Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 03:42 AM EST

PDB ID	:	2O8B
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 (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:

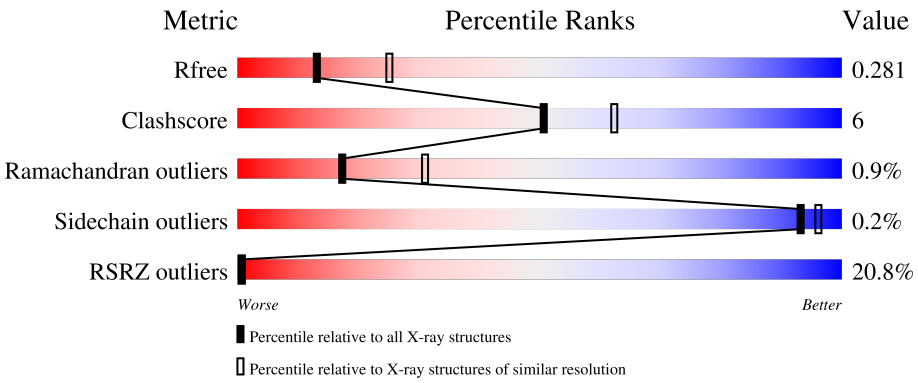
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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%, 53%, 13%
2	F	15	47%, 27%, 20%, 7%
3	A	934	26%; 76%, 13%, 11%
4	B	1022	13%; 77%, 13%, • 9%

2 Entry composition (i)

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*TP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	15	307	145	62	86	14	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	15	303	145	53	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	831	6536	4144	1113	1245	34	0	0	0

- 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	930	7447	4725	1279	1392	51	0	0	0

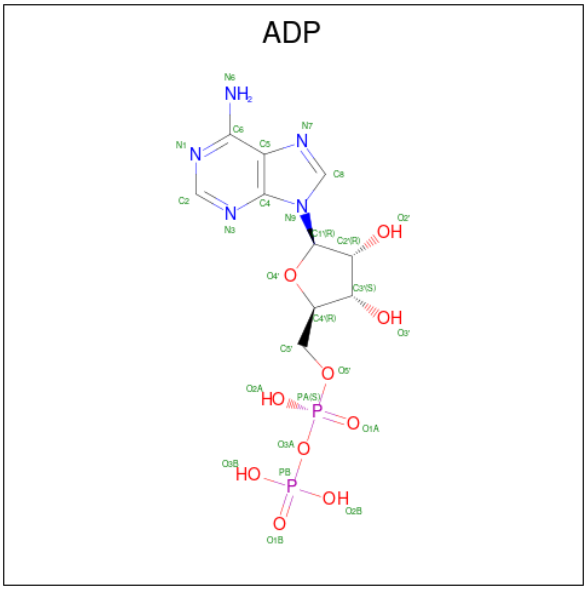
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	MET	-	initiating methionine	UNP P52701
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
			Total	Mg		
5	B	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
			Total	C	N	O	P		
6	B	1	27	10	5	10	2	0	0

- Molecule 7 is water.

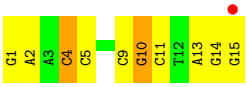
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	E	2	2	2	0	0
			Total	O		
7	F	1	1	1	0	0
			Total	O		
7	A	1	1	1	0	0
			Total	O		
7	B	39	39	39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain E: 7% 33% 53% 13%

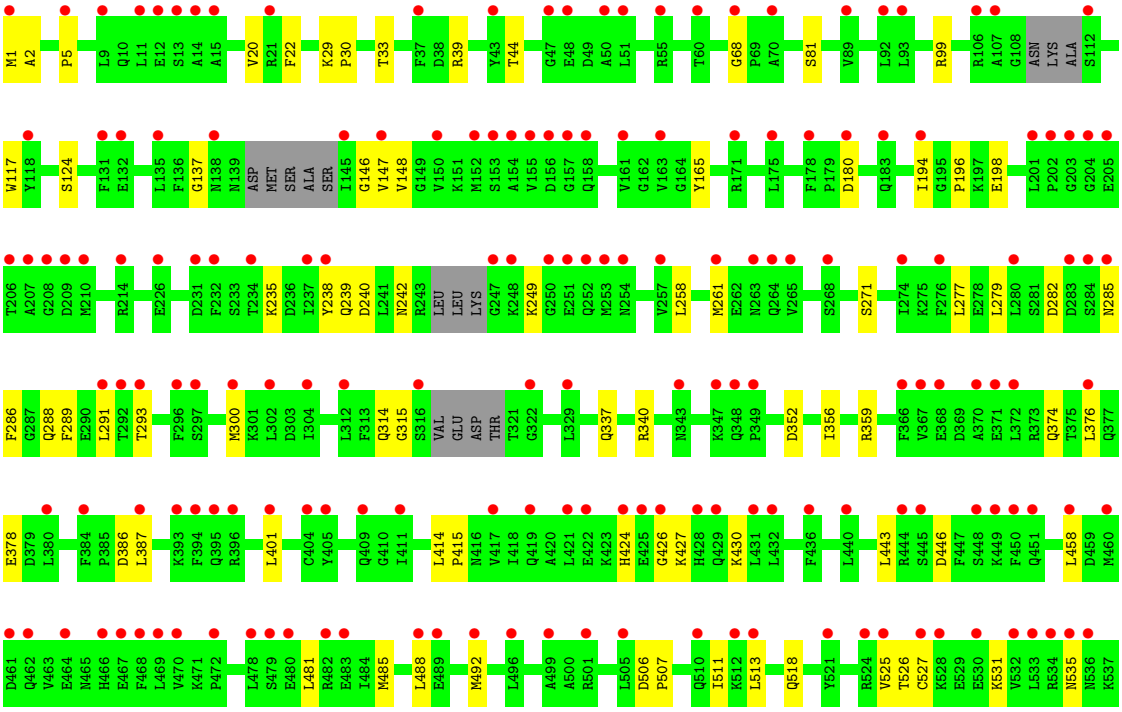


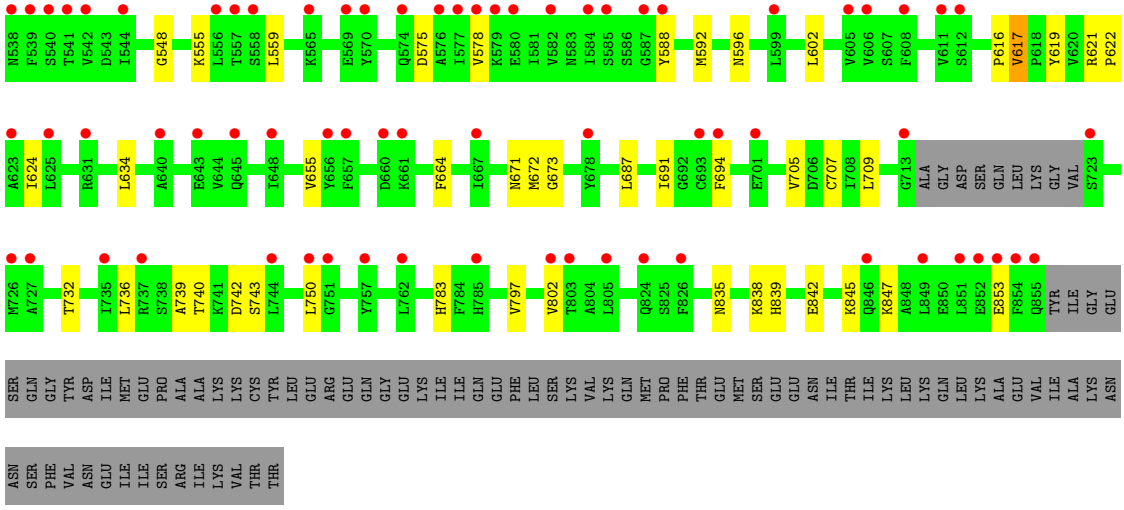
• Molecule 2: 5'-D(*CP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*TP*TP*C)-3'

Chain F: 47% 27% 20% 7%

• Molecule 3: DNA mismatch repair protein Msh2

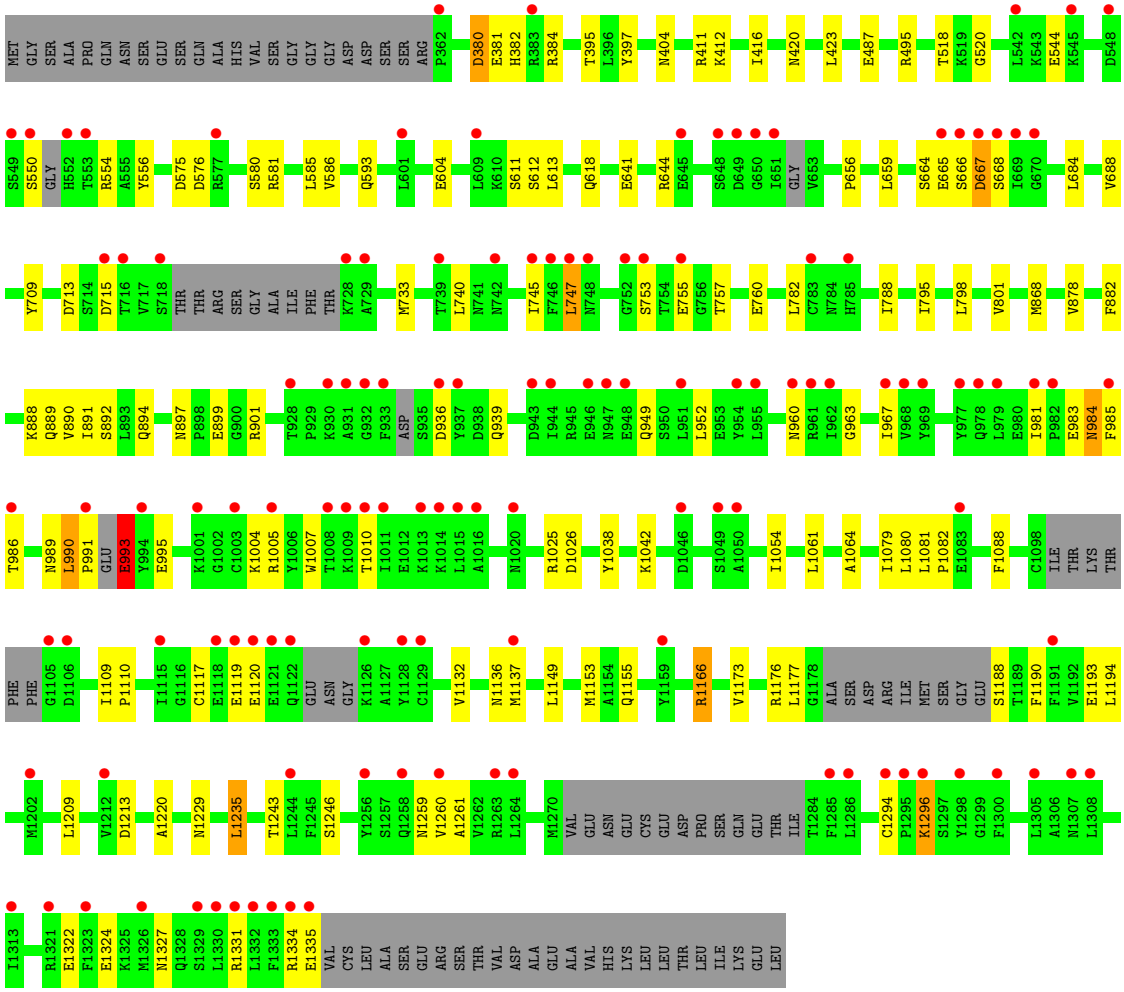
Chain A: 26% 76% 13% 11%





- Molecule 4: DNA mismatch repair protein MSH6

Chain B:



4 Data and refinement statistics (i)

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 48.05 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.75) 99.8 (48.05-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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 (5.07%)	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)	0.31 , 104.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	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.*

[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	1.71	6/345 (1.7%)	1.73	9/531 (1.7%)
2	F	5.11	17/338 (5.0%)	3.26	24/520 (4.6%)
3	A	0.39	2/6640 (0.0%)	0.63	0/8953
4	B	0.68	12/7591 (0.2%)	0.74	8/10228 (0.1%)
All	All	0.98	37/14914 (0.2%)	0.90	41/20232 (0.2%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	30	DC	N1-C6	80.97	1.85	1.37
2	F	30	DC	C4-C5	19.80	1.58	1.43
2	F	30	DC	N3-C4	19.45	1.47	1.33
4	B	1322	GLU	CD-OE2	19.43	1.47	1.25
4	B	1119	GLU	CD-OE1	16.43	1.43	1.25
4	B	1166	ARG	CZ-NH1	16.34	1.54	1.33
4	B	1322	GLU	CD-OE1	15.13	1.42	1.25
1	E	1	DG	C6-N1	12.60	1.48	1.39
1	E	1	DG	N3-C4	12.35	1.44	1.35
4	B	993	GLU	CG-CD	11.59	1.69	1.51
1	E	1	DG	N7-C5	11.02	1.45	1.39
2	F	29	DT	C5-C6	-10.99	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	30	DC	C5-C6	10.74	1.43	1.34
2	F	29	DT	N1-C6	10.46	1.45	1.38
2	F	30	DC	C2'-C1'	10.44	1.62	1.52
4	B	550	SER	C-O	9.55	1.41	1.23
2	F	28	DT	N1-C2	9.42	1.45	1.38
1	E	15	DG	C6-O6	9.30	1.32	1.24
2	F	30	DC	C4-N4	9.26	1.42	1.33
4	B	1335	GLU	C-O	8.85	1.40	1.23
4	B	984	ASN	CG-OD1	8.44	1.42	1.24
2	F	29	DT	C5-C7	8.39	1.55	1.50
4	B	963	GLY	C-O	8.32	1.36	1.23
3	A	853	GLU	CD-OE1	8.30	1.34	1.25
2	F	28	DT	C4-C5	7.99	1.52	1.45
4	B	1119	GLU	CD-OE2	7.96	1.34	1.25
2	F	30	DC	C1'-N1	7.48	1.58	1.49
4	B	993	GLU	CD-OE1	7.29	1.33	1.25
2	F	30	DC	C2-O2	7.24	1.30	1.24
3	A	853	GLU	CD-OE2	6.96	1.33	1.25
2	F	30	DC	C4'-O4'	6.63	1.51	1.45
2	F	30	DC	O4'-C1'	6.61	1.50	1.42
1	E	1	DG	N9-C8	6.38	1.42	1.37
2	F	30	DC	C2-N3	-6.11	1.30	1.35
4	B	990	LEU	CG-CD1	6.08	1.74	1.51
1	E	2	DA	N9-C4	6.01	1.41	1.37
2	F	30	DC	C4'-C3'	5.18	1.58	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	30	DC	C5-C6-N1	-40.48	100.76	121.00
2	F	30	DC	C6-N1-C2	34.16	133.96	120.30
4	B	1166	ARG	NE-CZ-NH2	-16.12	112.24	120.30
2	F	30	DC	C6-N1-C1'	-15.97	101.63	120.80
2	F	30	DC	N1-C2-N3	-15.90	108.07	119.20
2	F	30	DC	C2-N3-C4	14.96	127.38	119.90
1	E	14	DG	O4'-C1'-N9	12.31	116.62	108.00
2	F	30	DC	O4'-C1'-C2'	9.50	113.50	105.90
2	F	30	DC	O4'-C4'-C3'	9.44	111.67	106.00
4	B	993	GLU	CG-CD-OE1	-9.02	100.26	118.30
2	F	23	DT	O4'-C1'-N1	-8.98	101.71	108.00
2	F	30	DC	N1-C2-O2	8.55	124.03	118.90
4	B	984	ASN	CB-CG-OD1	-8.36	104.87	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	30	DC	N3-C2-O2	8.26	127.68	121.90
2	F	30	DC	C4-C5-C6	8.23	121.51	117.40
2	F	29	DT	N1-C2-N3	-7.43	110.14	114.60
4	B	990	LEU	CB-CG-CD2	-7.23	98.71	111.00
2	F	28	DT	C4-C5-C7	7.00	123.20	119.00
2	F	29	DT	C4-C5-C7	6.92	123.16	119.00
4	B	1235	LEU	CA-CB-CG	6.83	131.00	115.30
2	F	29	DT	C6-N1-C2	6.74	124.67	121.30
2	F	30	DC	C1'-O4'-C4'	-6.66	103.44	110.10
1	E	14	DG	C3'-C2'-C1'	-6.62	94.56	102.50
1	E	14	DG	C1'-O4'-C4'	-6.60	103.50	110.10
1	E	11	DC	O4'-C1'-N1	6.55	112.58	108.00
2	F	28	DT	N3-C4-C5	6.24	118.94	115.20
1	E	11	DC	C1'-O4'-C4'	-6.16	103.94	110.10
1	E	4	DC	O4'-C1'-N1	5.93	112.15	108.00
2	F	21	DC	P-O3'-C3'	5.75	126.60	119.70
2	F	28	DT	C5-C4-O4	-5.74	120.89	124.90
4	B	1166	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	F	21	DC	O4'-C1'-N1	5.70	111.99	108.00
1	E	13	DA	P-O3'-C3'	5.52	126.33	119.70
2	F	29	DT	N1-C2-O2	5.47	127.48	123.10
1	E	10	DG	O4'-C1'-N9	5.36	111.75	108.00
4	B	984	ASN	OD1-CG-ND2	5.35	134.21	121.90
2	F	28	DT	C6-N1-C2	5.35	123.97	121.30
2	F	28	DT	N3-C2-O2	-5.15	119.21	122.30
1	E	1	DG	N1-C2-N3	-5.14	120.82	123.90
4	B	990	LEU	CD1-CG-CD2	5.07	125.72	110.50
2	F	28	DT	C2-N3-C4	-5.05	124.17	127.20

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	72	0
4	B	7447	0	7444	87	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
7	A	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	164	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 (164) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1007:TRP:NE1	4:B:1010:THR:HB	2.12	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
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: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
4:B:1294:CYS:C	4:B:1296:LYS:H	2.06	0.58
3:A:39:ARG:HE	3:A:44:THR:CG2	2.14	0.58
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:1259:ASN:C	4:B:1261:ALA:H	2.10	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:518:THR:HG21	4:B:593:GLN:CD	2.29	0.53
4:B:1038:TYR:CE2	4:B:1042:LYS:HE3	2.43	0.53
4:B:991:PRO:O	4:B:993:GLU:N	2.42	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:733:MET:CE	4:B:1173:VAL:HG23	2.40	0.51
4:B:801:VAL:HG21	4:B:878:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.92	0.51
4:B:1213:ASP:OD1	4:B:1246:SER:OG	2.27	0.51
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.92	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
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: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: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
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
3:A:147:VAL:HG22	3:A:198:GLU:HB3	1.96	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
4:B:611:SER:OG	4:B:612:SER:N	2.43	0.46
3:A:575:ASP:HA	3:A:578:VAL:HB	1.98	0.46
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
3:A:492:MET:HE2	3:A:513:LEU:HD21	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:B:667:ASP:CG	4:B:668:SER:H	2.19	0.44
3:A:33:THR:HG22	3:A:99:ARG:CG	2.48	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:240:ASP:C	3:A:242:ASN:H	2.21	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:733:MET:HE3	4:B:1173:VAL:HG23	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
4:B:1294:CYS:C	4:B:1296:LYS:N	2.72	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:277:LEU:C	3:A:279:LEU:H	2.23	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
3:A:33:THR:CG2	3:A:99:ARG:HH11	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:424:HIS:HB2	3:A:427:LYS:H	1.85	0.42
3:A:783:HIS:HB2	4:B:1220:ALA:HA	2.01	0.41
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: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

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%)	22 39
4	B	910/1022 (89%)	834 (92%)	66 (7%)	10 (1%)	14 25
All	All	1729/1956 (88%)	1560 (90%)	153 (9%)	16 (1%)	17 31

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 (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	715/808 (88%)	714 (100%)	1 (0%)	93 96
4	B	822/899 (91%)	820 (100%)	2 (0%)	93 96
All	All	1537/1707 (90%)	1534 (100%)	3 (0%)	93 96

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

Mol	Chain	Res	Type
3	A	180	ASP
4	B	618	GLN
4	B	715	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	451	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	A	936	5	24,29,29	1.00	1 (4%)	29,45,45	1.28	5 (17%)
6	ADP	B	202	5	24,29,29	1.02	3 (12%)	29,45,45	1.35	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	-	1/12/32/32	0/3/3/3
6	ADP	B	202	5	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	2.62	1.47	1.40
6	B	202	ADP	C5-C4	2.60	1.47	1.40
6	B	202	ADP	C2-N3	2.04	1.35	1.32
6	B	202	ADP	O4'-C1'	2.00	1.43	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	202	ADP	N3-C2-N1	-3.45	123.29	128.68
6	A	936	ADP	N3-C2-N1	-3.37	123.41	128.68
6	B	202	ADP	C3'-C2'-C1'	2.97	105.45	100.98
6	B	202	ADP	PA-O3A-PB	-2.75	123.37	132.83
6	A	936	ADP	C3'-C2'-C1'	2.42	104.63	100.98
6	A	936	ADP	PA-O3A-PB	-2.42	124.53	132.83
6	B	202	ADP	C4-C5-N7	-2.33	106.97	109.40
6	A	936	ADP	C4-C5-N7	-2.20	107.11	109.40
6	A	936	ADP	C2-N1-C6	2.10	122.35	118.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

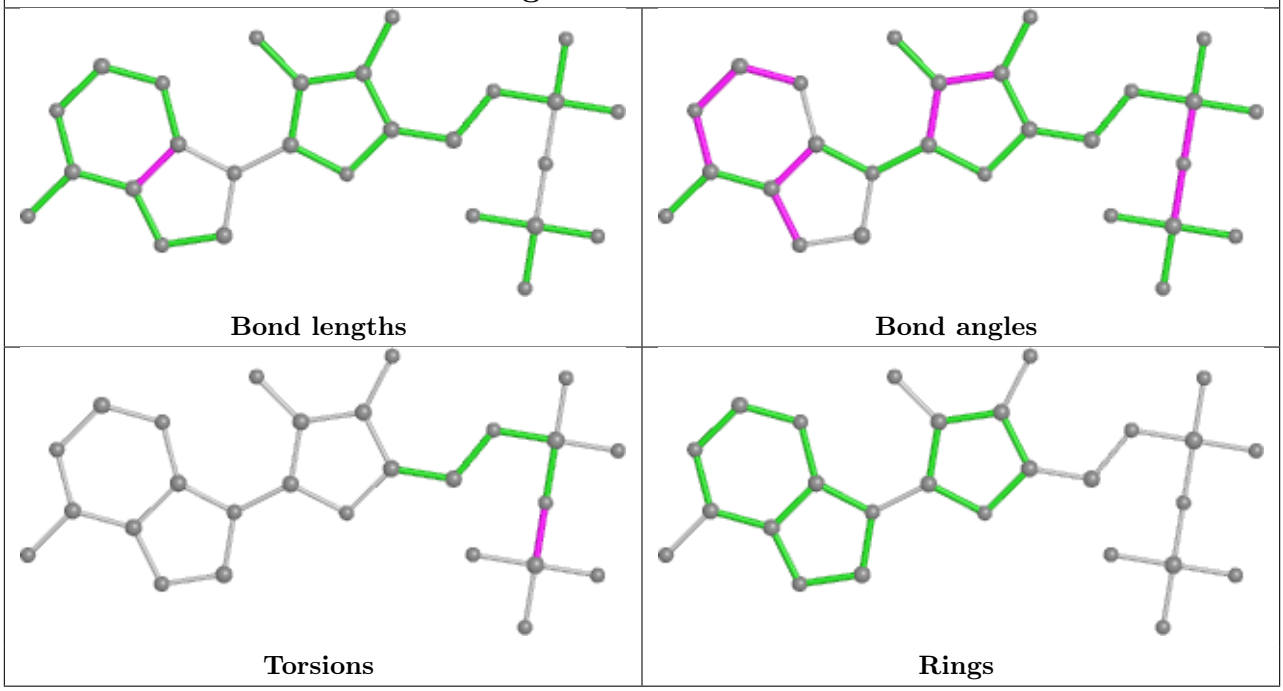
Mol	Chain	Res	Type	Atoms
6	B	202	ADP	PA-O3A-PB-O3B
6	A	936	ADP	PA-O3A-PB-O3B
6	B	202	ADP	PA-O3A-PB-O2B

There are no ring outliers.

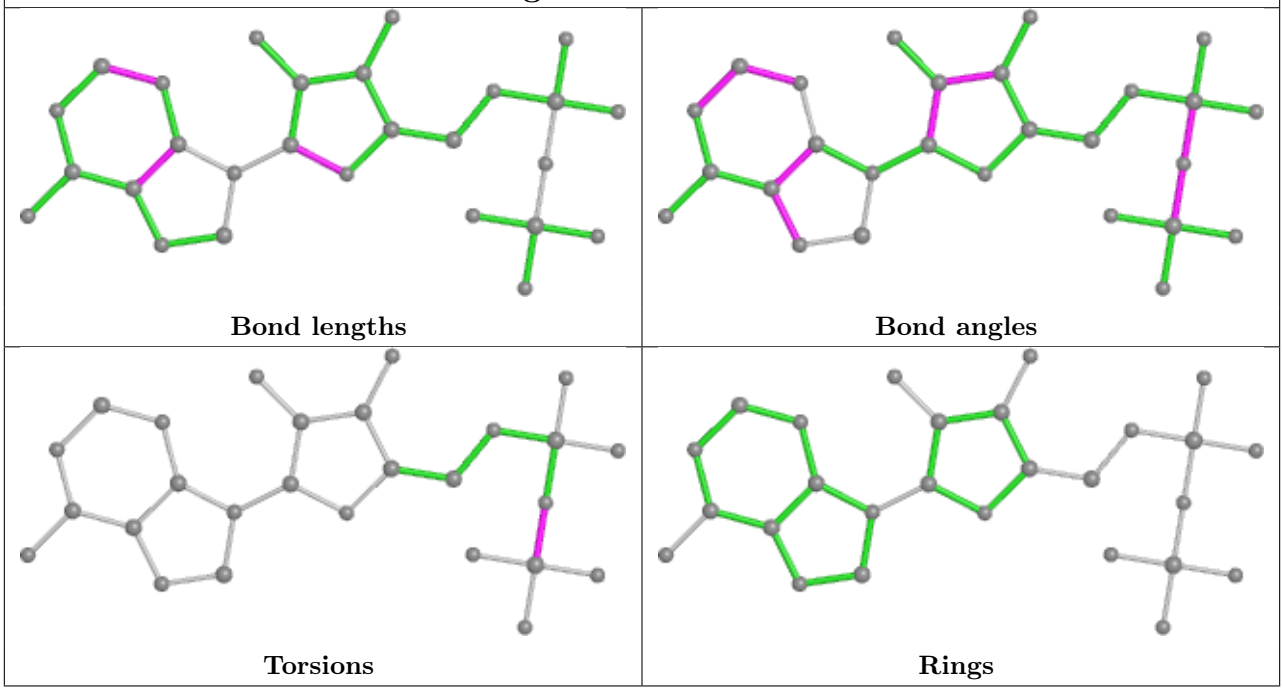
No monomer is involved in short contacts.

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 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.

Ligand ADP A 936



Ligand ADP B 202



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%)	0.48	1 (6%) 17 21	76, 81, 106, 113	0
2	F	15/15 (100%)	0.72	0 100 100	76, 80, 91, 92	0
3	A	831/934 (88%)	1.61	244 (29%) 0 0	32, 83, 92, 106	0
4	B	930/1022 (90%)	1.13	128 (13%) 2 3	65, 82, 97, 109	0
All	All	1791/1986 (90%)	1.34	373 (20%) 1 1	32, 83, 94, 113	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	541	THR	14.8
3	A	723	SER	13.3
4	B	1010	THR	12.4
4	B	550	SER	12.1
3	A	284	SER	10.6
3	A	206	THR	10.6
3	A	154	ALA	10.4
4	B	1333	PHE	9.2
4	B	753	SER	8.7
4	B	1121	GLU	8.6
4	B	954	TYR	8.6
4	B	1334	ARG	8.5
4	B	968	VAL	8.4
4	B	752	GLY	8.2
4	B	1326	MET	8.1
3	A	540	SER	7.5
3	A	569	GLU	7.3
4	B	552	HIS	7.2
4	B	1330	LEU	7.1
3	A	155	VAL	7.1
4	B	549	SER	6.8

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Mol	Chain	Res	Type	RSRZ
3	A	558	SER	6.7
3	A	426	GLY	6.7
4	B	747	LEU	6.7
3	A	570	TYR	6.6
3	A	424	HIS	6.6
3	A	587	GLY	6.6
3	A	533	LEU	6.6
4	B	718	SER	6.4
3	A	203	GLY	6.4
4	B	1009	LYS	6.3
3	A	467	GLU	6.3
4	B	715	ASP	6.3
4	B	1307	ASN	6.2
3	A	13	SER	6.1
3	A	640	ALA	6.0
3	A	204	GLY	6.0
4	B	1332	LEU	6.0
3	A	202	PRO	6.0
3	A	469	LEU	5.8
3	A	238	TYR	5.6
4	B	1258	GLN	5.6
4	B	716	THR	5.6
3	A	428	HIS	5.5
4	B	1008	THR	5.5
3	A	107	ALA	5.5
4	B	1126	LYS	5.4
3	A	727	ALA	5.4
3	A	263	ASN	5.3
4	B	728	LYS	5.3
4	B	1321	ARG	5.3
3	A	757	TYR	5.2
4	B	937	TYR	5.2
3	A	207	ALA	5.2
3	A	280	LEU	5.2
3	A	660	ASP	5.2
3	A	538	ASN	5.1
3	A	210	MET	5.1
3	A	535	ASN	5.1
4	B	1308	LEU	5.1
3	A	404	CYS	5.1
3	A	584	ILE	5.1
4	B	1295	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
4	B	1285	PHE	5.0
3	A	656	TYR	5.0
3	A	292	THR	5.0
4	B	948	GLU	5.0
4	B	1298	TYR	5.0
4	B	1120	GLU	5.0
3	A	158	GLN	5.0
3	A	557	THR	4.9
3	A	468	PHE	4.9
3	A	431	LEU	4.9
4	B	669	ILE	4.8
3	A	253	MET	4.8
3	A	112	SER	4.7
3	A	425	GLU	4.7
3	A	482	ARG	4.7
3	A	14	ALA	4.6
4	B	553	THR	4.6
3	A	606	VAL	4.6
3	A	366	PHE	4.6
3	A	201	LEU	4.6
4	B	1003	CYS	4.5
3	A	156	ASP	4.5
3	A	496	LEU	4.5
3	A	852	GLU	4.5
4	B	1137	MET	4.4
4	B	1119	GLU	4.4
3	A	585	SER	4.4
3	A	157	GLY	4.4
3	A	152	MET	4.4
3	A	380	LEU	4.4
3	A	479	SER	4.4
4	B	977	TYR	4.4
4	B	1105	GLY	4.3
3	A	458	LEU	4.3
3	A	851	LEU	4.3
3	A	265	VAL	4.3
3	A	826	PHE	4.3
3	A	648	ILE	4.3
3	A	539	PHE	4.3
3	A	785	HIS	4.2
3	A	661	LYS	4.2
3	A	480	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
3	A	393	LYS	4.2
4	B	1331	ARG	4.1
3	A	528	LYS	4.1
4	B	967	ILE	4.1
3	A	254	ASN	4.1
3	A	510	GLN	4.0
3	A	367	VAL	4.0
4	B	969	TYR	4.0
3	A	283	ASP	4.0
3	A	478	LEU	4.0
3	A	432	LEU	4.0
4	B	1016	ALA	3.9
4	B	542	LEU	3.9
3	A	417	VAL	3.9
4	B	982	PRO	3.9
3	A	472	PRO	3.8
3	A	371	GLU	3.8
3	A	737	ARG	3.8
4	B	994	TYR	3.8
3	A	387	LEU	3.7
3	A	276	PHE	3.7
3	A	384	PHE	3.7
3	A	505	LEU	3.7
3	A	492	MET	3.6
4	B	548	ASP	3.6
4	B	955	LEU	3.6
4	B	383	ARG	3.6
3	A	532	VAL	3.6
3	A	9	LEU	3.5
3	A	466	HIS	3.5
3	A	611	VAL	3.5
4	B	1129	CYS	3.5
3	A	461	ASP	3.5
3	A	530	GLU	3.5
4	B	981	ILE	3.5
3	A	55	ARG	3.5
3	A	161	VAL	3.4
3	A	304	ILE	3.4
3	A	234	THR	3.4
4	B	1015	LEU	3.4
4	B	1323	PHE	3.4
3	A	460	MET	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	693	CYS	3.4
4	B	665	GLU	3.4
3	A	499	ALA	3.4
3	A	208	GLY	3.4
3	A	153	SER	3.3
3	A	657	PHE	3.3
3	A	744	LEU	3.3
3	A	436	PHE	3.3
3	A	257	VAL	3.3
3	A	631	ARG	3.3
3	A	132	GLU	3.3
4	B	666	SER	3.2
3	A	232	PHE	3.2
3	A	394	PHE	3.2
4	B	577	ARG	3.2
3	A	316	SER	3.2
4	B	1128	TYR	3.2
3	A	524	ARG	3.2
3	A	297	SER	3.2
3	A	422	GLU	3.2
4	B	1005	ARG	3.2
3	A	248	LYS	3.2
3	A	247	GLY	3.2
3	A	849	LEU	3.2
4	B	947	ASN	3.2
4	B	1001	LYS	3.2
4	B	931	ALA	3.2
4	B	1122	GLN	3.1
3	A	368	GLU	3.1
3	A	343	ASN	3.1
4	B	1013	LYS	3.1
4	B	545	LYS	3.1
3	A	625	LEU	3.1
3	A	501	ARG	3.1
3	A	605	VAL	3.1
4	B	649	ASP	3.1
3	A	1	MET	3.0
4	B	1335	GLU	3.0
4	B	1313	ILE	3.0
3	A	565	LYS	3.0
3	A	293	THR	3.0
3	A	409	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	106	ARG	3.0
3	A	268	SER	3.0
3	A	175	LEU	3.0
4	B	1296	LYS	3.0
3	A	421	LEU	3.0
4	B	944	ILE	2.9
3	A	12	GLU	2.9
3	A	419	GLN	2.9
4	B	1329	SER	2.9
3	A	396	ARG	2.9
3	A	429	GLN	2.9
3	A	525	VAL	2.9
3	A	542	VAL	2.9
3	A	138	ASN	2.9
3	A	726	MET	2.9
3	A	11	LEU	2.9
3	A	580	GLU	2.8
4	B	962	ILE	2.8
4	B	1014	LYS	2.8
3	A	450	PHE	2.8
4	B	1264	LEU	2.8
3	A	462	GLN	2.8
3	A	43	TYR	2.8
3	A	405	TYR	2.8
3	A	577	ILE	2.8
3	A	376	LEU	2.8
3	A	171	ARG	2.8
3	A	264	GLN	2.8
3	A	608	PHE	2.8
4	B	951	LEU	2.8
3	A	444	ARG	2.7
4	B	986	THR	2.7
4	B	1260	VAL	2.7
3	A	853	GLU	2.7
3	A	574	GLN	2.7
3	A	147	VAL	2.7
3	A	802	VAL	2.7
3	A	285	ASN	2.7
3	A	92	LEU	2.7
3	A	449	LYS	2.7
4	B	667	ASP	2.7
3	A	534	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
4	B	1300	PHE	2.7
3	A	296	PHE	2.7
4	B	1083	GLU	2.7
3	A	180	ASP	2.7
4	B	651	ILE	2.7
3	A	854	PHE	2.6
3	A	521	TYR	2.6
3	A	667	ILE	2.6
3	A	578	VAL	2.6
3	A	135	LEU	2.6
4	B	933	PHE	2.6
4	B	1159	TYR	2.6
3	A	470	VAL	2.6
3	A	214	ARG	2.6
3	A	582	VAL	2.6
4	B	1263	ARG	2.6
3	A	512	LYS	2.6
3	A	145	ILE	2.5
3	A	131	PHE	2.5
3	A	579	LYS	2.5
4	B	1049	SER	2.5
3	A	395	GLN	2.5
3	A	855	GLN	2.5
3	A	612	SER	2.5
3	A	701	GLU	2.5
4	B	650	GLY	2.5
3	A	150	VAL	2.5
1	E	15	DG	2.5
3	A	205	GLU	2.5
3	A	451	GLN	2.5
4	B	946	GLU	2.5
3	A	645	GLN	2.5
3	A	588	TYR	2.5
3	A	401	LEU	2.5
3	A	556	LEU	2.5
4	B	928	THR	2.4
3	A	513	LEU	2.4
3	A	250	GLY	2.4
4	B	1011	ILE	2.4
3	A	370	ALA	2.4
3	A	291	LEU	2.4
3	A	750	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	713	GLY	2.4
3	A	231	ASP	2.4
3	A	252	GLN	2.4
4	B	668	SER	2.4
3	A	527	CYS	2.4
3	A	194	ILE	2.4
3	A	751	GLY	2.4
4	B	1118	GLU	2.4
3	A	15	ALA	2.4
3	A	209	ASP	2.4
4	B	1294	CYS	2.4
3	A	226	GLU	2.3
3	A	183	GLN	2.3
3	A	163	VAL	2.3
3	A	60	THR	2.3
4	B	930	LYS	2.3
4	B	1286	LEU	2.3
4	B	978	GLN	2.3
4	B	1191	PHE	2.3
4	B	362	PRO	2.3
3	A	762	LEU	2.3
4	B	601	LEU	2.3
4	B	648	SER	2.3
4	B	1256	TYR	2.3
3	A	483	GLU	2.3
3	A	237	ILE	2.3
3	A	694	PHE	2.3
4	B	943	ASP	2.3
3	A	347	LYS	2.3
4	B	1106	ASP	2.3
3	A	349	PRO	2.2
3	A	372	LEU	2.2
4	B	645	GLU	2.2
3	A	623	ALA	2.2
4	B	961	ARG	2.2
3	A	544	ILE	2.2
4	B	936	ASP	2.2
3	A	51	LEU	2.2
3	A	312	LEU	2.2
4	B	785	HIS	2.2
4	B	979	LEU	2.2
3	A	89	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	348	GLN	2.2
3	A	5	PRO	2.2
4	B	1046	ASP	2.2
3	A	47	GLY	2.2
3	A	322	GLY	2.2
4	B	985	PHE	2.2
4	B	1212	VAL	2.2
3	A	50	ALA	2.2
3	A	274	ILE	2.2
4	B	670	GLY	2.2
4	B	739	THR	2.2
3	A	536	ASN	2.2
3	A	643	GLU	2.2
3	A	824	GLN	2.2
4	B	783	CYS	2.2
3	A	118	TYR	2.2
3	A	48	GLU	2.2
3	A	93	LEU	2.2
3	A	440	LEU	2.2
3	A	488	LEU	2.2
3	A	576	ALA	2.2
4	B	748	ASN	2.1
3	A	489	GLU	2.1
3	A	678	TYR	2.1
4	B	1305	LEU	2.1
3	A	261	MET	2.1
3	A	300	MET	2.1
4	B	1115	ILE	2.1
4	B	991	PRO	2.1
4	B	960	ASN	2.1
3	A	448	SER	2.1
3	A	21	ARG	2.1
4	B	745	ILE	2.1
4	B	1020	ASN	2.1
4	B	746	PHE	2.1
4	B	609	LEU	2.1
4	B	742	ASN	2.1
3	A	805	LEU	2.1
4	B	755	GLU	2.1
4	B	729	ALA	2.1
3	A	37	PHE	2.1
3	A	68	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	599	LEU	2.0
3	A	411	ILE	2.0
4	B	1050	ALA	2.0
3	A	302	LEU	2.0
4	B	1244	LEU	2.0
3	A	251	GLU	2.0
3	A	70	ALA	2.0
3	A	803	THR	2.0
4	B	932	GLY	2.0
3	A	178	PHE	2.0
3	A	846	GLN	2.0
3	A	329	LEU	2.0
3	A	464	GLU	2.0
3	A	735	ILE	2.0
3	A	445	SER	2.0
4	B	1202	MET	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.

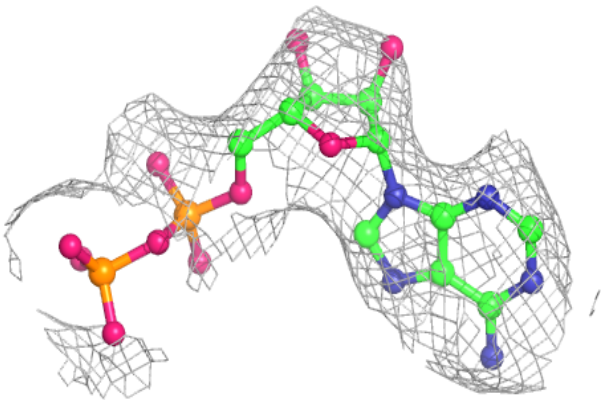
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ADP	A	936	27/27	0.90	0.20	70,71,73,73	0
6	ADP	B	202	27/27	0.92	0.24	79,80,81,81	0
5	MG	B	102	1/1	0.93	0.20	76,76,76,76	0
5	MG	A	935	1/1	0.95	0.43	100,100,100,100	0

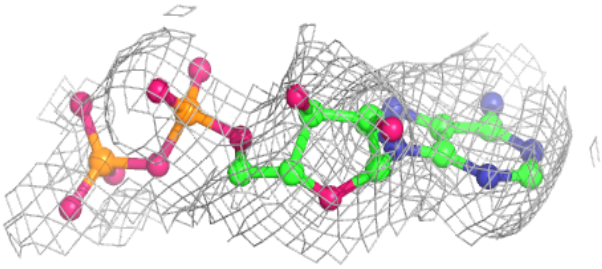
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

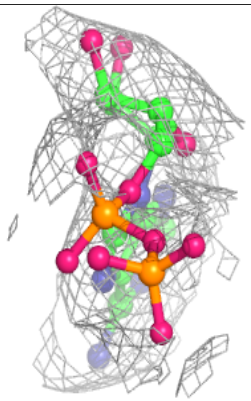
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

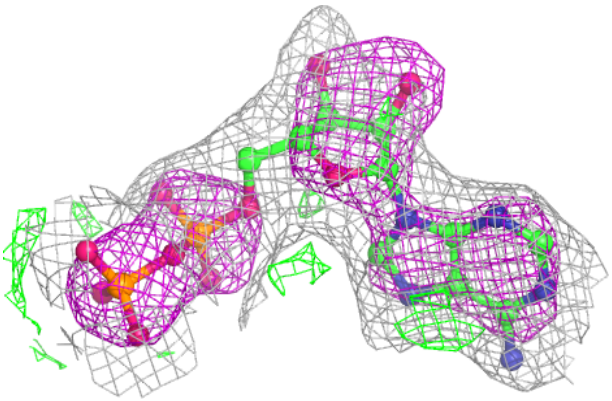


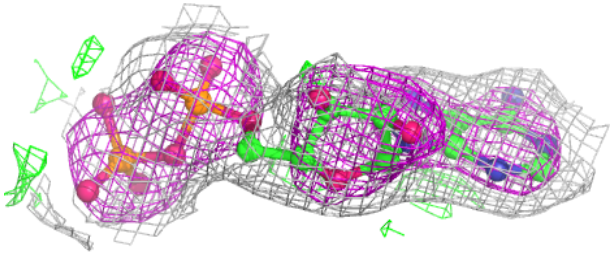


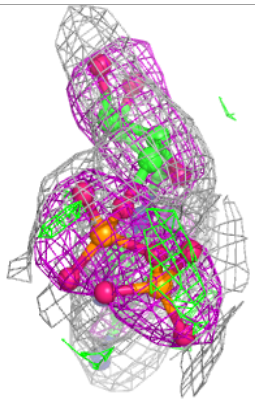


Electron density around ADP B 202:

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







6.5 Other polymers (i)

There are no such residues in this entry.