



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 04:54 pm BST

PDB ID : 8PO8
Title : Structure of Escherichia coli HrpA in complex with ADP and oligonucleotide poly(dC)11 forming an i-motif
Authors : Xin, B.G.; Yuan, L.G.; Zhang, L.L.; Xie, S.M.; Liu, N.N.; Ai, X.; Li, H.H.; Rety, S.; Xi, X.G.
Deposited on : 2023-07-03
Resolution : 2.52 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

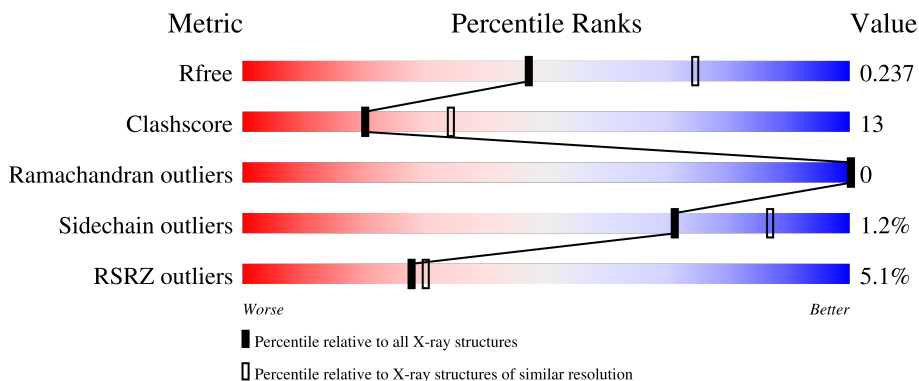
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	A	758	 2% 61% 18% 19%
1	B	758	 5% 60% 20% 15%
2	C	11	 45% 27% 64% 9%
2	D	11	 45% 36% 55% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10342 atoms, of which 8 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 protein called ATP-dependent RNA helicase HrpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	603	4812	3016	875	905	16	0	0	0
1	B	615	4920	3084	901	918	17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	ASN	ASP	conflict	UNP P43329
A	290	PRO	HIS	conflict	UNP P43329
B	162	ASN	ASP	conflict	UNP P43329
B	290	PRO	HIS	conflict	UNP P43329

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	11	209	99	33	66	11	0	0	0
2	D	10	190	90	30	60	10	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

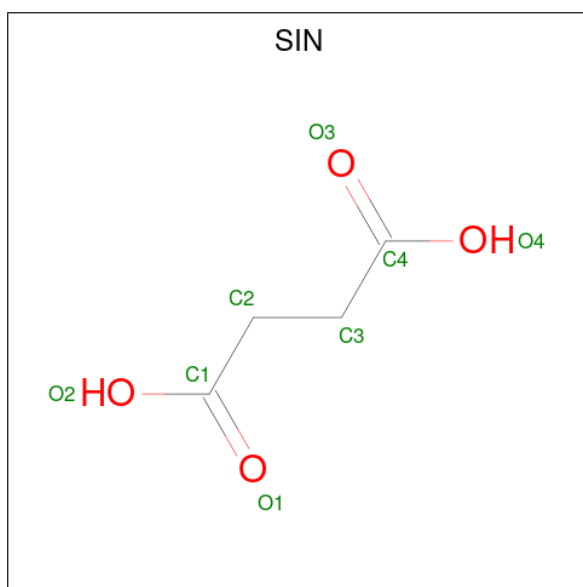


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	27	10	5	10	2	0	0
3	B	1	27	10	5	10	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

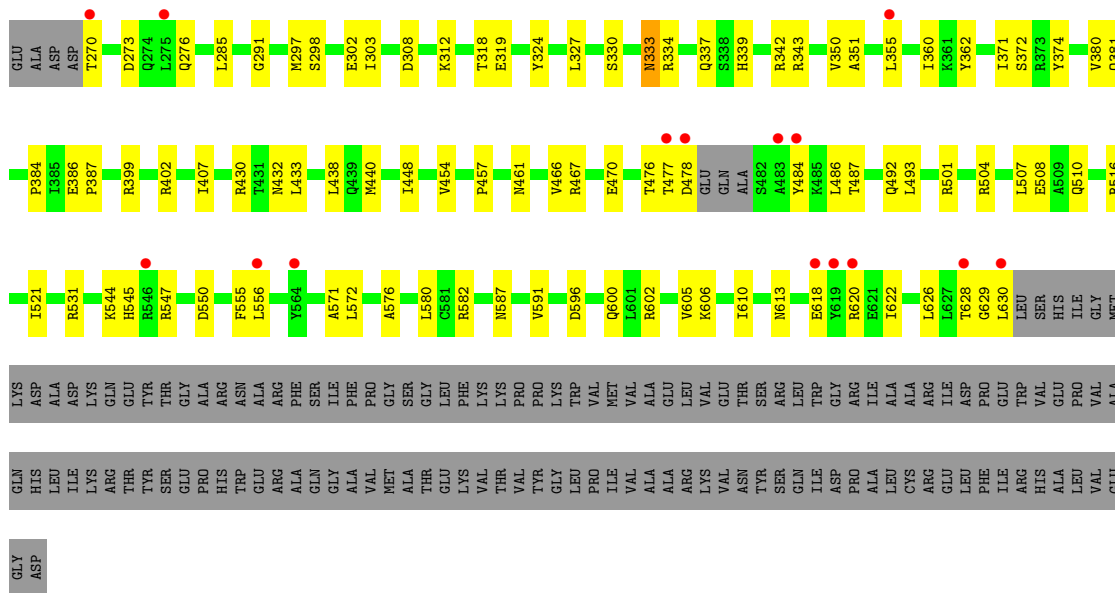
- Molecule 5 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).



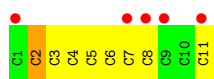
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
5	A	1	Total	C	H	O	0	0
			12	4	4	4		
5	A	1	Total	C	H	O	0	0
			12	4	4	4		

- Molecule 6 is water.

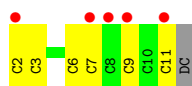
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total	O	0	0
			56	56		
6	B	73	Total	O	0	0
			73	73		
6	C	2	Total	O	0	0
			2	2		



● Molecule 2: DNA (5'-D(P*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')



● Molecule 2: DNA (5'-D(P*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.26Å 105.97Å 177.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.98 – 2.52 91.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	93.9 (63.98-2.52) 94.0 (91.00-2.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.210 , 0.243 0.207 , 0.237	Depositor DCC
R_{free} test set	2394 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10342	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	A	0.27	0/4887	0.52	0/6607
1	B	0.26	0/4998	0.53	0/6751
2	C	0.57	0/230	0.88	1/348 (0.3%)
2	D	0.52	0/209	0.74	0/316
All	All	0.28	0/10324	0.55	1/14022 (0.0%)

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
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	2	DC	OP1-P-OP2	5.01	127.12	119.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	478	ASP	Peptide
1	B	37	VAL	Peptide
1	B	38	LYS	Peptide

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	A	4812	0	4896	122	0
1	B	4920	0	5012	122	0
2	C	209	0	122	21	0
2	D	190	0	111	16	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	8	8	3	0
6	A	56	0	0	4	0
6	B	73	0	0	4	0
6	C	2	0	0	0	0
All	All	10334	8	10173	255	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 13.

All (255) 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)
1:B:508:GLU:HG2	1:B:628:THR:HG21	1.34	1.09
1:A:572:LEU:HD13	1:A:576:ALA:HB1	1.38	1.02
1:B:351:ALA:HA	1:B:355:LEU:HB2	1.47	0.96
1:A:370:ARG:HG2	1:A:385:ILE:HD13	1.52	0.92
1:B:501:ARG:HE	1:B:630:LEU:HD12	1.39	0.87
1:A:15:ARG:NH2	1:A:55:ASP:OD1	2.11	0.84
1:A:132:ARG:HB3	5:A:2004:SIN:H32	1.58	0.84
1:B:521:ILE:HD13	1:B:555:PHE:HB3	1.61	0.82
1:A:606:LYS:HG3	1:B:149:GLU:HG3	1.62	0.82
1:A:286:SER:HB3	1:A:342:ARG:HH12	1.43	0.82
1:A:29:ARG:CZ	2:C:11:DC:H3'	2.09	0.81
1:A:215:GLU:HG3	1:A:452:PRO:HG2	1.61	0.81
1:A:271:GLU:HG3	1:A:589:LEU:HD21	1.63	0.80
1:A:336:PHE:O	6:A:2101:HOH:O	1.98	0.80
1:B:213:LEU:HD13	1:B:225:ILE:HD12	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:SER:HB3	1:A:342:ARG:NH1	1.98	0.78
1:B:298:SER:OG	1:B:302:GLU:OE2	2.00	0.78
1:A:15:ARG:NH1	6:A:2102:HOH:O	2.11	0.77
1:B:433:LEU:HD12	1:B:461:ASN:HB2	1.65	0.77
1:B:433:LEU:HD21	1:B:457:PRO:HB2	1.68	0.75
1:A:370:ARG:HG2	1:A:385:ILE:CD1	2.16	0.75
1:B:571:ALA:O	6:B:2101:HOH:O	2.04	0.75
1:A:615:GLU:N	1:A:615:GLU:OE2	2.21	0.74
1:B:23:ASP:HA	2:C:8:DC:H41	1.51	0.74
1:B:501:ARG:NE	1:B:630:LEU:HD12	2.02	0.74
1:B:508:GLU:CG	1:B:628:THR:HG21	2.16	0.73
1:B:23:ASP:HA	2:C:8:DC:N4	2.03	0.73
1:B:297:MET:HE3	1:B:302:GLU:HG2	1.71	0.73
1:B:13:GLN:NE2	1:B:31:LEU:HD12	2.05	0.71
1:A:516:ARG:O	1:A:520:ILE:HG13	1.91	0.71
2:C:5:DC:H5''	2:C:5:DC:H6	1.56	0.71
1:B:185:ASP:OD1	6:B:2102:HOH:O	2.09	0.71
1:A:73:TYR:CE2	1:A:83:LYS:HD3	2.26	0.70
1:A:73:TYR:CZ	1:A:83:LYS:HD3	2.27	0.70
1:B:112:LYS:NZ	1:B:145:GLU:OE1	2.22	0.70
1:A:614:SER:HB2	1:A:615:GLU:OE2	1.91	0.69
1:B:57:ALA:O	1:B:60:LYS:HG2	1.92	0.69
1:A:383:LEU:HD23	1:A:597:ILE:HD12	1.75	0.69
1:B:297:MET:CE	1:B:302:GLU:HG2	2.23	0.69
1:B:26:ARG:HG3	2:D:11:DC:C5	2.28	0.69
1:B:433:LEU:HD12	1:B:461:ASN:CB	2.23	0.69
1:A:504:ARG:NH2	1:A:508:GLU:OE1	2.27	0.68
1:B:13:GLN:HE21	1:B:31:LEU:HD12	1.59	0.68
2:C:3:DC:H2''	2:C:11:DC:O2	1.95	0.67
1:B:37:VAL:HG22	1:B:43:GLN:NE2	2.10	0.67
1:A:29:ARG:HD3	2:C:11:DC:C2'	2.25	0.67
1:A:529:ASP:O	1:A:590:ARG:HD3	1.94	0.67
1:A:96:VAL:CG1	1:A:247:ILE:HD13	2.25	0.66
1:A:190:GLN:NE2	6:A:2104:HOH:O	2.27	0.66
1:A:350:VAL:HG22	1:A:355:LEU:HD12	1.77	0.66
1:B:470:GLU:OE2	1:B:477:THR:OG1	2.12	0.66
1:B:7:LEU:HD13	1:B:12:LEU:HD21	1.77	0.66
1:B:618:GLU:OE1	1:B:620:ARG:NH2	2.29	0.65
1:B:37:VAL:HG22	1:B:43:GLN:CD	2.17	0.65
1:A:29:ARG:NH1	2:C:11:DC:H3'	2.11	0.65
1:B:26:ARG:NH1	2:D:3:DC:N3	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ILE:HD12	1:A:622:ILE:H	1.61	0.64
1:A:477:THR:HG22	1:A:481:ALA:HA	1.80	0.64
1:A:356:THR:HG23	6:A:2103:HOH:O	1.97	0.64
1:B:184:GLN:NE2	2:D:9:DC:OP2	2.31	0.63
1:A:572:LEU:HD22	1:A:576:ALA:CB	2.29	0.63
1:B:605:VAL:HG13	1:B:610:ILE:HB	1.81	0.63
1:A:91:ARG:HB2	1:A:117:LEU:HD21	1.80	0.62
1:A:602:ARG:O	1:A:606:LYS:HD3	2.00	0.62
1:B:507:LEU:O	1:B:510:GLN:HG2	1.97	0.62
2:C:4:DC:O4'	2:C:11:DC:H1'	2.00	0.62
1:B:26:ARG:O	1:B:30:ARG:HB2	2.00	0.62
1:B:350:VAL:HG23	1:B:355:LEU:HD12	1.82	0.62
1:A:29:ARG:HD3	2:C:11:DC:H2'	1.81	0.61
1:A:324:TYR:H	1:A:327:LEU:HD13	1.65	0.61
1:B:319:GLU:OE1	1:B:334:ARG:NH1	2.34	0.61
1:A:271:GLU:HG3	1:A:589:LEU:CD2	2.30	0.61
1:A:605:VAL:HG13	1:A:610:ILE:HB	1.83	0.61
1:B:399:ARG:HE	1:B:399:ARG:HA	1.66	0.61
1:A:371:ILE:O	1:A:384:PRO:HD2	2.00	0.60
1:A:299:GLY:O	1:A:303:ILE:HG13	2.01	0.60
1:B:596:ASP:O	1:B:600:GLN:HG3	2.02	0.60
1:A:29:ARG:HD3	2:C:11:DC:C3'	2.31	0.60
2:C:4:DC:P	2:C:11:DC:H2''	2.42	0.60
2:D:2:DC:H2''	2:D:3:DC:H5'	1.83	0.60
1:A:96:VAL:HG13	1:A:247:ILE:HD13	1.82	0.59
1:A:383:LEU:HD23	1:A:597:ILE:CD1	2.32	0.59
1:A:477:THR:CG2	1:A:481:ALA:HA	2.31	0.59
1:A:485:LYS:HD3	2:C:7:DC:N3	2.18	0.59
1:B:34:VAL:CG1	1:B:43:GLN:HB3	2.33	0.58
1:A:78:PRO:O	1:A:82:LYS:HG3	2.03	0.58
1:A:563:ASN:O	1:A:567:GLU:HG3	2.04	0.57
1:B:374:TYR:CD1	1:B:432:ASN:HB3	2.39	0.57
1:B:291:GLY:O	1:B:342:ARG:HD3	2.04	0.57
1:B:508:GLU:HG2	1:B:628:THR:CG2	2.22	0.57
1:B:433:LEU:CD1	1:B:461:ASN:HB2	2.35	0.57
1:B:544:LYS:O	1:B:547:ARG:NE	2.38	0.56
1:A:213:LEU:O	1:A:217:LEU:HG	2.06	0.56
1:B:102:THR:HB	1:B:399:ARG:CZ	2.35	0.56
1:A:83:LYS:HG3	1:A:113:ILE:HG12	1.86	0.56
2:D:6:DC:H2''	2:D:7:DC:H5''	1.88	0.56
1:A:339:HIS:HB3	1:A:343:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:GLN:NE2	6:B:2108:HOH:O	2.39	0.55
1:A:247:ILE:HD12	1:A:247:ILE:N	2.21	0.55
1:B:199:ALA:HA	1:B:206:ILE:HD13	1.88	0.55
1:B:21:LEU:HD11	1:B:192:ASP:HB3	1.87	0.55
1:B:399:ARG:HA	1:B:399:ARG:NE	2.22	0.54
1:A:159:ARG:HG3	5:A:2004:SIN:C1	2.37	0.54
1:A:583:THR:HG22	1:A:583:THR:O	2.07	0.54
1:A:572:LEU:HD22	1:A:576:ALA:HB3	1.87	0.54
1:B:572:LEU:HD22	1:B:576:ALA:HB1	1.89	0.54
1:B:58:ALA:O	1:B:62:LEU:HD23	2.07	0.54
1:B:19:LEU:HD11	1:B:54:ILE:HG23	1.89	0.54
1:B:285:LEU:HD13	1:B:362:TYR:HB3	1.90	0.54
2:C:3:DC:O3'	2:C:11:DC:H2''	2.08	0.54
1:B:477:THR:O	1:B:478:ASP:HB3	2.09	0.53
1:A:572:LEU:HD13	1:A:576:ALA:CB	2.25	0.53
1:A:363:VAL:HG23	1:A:400:CYS:HB3	1.91	0.53
1:A:271:GLU:CG	1:A:589:LEU:HD21	2.33	0.53
1:A:497:PRO:CD	1:A:604:VAL:HG11	2.39	0.53
1:B:351:ALA:CA	1:B:355:LEU:HB2	2.31	0.53
1:A:334:ARG:HA	1:A:337:GLN:OE1	2.09	0.53
1:B:440:MET:SD	1:B:448:ILE:HG13	2.50	0.52
1:B:16:LEU:HB3	1:B:24:ARG:HG3	1.90	0.52
1:A:69:PRO:CG	1:A:115:MET:HE1	2.38	0.52
1:A:29:ARG:NE	2:C:11:DC:H3'	2.23	0.52
1:A:622:ILE:HD12	1:A:622:ILE:N	2.24	0.52
1:B:587:ASN:O	1:B:591:VAL:HG23	2.09	0.52
1:B:262:PRO:O	1:B:263:ILE:HG12	2.10	0.52
1:B:44:GLN:O	1:B:48:GLN:HG2	2.10	0.51
1:B:476:THR:HG23	1:B:487:THR:HG22	1.92	0.51
1:B:26:ARG:HG3	2:D:11:DC:C6	2.44	0.51
1:B:34:VAL:O	1:B:43:GLN:NE2	2.44	0.51
1:B:622:ILE:O	1:B:626:LEU:HG	2.11	0.51
2:C:5:DC:H6	2:C:5:DC:C5'	2.22	0.51
1:A:516:ARG:NH1	1:A:517:GLU:OE2	2.43	0.50
1:A:399:ARG:HA	1:A:399:ARG:NE	2.26	0.50
1:A:399:ARG:HA	1:A:399:ARG:HE	1.77	0.50
1:B:34:VAL:HG11	1:B:47:PHE:CE1	2.47	0.50
1:A:606:LYS:CG	1:B:149:GLU:HG3	2.39	0.50
1:B:516:ARG:HB3	1:B:613:ASN:ND2	2.27	0.49
1:A:99:ALA:O	1:A:248:GLU:HA	2.11	0.49
1:A:159:ARG:HD3	5:A:2004:SIN:H22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ARG:NH1	1:A:616:PRO:HA	2.27	0.49
1:B:30:ARG:HH21	2:D:3:DC:N4	2.10	0.49
1:B:339:HIS:HB3	1:B:343:ARG:NH2	2.28	0.49
1:B:371:ILE:O	1:B:384:PRO:HD2	2.12	0.49
1:A:331:GLU:O	1:A:334:ARG:HG2	2.12	0.49
1:A:464:ASP:OD1	1:A:467:ARG:NH2	2.42	0.49
1:B:99:ALA:O	1:B:248:GLU:HA	2.12	0.49
2:D:6:DC:H2''	2:D:7:DC:OP1	2.12	0.49
1:B:476:THR:HG23	1:B:487:THR:CG2	2.43	0.49
1:B:493:LEU:HD21	1:B:504:ARG:HA	1.93	0.49
1:A:29:ARG:HD3	2:C:11:DC:H3'	1.95	0.49
1:B:26:ARG:HG2	2:D:3:DC:O2	2.12	0.49
1:B:129:GLN:O	1:B:174:THR:HA	2.13	0.49
1:B:34:VAL:HG12	1:B:43:GLN:HB3	1.94	0.48
1:B:152:GLY:O	1:B:168:THR:HA	2.13	0.48
1:B:372:SER:O	1:B:430:ARG:HD2	2.13	0.48
2:C:6:DC:H2''	2:C:7:DC:H4'	1.95	0.48
1:A:318:THR:HA	1:A:342:ARG:O	2.13	0.48
1:A:584:ASP:OD1	1:A:585:TYR:N	2.46	0.48
1:A:587:ASN:O	1:A:591:VAL:HG23	2.13	0.48
1:A:278:ILE:O	1:A:282:VAL:HG23	2.13	0.48
1:B:23:ASP:OD2	1:B:60:LYS:HD3	2.12	0.48
1:B:466:VAL:HG13	1:B:484:TYR:HE1	1.77	0.48
1:A:561:LEU:HD11	1:A:565:LEU:HD11	1.96	0.48
1:A:402:ARG:HG3	1:A:403:VAL:HG13	1.96	0.48
1:B:516:ARG:HB3	1:B:613:ASN:HD21	1.79	0.48
1:B:273:ASP:HB3	1:B:276:GLN:HB2	1.96	0.48
1:B:550:ASP:OD2	1:B:556:LEU:HD12	2.14	0.48
1:A:73:TYR:CZ	1:A:83:LYS:CD	2.96	0.48
1:B:360:ILE:O	1:B:402:ARG:HD3	2.15	0.47
1:B:324:TYR:HD2	1:B:327:LEU:HD21	1.80	0.47
1:B:297:MET:HE3	1:B:302:GLU:CG	2.41	0.47
1:B:629:GLY:O	1:B:630:LEU:HG	2.15	0.47
1:B:330:SER:HA	1:B:333:ASN:OD1	2.14	0.46
2:D:6:DC:H4'	2:D:7:DC:OP1	2.14	0.46
1:A:29:ARG:CD	2:C:11:DC:H3'	2.46	0.46
1:A:294:LEU:HB2	1:A:360:ILE:HD12	1.96	0.46
1:B:318:THR:HA	1:B:342:ARG:O	2.15	0.46
1:A:488:PRO:HG2	1:B:56:GLN:HB3	1.97	0.46
1:A:73:TYR:CE2	1:A:83:LYS:CD	2.98	0.46
1:B:580:LEU:HD13	1:B:580:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:HA	1:B:467:ARG:HD3	1.69	0.46
1:A:83:LYS:HB3	1:A:83:LYS:HE3	1.61	0.46
2:D:2:DC:H5'	2:D:2:DC:C6	2.50	0.46
1:A:596:ASP:O	1:A:600:GLN:HG2	2.16	0.46
1:B:240:HIS:CG	1:B:454:VAL:HG22	2.50	0.46
1:B:362:TYR:HD1	1:B:407:ILE:HB	1.81	0.46
1:B:438:LEU:HD12	1:B:486:LEU:HD21	1.98	0.46
1:A:386:GLU:HB2	1:A:387:PRO:HD2	1.98	0.45
1:A:572:LEU:CD2	1:A:573:SER:H	2.28	0.45
1:B:79:VAL:HG23	1:B:104:SER:O	2.16	0.45
1:A:279:PHE:HE1	1:A:310:LEU:HD23	1.81	0.45
1:A:576:ALA:O	1:A:580:LEU:HG	2.16	0.45
1:B:26:ARG:HG3	2:D:11:DC:C4	2.51	0.45
1:A:352:GLU:O	1:A:399:ARG:HD2	2.16	0.45
1:B:34:VAL:HG22	2:D:2:DC:O4'	2.17	0.45
2:D:6:DC:C2'	2:D:7:DC:H5''	2.47	0.45
1:A:618:GLU:O	1:A:621:GLU:HB2	2.17	0.45
1:B:7:LEU:CD1	1:B:12:LEU:HD21	2.46	0.45
1:A:265:GLU:HA	1:A:273:ASP:OD2	2.17	0.45
1:B:49:GLU:OE1	1:B:49:GLU:HA	2.17	0.45
1:A:279:PHE:CE1	1:A:310:LEU:HD23	2.52	0.45
1:A:279:PHE:CD1	1:A:313:LEU:HD11	2.52	0.44
1:B:333:ASN:O	1:B:337:GLN:HG3	2.16	0.44
1:A:527:ILE:HD12	1:A:528:GLN:N	2.32	0.44
1:B:531:ARG:HB3	1:B:545:HIS:CD2	2.52	0.44
1:B:27:PHE:HE1	1:B:30:ARG:NH1	2.16	0.44
1:A:519:MET:HE1	1:A:612:VAL:CG2	2.48	0.44
1:B:128:THR:HA	1:B:173:MET:O	2.18	0.44
1:B:259:ARG:NH2	1:B:407:ILE:HD13	2.33	0.44
1:A:87:LEU:HG	1:A:117:LEU:HG	2.00	0.44
1:B:380:VAL:HG12	1:B:381:GLN:O	2.18	0.44
1:B:40:PRO:HB2	1:B:44:GLN:NE2	2.33	0.43
1:A:371:ILE:HG22	1:A:386:GLU:HG2	2.01	0.43
2:C:6:DC:O3'	2:C:7:DC:H4'	2.18	0.43
1:A:156:TYR:HA	1:A:172:LEU:O	2.18	0.43
1:A:373:ARG:NH2	1:A:386:GLU:OE2	2.45	0.43
1:A:587:ASN:OD1	1:A:589:LEU:HB2	2.18	0.43
1:B:297:MET:HG3	1:B:303:ILE:CG1	2.49	0.43
1:B:27:PHE:HD1	1:B:30:ARG:HD2	1.83	0.43
1:B:198:GLU:OE1	6:B:2103:HOH:O	2.21	0.43
1:A:478:ASP:OD2	2:C:7:DC:N3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HA	1:A:332:GLN:HB3	2.01	0.43
1:A:25:LEU:HD22	1:A:189:MET:HG3	1.99	0.43
1:B:132:ARG:HG3	1:B:133:LEU:N	2.34	0.43
1:B:297:MET:HG3	1:B:303:ILE:HG12	2.00	0.43
1:A:30:ARG:HB3	2:C:2:DC:O2	2.18	0.42
1:A:215:GLU:HG3	1:A:452:PRO:CG	2.39	0.42
1:A:432:ASN:OD1	1:A:434:ALA:HB3	2.19	0.42
1:A:163:HIS:CE1	1:B:160:PHE:HB3	2.54	0.42
1:B:602:ARG:O	1:B:606:LYS:HG3	2.20	0.42
1:B:120:GLY:HA2	1:B:123:GLY:O	2.19	0.42
2:D:2:DC:H5'	2:D:2:DC:H6	1.85	0.42
1:B:62:LEU:HD13	1:B:62:LEU:HA	1.91	0.42
1:B:312:LYS:HB3	1:B:312:LYS:HE2	1.85	0.42
1:A:69:PRO:CD	1:A:115:MET:HE1	2.49	0.42
1:A:267:ALA:O	1:A:268:ASP:HB3	2.19	0.42
1:A:281:ALA:HB3	1:A:364:ILE:HD13	2.02	0.42
1:B:477:THR:O	1:B:478:ASP:CB	2.68	0.42
1:A:69:PRO:HD2	1:A:115:MET:CE	2.49	0.42
1:A:292:ASP:OD2	1:A:339:HIS:NE2	2.44	0.42
1:B:386:GLU:HB2	1:B:387:PRO:HD2	2.02	0.42
1:A:378:THR:O	1:A:380:VAL:HG23	2.19	0.41
1:B:115:MET:HG2	1:B:169:MET:HE2	2.01	0.41
1:A:380:VAL:HA	1:A:499:ASP:OD2	2.21	0.41
1:A:42:ALA:O	1:A:46:ILE:HG13	2.20	0.41
1:B:50:MET:HE2	2:D:2:DC:O2	2.21	0.41
1:A:248:GLU:OE2	1:A:250:SER:OG	2.35	0.41
1:A:527:ILE:HD12	1:A:527:ILE:C	2.41	0.41
1:B:270:THR:O	1:B:582:ARG:NH1	2.54	0.41
1:A:377:ARG:HE	1:A:378:THR:HG23	1.86	0.40
1:A:555:PHE:O	1:A:558:PHE:HB2	2.21	0.40
1:A:44:GLN:O	1:A:48:GLN:HG2	2.21	0.40
1:A:248:GLU:OE2	1:A:250:SER:CB	2.69	0.40
1:A:210:LEU:CD2	1:A:227:ILE:HD12	2.51	0.40
1:A:511:LYS:HB2	1:A:512:HIS:ND1	2.36	0.40
1:B:371:ILE:HD11	1:B:430:ARG:NE	2.36	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	
1	A	599/758 (79%)	592 (99%)	7 (1%)	0	100	100
1	B	609/758 (80%)	598 (98%)	11 (2%)	0	100	100
All	All	1208/1516 (80%)	1190 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	526/657 (80%)	518 (98%)	8 (2%)	65	83
1	B	538/657 (82%)	533 (99%)	5 (1%)	78	91
All	All	1064/1314 (81%)	1051 (99%)	13 (1%)	71	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	175	ASP
1	A	271	GLU
1	A	329	ASN
1	A	487	THR
1	A	504	ARG
1	A	528	GLN
1	A	572	LEU

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Mol	Chain	Res	Type
1	B	9	PHE
1	B	46	ILE
1	B	229	SER
1	B	308	ASP
1	B	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	B	13	GLN
1	B	43	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
5	SIN	A	2004	-	7,7,7	1.01	0	8,8,8	1.58	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	2001	4	24,29,29	0.98	1 (4%)	29,45,45	1.31	5 (17%)
3	ADP	B	2001	4	24,29,29	0.94	1 (4%)	29,45,45	1.39	4 (13%)
5	SIN	A	2003	-	7,7,7	1.08	0	8,8,8	1.67	2 (25%)

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
5	SIN	A	2004	-	-	3/5/5/5	-
3	ADP	A	2001	4	-	3/12/32/32	0/3/3/3
3	ADP	B	2001	4	-	0/12/32/32	0/3/3/3
5	SIN	A	2003	-	-	3/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	ADP	C5-C4	2.53	1.47	1.40
3	B	2001	ADP	C5-C4	2.45	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	ADP	N3-C2-N1	-3.44	123.30	128.68
3	B	2001	ADP	N3-C2-N1	-3.23	123.64	128.68
3	B	2001	ADP	C3'-C2'-C1'	3.14	105.70	100.98
3	B	2001	ADP	C4-C5-N7	-2.58	106.71	109.40
3	A	2001	ADP	C3'-C2'-C1'	2.48	104.70	100.98
3	B	2001	ADP	PA-O3A-PB	-2.48	124.33	132.83
3	A	2001	ADP	C4-C5-N7	-2.31	106.99	109.40
5	A	2004	SIN	O2-C1-C2	2.24	121.24	114.03
5	A	2003	SIN	O2-C1-O1	-2.24	117.73	123.30
3	A	2001	ADP	PA-O3A-PB	-2.23	125.19	132.83
5	A	2003	SIN	O2-C1-C2	2.10	120.77	114.03
3	A	2001	ADP	C2-N1-C6	2.08	122.31	118.75

There are no chirality outliers.

All (9) torsion outliers are listed below:

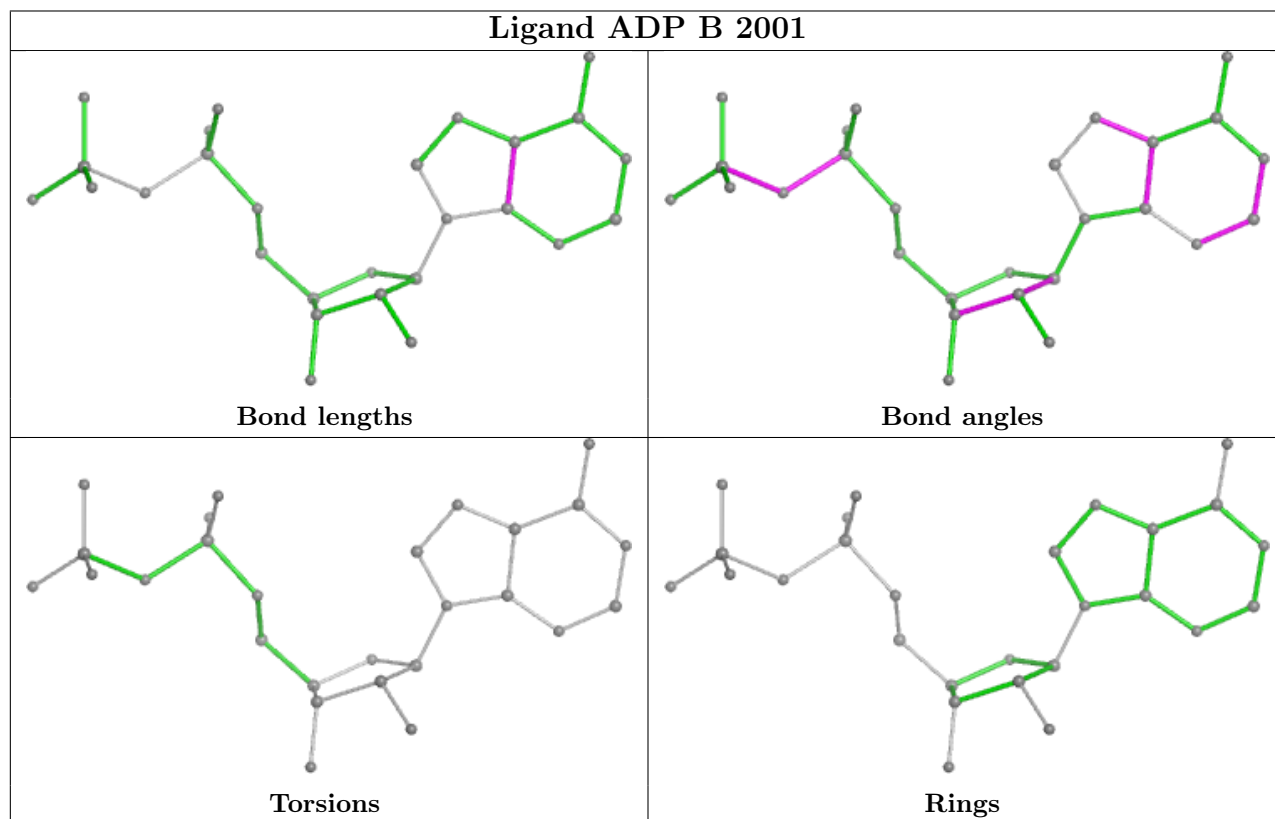
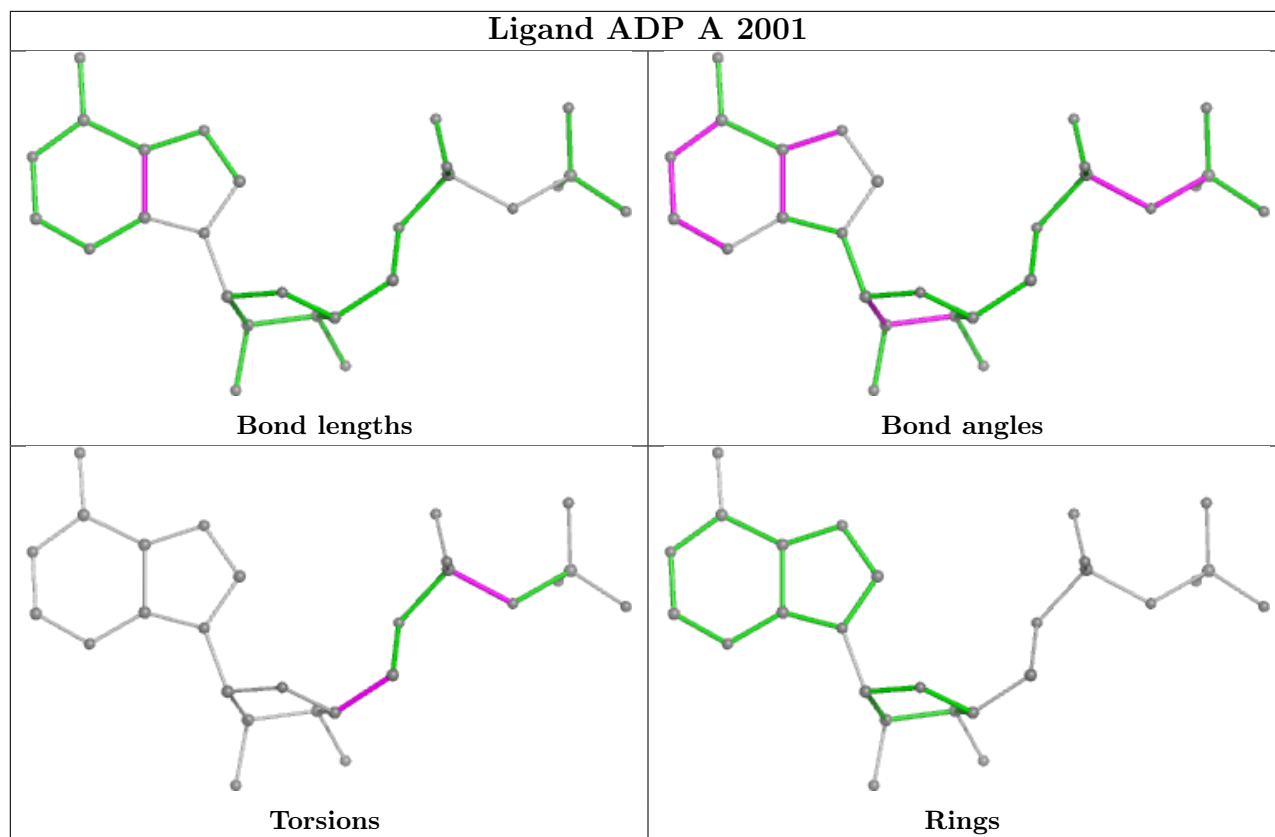
Mol	Chain	Res	Type	Atoms
5	A	2003	SIN	C1-C2-C3-C4
5	A	2004	SIN	C1-C2-C3-C4
3	A	2001	ADP	O4'-C4'-C5'-O5'
5	A	2003	SIN	O1-C1-C2-C3
3	A	2001	ADP	C3'-C4'-C5'-O5'
5	A	2003	SIN	O2-C1-C2-C3
5	A	2004	SIN	O1-C1-C2-C3
5	A	2004	SIN	O2-C1-C2-C3
3	A	2001	ADP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2004	SIN	3	0

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	A	603/758 (79%)	0.24	18 (2%) 50 54	29, 50, 107, 176	0
1	B	615/758 (81%)	0.32	35 (5%) 23 25	27, 51, 117, 159	0
2	C	11/11 (100%)	1.94	5 (45%) 0 0	75, 109, 143, 183	0
2	D	10/11 (90%)	1.94	5 (50%) 0 0	109, 114, 128, 141	0
All	All	1239/1538 (80%)	0.31	63 (5%) 28 30	27, 51, 115, 183	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	619	TYR	9.6
1	A	481	ALA	8.7
1	B	37	VAL	7.7
1	A	479	GLU	6.9
1	A	480	GLN	6.6
1	B	38	LYS	5.7
1	B	43	GLN	5.3
1	A	478	ASP	5.3
1	B	34	VAL	5.0
2	C	7	DC	5.0
1	B	478	ASP	4.8
1	B	619	TYR	4.6
1	A	620	ARG	4.3
1	B	36	LYS	4.1
1	B	47	PHE	4.0
1	A	4	GLN	3.9
1	B	39	ASN	3.9
1	B	477	THR	3.8
1	B	29	ARG	3.7
1	B	628	THR	3.7
2	C	11	DC	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	9	PHE	3.6
1	B	7	LEU	3.3
1	B	32	HIS	3.3
1	A	327	LEU	3.2
1	B	355	LEU	3.2
1	B	35	LYS	3.2
2	C	1	DC	3.1
2	D	9	DC	2.9
1	B	484	TYR	2.9
1	B	620	ARG	2.9
2	D	7	DC	2.8
1	B	50	MET	2.8
1	B	28	SER	2.8
1	B	25	LEU	2.8
1	B	270	THR	2.8
1	B	22	ARG	2.8
1	A	483	ALA	2.7
1	B	630	LEU	2.6
1	A	585	TYR	2.6
1	A	485	LYS	2.5
1	A	531	ARG	2.5
1	B	618	GLU	2.5
1	B	12	LEU	2.4
2	D	2	DC	2.4
1	A	484	TYR	2.4
2	D	11	DC	2.4
2	C	9	DC	2.4
1	B	8	THR	2.3
1	B	275	LEU	2.3
2	C	8	DC	2.3
1	A	578	ARG	2.2
1	A	272	ARG	2.2
1	A	618	GLU	2.2
1	B	483	ALA	2.2
1	B	564	TYR	2.2
1	A	477	THR	2.2
1	B	14	GLN	2.1
1	B	21	LEU	2.1
1	A	590	ARG	2.1
1	B	556	LEU	2.1
2	D	8	DC	2.0
1	B	546	ARG	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](#)

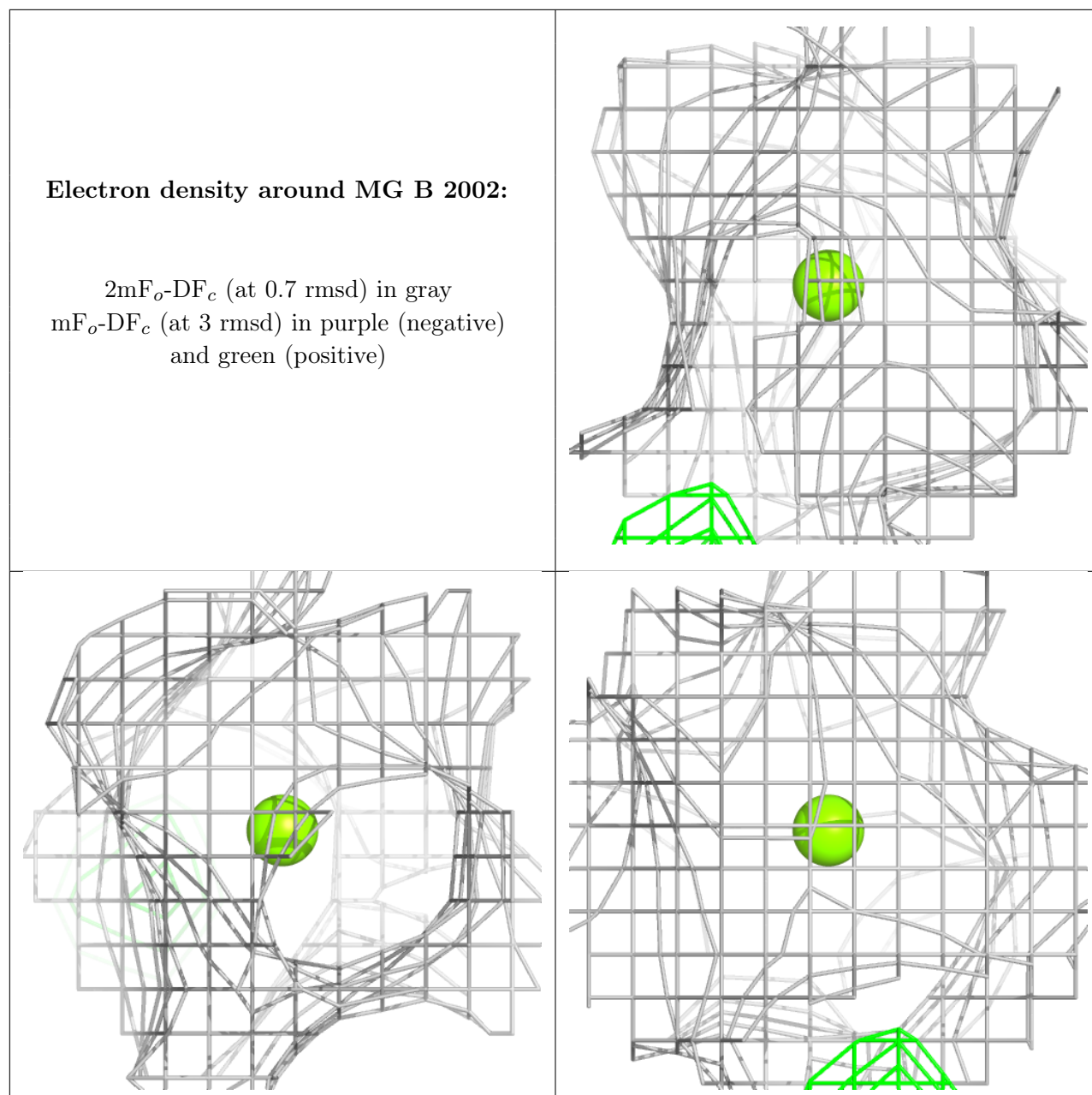
There are no monosaccharides in this entry.

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.

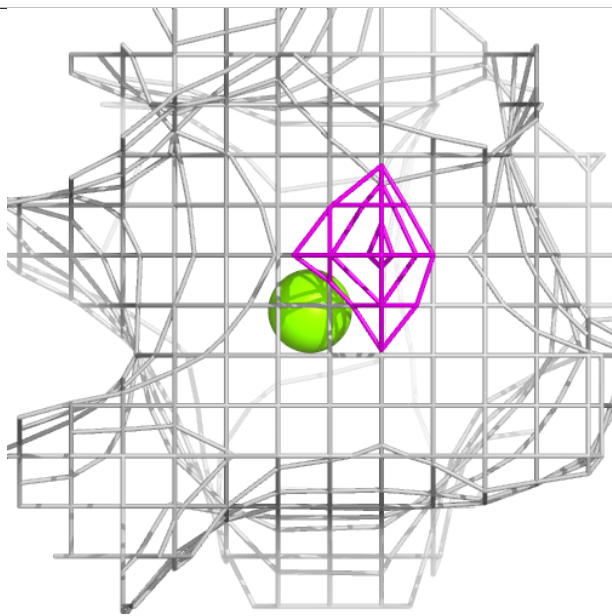
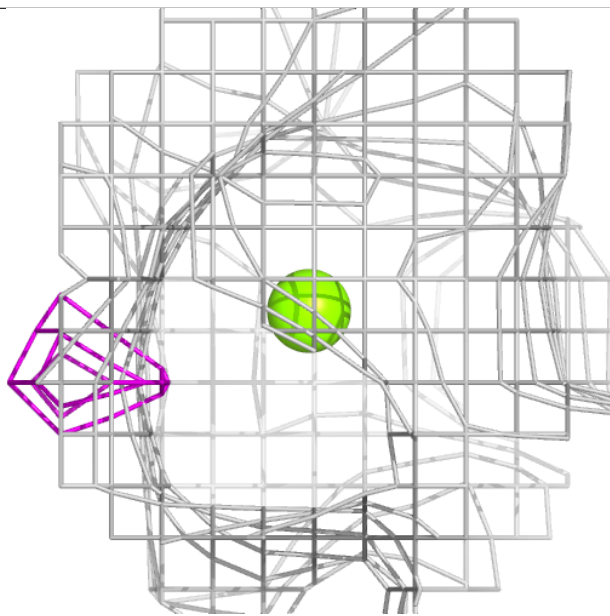
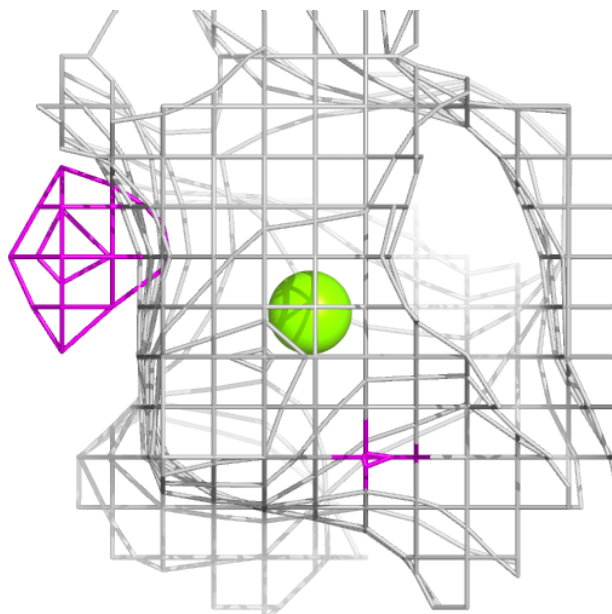
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SIN	A	2004	8/8	0.79	0.30	48,60,70,70	0
5	SIN	A	2003	8/8	0.82	0.48	43,52,56,56	0
4	MG	B	2002	1/1	0.93	0.13	36,36,36,36	0
4	MG	A	2002	1/1	0.94	0.12	37,37,37,37	0
3	ADP	A	2001	27/27	0.97	0.17	33,50,54,58	0
3	ADP	B	2001	27/27	0.97	0.18	29,45,51,54	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.



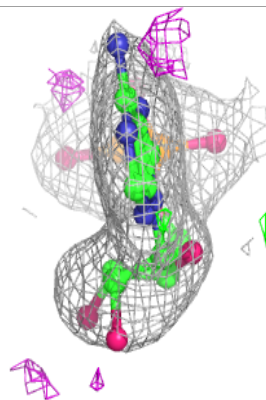
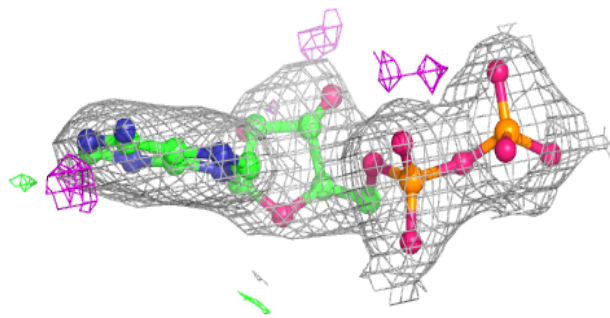
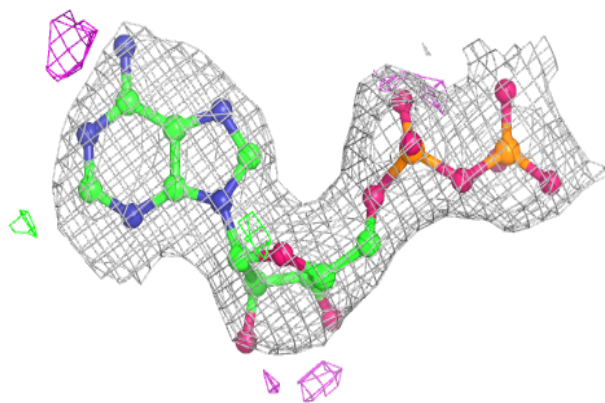
Electron density around MG A 2002:

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

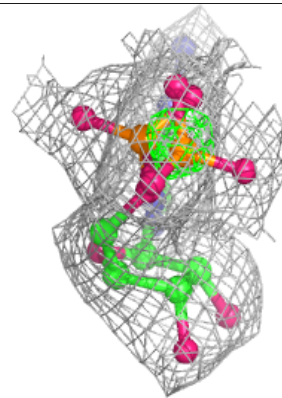
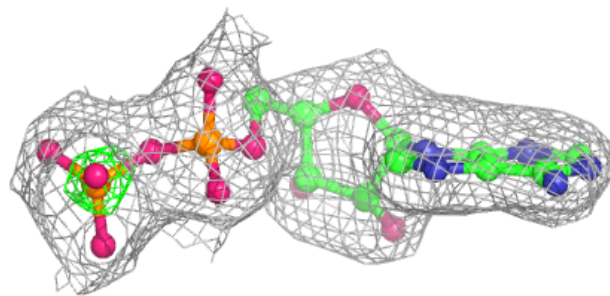
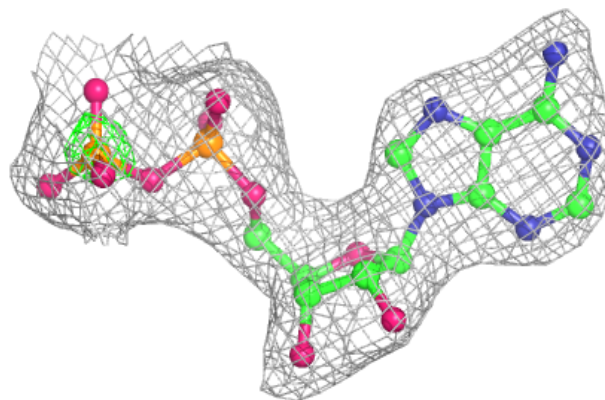


Electron density around ADP A 2001:

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

**Electron density around ADP B 2001:**

$2mF_o-DF_c$ (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.