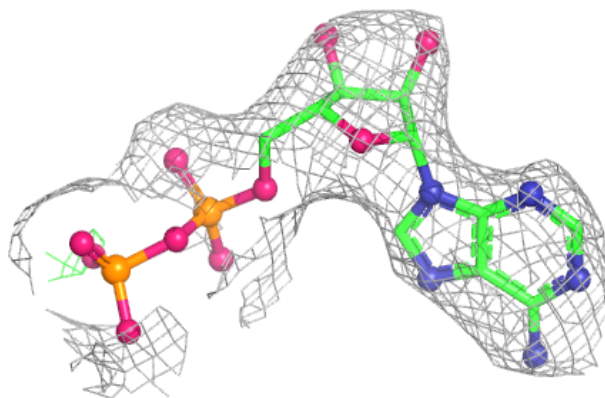
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 202:

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

**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.