



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:43 AM UTC

PDB ID : 4A1Z / pdb_00004a1z
Title : Eg5-1
Authors : Talapatra, S.K.; Kozielski, F.
Deposited on : 2011-09-20
Resolution : 2.80 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

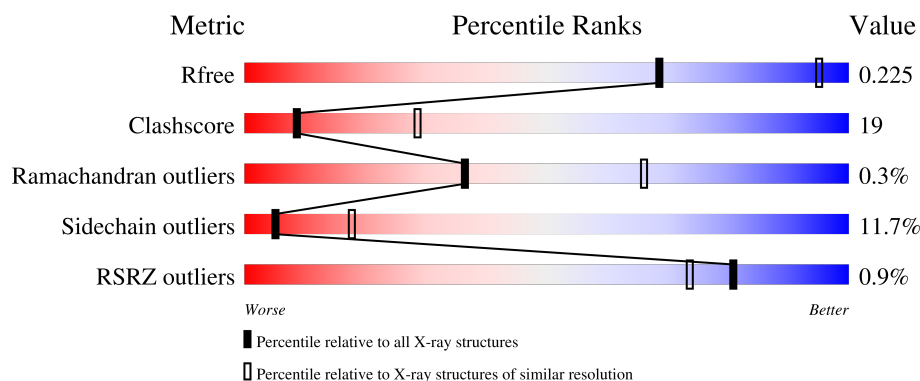
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	368	% 56% 25% 8% 11%
1	B	368	% 55% 27% 5% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	A	2000	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5255 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 protein called KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	1	0
			2521	1587	434	490	10			
1	B	321	Total	C	N	O	S	0	0	0
			2500	1572	436	482	10			

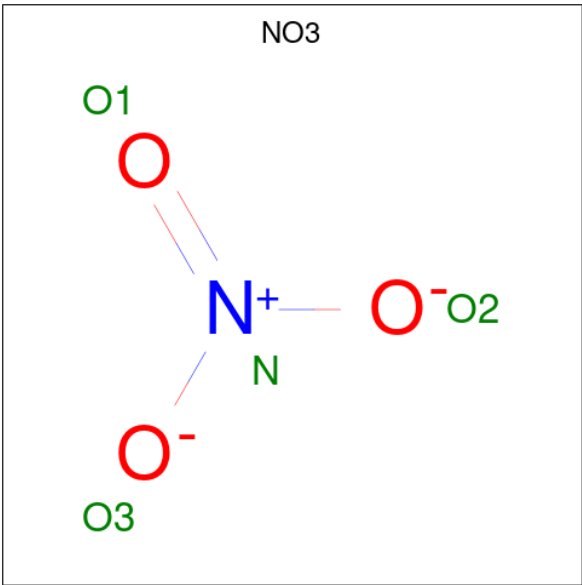
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	VAL	ASP	engineered mutation	UNP P52732
B	130	VAL	ASP	engineered mutation	UNP P52732

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

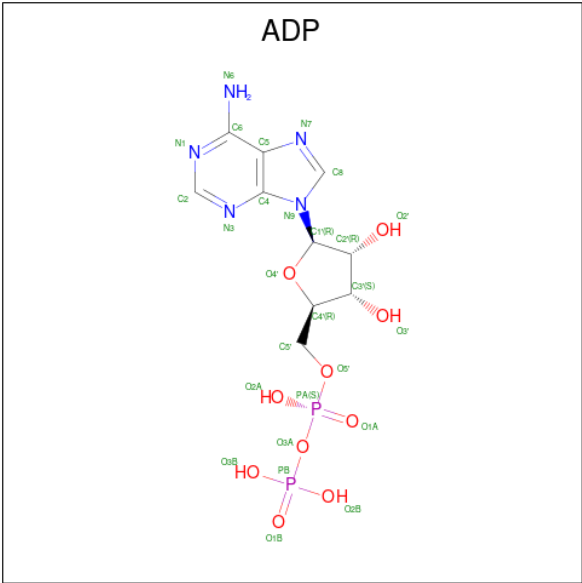
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total 89	O 89	0	0
5	B	81	Total 81	O 81	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.48Å 78.39Å 93.27Å 90.00° 93.47° 90.00°	Depositor
Resolution (Å)	29.23 – 2.80 29.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.23-2.80) 99.8 (29.23-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.173 , 0.257 (Not available) , 0.225	Depositor DCC
R_{free} test set	941 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5255	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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, NO3, 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	A	0.69	0/2559	1.10	11/3463 (0.3%)
1	B	0.75	0/2535	1.09	7/3426 (0.2%)
All	All	0.72	0/5094	1.10	18/6889 (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
1	B	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	362	LYS	CA-C-N	7.42	127.47	119.90
1	B	362	LYS	C-N-CA	7.42	127.47	119.90
1	A	180	GLU	N-CA-C	7.41	120.28	111.02
1	A	362	LYS	CA-C-N	7.38	129.06	119.84
1	A	362	LYS	C-N-CA	7.38	129.06	119.84
1	A	84	SER	N-CA-C	6.33	117.97	111.14
1	B	323	SER	N-CA-C	-5.97	98.08	110.80
1	B	235	SER	N-CA-C	5.93	118.71	109.52
1	A	229	ASN	CA-C-N	-5.84	114.74	122.85
1	A	229	ASN	C-N-CA	-5.84	114.74	122.85
1	A	127	TRP	N-CA-C	5.71	117.30	111.14
1	A	177	ASP	N-CA-C	-5.43	98.43	107.99
1	A	110	GLY	N-CA-C	5.38	123.84	115.72
1	B	227	LEU	N-CA-C	5.30	118.21	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLY	N-CA-C	5.17	124.80	115.80
1	A	154	PHE	N-CA-C	5.13	116.64	108.79
1	B	135	ILE	N-CA-C	5.08	115.30	110.42
1	B	193	GLY	N-CA-C	5.02	118.97	112.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	325	GLY	Peptide

5.2 Too-close contacts ⓘ

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	2521	0	2531	103	0
1	B	2500	0	2527	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	3	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	89	0	0	7	0
5	B	81	0	0	6	0
All	All	5255	0	5082	191	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 19.

All (191) 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:A:304:GLU:HB2	1:A:306:THR:HG23	1.34	1.05
1:B:53:ARG:HH11	1:B:53:ARG:HG3	1.27	0.99
1:A:206:ASN:HD21	1:A:208:ASP:HB2	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:SER:HB2	1:A:181:ARG:NH2	1.87	0.90
1:A:312:ARG:H	1:A:312:ARG:HD3	1.38	0.89
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.53	0.89
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.55	0.88
1:A:249:THR:HB	1:A:252:GLY:HA3	1.57	0.87
1:B:73:GLY:O	1:B:76:THR:HG23	1.78	0.83
1:B:362:LYS:H	1:B:362:LYS:NZ	1.75	0.83
1:A:305:ARG:HG2	1:A:305:ARG:HH11	1.48	0.79
1:B:105:GLY:C	1:B:269:SER:HB2	2.08	0.79
1:A:312:ARG:HD3	1:A:312:ARG:N	1.98	0.79
1:A:127:TRP:CZ2	1:A:145:GLU:HG3	2.19	0.77
1:A:169:PHE:CE1	1:A:228:MET:HE1	2.20	0.76
1:B:168:LEU:O	1:B:181:ARG:HB2	1.84	0.76
1:B:344:GLU:H	1:B:344:GLU:CD	1.94	0.76
1:A:304:GLU:HB2	1:A:306:THR:CG2	2.15	0.74
1:B:53:ARG:HH11	1:B:53:ARG:CG	1.99	0.74
1:B:40:ILE:HD12	1:B:41:VAL:HG23	1.70	0.73
1:A:57:LEU:HB2	1:B:164:TYR:HE2	1.54	0.71
1:A:100:THR:HG23	1:A:262:ASN:HB2	1.70	0.71
1:A:223:THR:HG23	1:A:227:LEU:HD23	1.72	0.71
1:B:17:LYS:HG3	1:B:18:ASN:H	1.56	0.70
1:A:127:TRP:CH2	1:A:145:GLU:HG3	2.28	0.69
1:A:305:ARG:HH11	1:A:305:ARG:CG	2.04	0.69
1:A:305:ARG:HG2	1:A:305:ARG:NH1	2.05	0.67
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.76	0.66
1:B:362:LYS:H	1:B:362:LYS:HZ2	1.39	0.66
1:A:146:LYS:O	1:A:150:ASN:HB2	1.96	0.65
1:A:206:ASN:HD21	1:A:208:ASP:CB	2.07	0.65
1:A:143:ILE:CD1	1:A:243:ILE:HD11	2.27	0.65
1:A:179:SER:HB2	1:A:181:ARG:HH21	1.60	0.64
1:B:321:GLN:HG2	1:B:321:GLN:O	1.98	0.64
1:B:311:TYR:CG	1:B:321:GLN:HG3	2.33	0.63
1:A:264:VAL:HG21	1:A:320:LEU:HD11	1.79	0.63
1:A:362:LYS:HG2	5:A:2020:HOH:O	1.98	0.63
1:A:58:ALA:HB2	1:B:228:MET:CE	2.29	0.63
1:B:272:ILE:HG23	1:B:293:LEU:HD21	1.81	0.63
1:A:169:PHE:CZ	1:A:228:MET:HE1	2.34	0.62
1:B:184:MET:HE2	1:B:194:VAL:HG21	1.82	0.61
1:B:362:LYS:NZ	1:B:362:LYS:N	2.49	0.60
1:A:172:LEU:HB2	5:A:2064:HOH:O	2.02	0.59
1:A:187:ASP:HB2	1:A:195:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLN:HA	1:B:293:LEU:HD23	1.84	0.59
1:A:161:LEU:HD12	1:A:161:LEU:O	2.01	0.59
1:B:311:TYR:CD1	1:B:321:GLN:HG3	2.38	0.59
1:A:87:CYS:HB2	1:A:88:PRO:HD3	1.84	0.58
1:A:340:SER:OG	3:A:2000:NO3:O1	2.15	0.58
1:B:143:ILE:CD1	1:B:243:ILE:HD11	2.33	0.58
1:B:243:ILE:HG22	1:B:245:MET:HG3	1.86	0.57
1:A:117:GLY:O	1:A:118:GLU:HG3	2.05	0.57
1:A:298:VAL:HG21	1:A:317:THR:HG21	1.86	0.56
1:A:172:LEU:HD13	1:A:202:ILE:HG12	1.87	0.56
1:B:357:LYS:HE2	1:B:359:ILE:HD11	1.87	0.56
1:A:179:SER:HB2	1:A:181:ARG:HH22	1.71	0.56
1:A:30:LEU:HG	1:A:34:LYS:HE3	1.88	0.56
1:A:21:VAL:HG22	1:A:332:ILE:HD12	1.88	0.56
1:B:247:GLU:HG2	5:B:2065:HOH:O	2.05	0.55
1:B:17:LYS:CG	1:B:18:ASN:H	2.19	0.55
1:B:244:HIS:ND1	1:B:258:ILE:HG12	2.21	0.55
1:A:207:LYS:HG3	1:A:208:ASP:N	2.21	0.55
1:A:61:SER:HA	5:A:2023:HOH:O	2.07	0.54
1:B:143:ILE:HD13	1:B:243:ILE:HD11	1.88	0.54
1:B:19:ILE:HD11	1:B:302:LEU:HB3	1.90	0.54
1:B:18:ASN:HD21	1:B:327:ARG:HA	1.73	0.54
1:A:194:VAL:HG21	1:A:318:ARG:HD2	1.89	0.54
1:A:173:ASN:OD1	1:A:174:PRO:HD2	2.08	0.53
1:A:252:GLY:O	1:A:253:GLU:HB3	2.09	0.53
1:B:142:GLN:O	1:B:146:LYS:HG3	2.08	0.52
1:B:294:THR:O	1:B:295:LEU:C	2.51	0.52
1:B:40:ILE:CD1	1:B:41:VAL:HG23	2.39	0.52
1:B:264:VAL:HG21	1:B:320:LEU:HD21	1.90	0.52
1:B:362:LYS:N	1:B:362:LYS:HZ3	2.07	0.52
1:B:129:GLU:OE2	1:B:141:HIS:HD2	1.92	0.52
1:B:184:MET:HA	1:B:195:ILE:O	2.09	0.52
1:A:100:THR:HG23	1:A:262:ASN:CB	2.40	0.52
1:A:161:LEU:HD12	1:A:161:LEU:C	2.35	0.52
1:A:98[B]:ASN:HD21	1:A:260:LYS:NZ	2.08	0.52
1:A:57:LEU:HB2	1:B:164:TYR:CE2	2.41	0.51
1:B:244:HIS:HD2	5:B:2039:HOH:O	1.94	0.51
1:B:129:GLU:OE2	1:B:141:HIS:CD2	2.63	0.51
1:B:165:ASN:N	5:B:2046:HOH:O	2.26	0.51
1:A:127:TRP:HZ2	1:A:145:GLU:HG3	1.69	0.51
1:B:105:GLY:C	1:B:269:SER:CB	2.81	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLU:OE1	1:B:63:ARG:NH1	2.44	0.50
1:B:134:GLY:O	1:B:137:PRO:HD2	2.11	0.50
1:A:322:ASP:HB2	5:A:2080:HOH:O	2.10	0.50
1:B:18:ASN:HB3	1:B:328:THR:O	2.11	0.50
1:B:72:PHE:HB3	1:B:76:THR:HG21	1.93	0.50
1:B:244:HIS:CE1	1:B:258:ILE:HG12	2.47	0.50
1:A:209:GLU:O	1:A:213:ILE:HG13	2.12	0.50
1:A:50:VAL:CG1	1:A:68:PHE:HE2	2.26	0.49
1:A:154:PHE:HA	1:A:244:HIS:O	2.12	0.49
1:A:329:ARG:HB3	5:A:2003:HOH:O	2.11	0.49
1:B:92:GLU:OE2	1:B:329:ARG:HG2	2.12	0.49
1:B:205:HIS:O	1:B:206:ASN:HB3	2.12	0.49
1:B:329:ARG:HH11	1:B:329:ARG:HB3	1.77	0.49
1:B:17:LYS:HG3	1:B:18:ASN:N	2.25	0.49
1:B:53:ARG:HG3	1:B:53:ARG:NH1	2.09	0.49
1:A:297:ARG:HH22	1:A:313:GLU:CD	2.21	0.49
1:B:207:LYS:HB2	1:B:207:LYS:NZ	2.28	0.49
1:A:241:VAL:HG13	1:A:261:LEU:HB3	1.94	0.48
1:B:215:GLU:O	1:B:216:LYS:C	2.56	0.48
1:A:297:ARG:NH2	1:A:313:GLU:OE2	2.46	0.48
1:B:134:GLY:O	1:B:138:ARG:HG3	2.13	0.48
1:B:20:GLN:HA	1:B:69:ASP:OD2	2.14	0.48
1:B:250:ILE:O	1:B:251:ASP:HB2	2.14	0.48
1:A:48:LYS:HE3	1:A:68:PHE:O	2.13	0.48
1:B:184:MET:HE3	1:B:319:ILE:CG1	2.44	0.48
1:A:212:GLN:HG2	1:A:213:ILE:N	2.25	0.47
1:A:53:ARG:HD2	5:A:2021:HOH:O	2.14	0.47
1:B:320:LEU:HA	1:B:320:LEU:HD12	1.65	0.47
1:A:67:THR:HG22	1:A:359:ILE:HD11	1.97	0.47
1:A:168:LEU:HD11	1:A:319:ILE:HD11	1.97	0.47
1:B:104:TYR:O	1:B:334:ALA:HA	2.14	0.47
1:A:160:LEU:HB3	1:A:172:LEU:HG	1.95	0.46
1:B:185:PHE:HE2	1:B:197:LYS:HE3	1.80	0.46
1:B:305:ARG:HE	1:B:305:ARG:HB2	1.48	0.46
1:A:40:ILE:CD1	1:A:343:LEU:HB2	2.44	0.46
1:B:161:LEU:C	1:B:161:LEU:HD12	2.41	0.46
1:B:187:ASP:OD1	1:B:189:ARG:NH1	2.49	0.46
1:A:141:HIS:ND1	1:A:207:LYS:HE3	2.31	0.46
1:A:294:THR:O	1:A:295:LEU:C	2.57	0.46
1:A:295:LEU:HD11	1:A:299:ILE:HD11	1.97	0.46
1:B:164:TYR:O	1:B:165:ASN:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:HD2	1:B:175:SER:H	1.81	0.46
1:B:53:ARG:CG	1:B:53:ARG:NH1	2.66	0.45
1:A:35:ALA:O	1:A:36:SER:HB2	2.15	0.45
1:B:26:ARG:HD2	1:B:27:PRO:O	2.16	0.45
1:A:58:ALA:HB2	1:B:228:MET:HE1	1.98	0.45
1:B:105:GLY:CA	1:B:269:SER:HB2	2.46	0.45
1:A:106:GLN:HG2	1:A:107:THR:O	2.16	0.45
1:A:238:VAL:HG22	1:A:264:VAL:HG22	1.98	0.45
1:A:26:ARG:HB2	1:A:27:PRO:HD2	1.99	0.45
1:A:98[B]:ASN:ND2	1:A:322:ASP:HB3	2.31	0.45
1:A:138:ARG:O	1:A:141:HIS:HB3	2.17	0.44
1:A:176:SER:O	1:A:176:SER:OG	2.32	0.44
1:A:98[B]:ASN:CG	1:A:323:SER:OG	2.61	0.44
1:A:184:MET:HE1	1:A:315:LYS:HG2	2.00	0.44
1:B:221:ARG:HD3	5:B:2043:HOH:O	2.16	0.44
1:A:40:ILE:HD13	1:A:340:SER:HA	1.99	0.44
1:A:143:ILE:HD13	1:A:243:ILE:CD1	2.37	0.44
1:A:298:VAL:HG21	1:A:317:THR:CG2	2.46	0.44
1:A:309:VAL:HG22	1:A:311:TYR:CE2	2.53	0.44
1:B:138:ARG:HD2	5:B:2015:HOH:O	2.18	0.44
1:A:187:ASP:HB2	1:A:195:ILE:CD1	2.48	0.44
1:B:322:ASP:C	1:B:323:SER:O	2.58	0.43
1:B:82:TYR:CE1	1:B:86:VAL:HG11	2.53	0.43
1:A:157:LYS:HG2	5:A:2059:HOH:O	2.19	0.43
1:B:26:ARG:HH12	1:B:32:GLU:CD	2.25	0.43
1:A:25:CYS:O	1:A:74:ALA:HA	2.17	0.43
1:B:163:ILE:HG12	1:B:168:LEU:HD12	2.00	0.43
1:A:98[B]:ASN:OD1	1:A:260:LYS:HG2	2.18	0.43
1:B:163:ILE:O	1:B:235:SER:HB2	2.19	0.43
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.88	0.43
1:B:228:MET:HE3	1:B:228:MET:HB3	1.95	0.43
1:A:309:VAL:HG22	1:A:311:TYR:CD2	2.54	0.43
1:B:92:GLU:CD	1:B:329:ARG:HG2	2.44	0.42
1:A:309:VAL:HA	1:A:310:PRO:HD3	1.75	0.42
1:A:104:TYR:CD1	1:A:104:TYR:C	2.97	0.42
1:A:88:PRO:HB3	1:A:329:ARG:NH2	2.35	0.42
1:A:206:ASN:ND2	1:A:208:ASP:HB2	2.15	0.42
1:A:59:ASP:O	1:B:229:ASN:ND2	2.53	0.41
1:A:173:ASN:ND2	1:A:176:SER:HB3	2.35	0.41
1:A:244:HIS:CD2	1:A:258:ILE:HG12	2.55	0.41
1:B:18:ASN:ND2	1:B:327:ARG:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:HB2	1:A:111:LYS:HE2	1.67	0.41
1:A:115:MET:HE3	1:A:263:LEU:HD22	2.02	0.41
1:A:340:SER:CB	3:A:2000:NO3:O1	2.67	0.41
1:B:94:ILE:C	1:B:96:GLY:H	2.27	0.41
1:B:221:ARG:HD2	1:B:232:SER:HB3	2.02	0.41
1:A:341:LEU:HA	3:A:2000:NO3:O2	2.20	0.41
1:A:304:GLU:C	1:A:306:THR:H	2.28	0.41
1:B:173:ASN:OD1	1:B:174:PRO:HD2	2.20	0.41
1:B:247:GLU:CD	5:B:2035:HOH:O	2.62	0.41
1:B:104:TYR:CD1	1:B:104:TYR:C	2.99	0.41
1:A:215:GLU:O	1:A:216:LYS:C	2.62	0.41
1:A:100:THR:OG1	1:A:323:SER:HB2	2.21	0.41
1:A:161:LEU:C	1:A:161:LEU:CD1	2.94	0.41
1:B:184:MET:HE3	1:B:319:ILE:HG12	2.02	0.41
1:B:236:HIS:CD2	1:B:316:LEU:HD22	2.56	0.41
1:B:302:LEU:HD12	1:B:302:LEU:HA	1.99	0.41
1:B:174:PRO:CD	1:B:175:SER:H	2.35	0.40
1:B:298:VAL:HG22	1:B:309:VAL:HG12	2.03	0.40
1:B:140:LEU:HD13	1:B:140:LEU:HA	1.87	0.40
1:A:98[B]:ASN:HD21	1:A:260:LYS:HZ3	1.69	0.40
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.78	0.40
1:A:186:ASP:OD2	1:A:318:ARG:NH1	2.49	0.40
1:A:250:ILE:O	1:A:251:ASP:HB2	2.21	0.40
1:B:103:ALA:HB2	1:B:115:MET:HE2	2.03	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	320/368 (87%)	308 (96%)	10 (3%)	2 (1%)	21 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	313/368 (85%)	305 (97%)	8 (3%)	0	100	100
All	All	633/736 (86%)	613 (97%)	18 (3%)	2 (0%)	36	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	VAL
1	A	179	SER

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	
1	A	279/322 (87%)	247 (88%)	32 (12%)	5	18
1	B	279/322 (87%)	246 (88%)	33 (12%)	5	17
All	All	558/644 (87%)	493 (88%)	65 (12%)	5	18

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	48	LYS
1	A	100	THR
1	A	115	MET
1	A	130	VAL
1	A	142	GLN
1	A	145	GLU
1	A	161	LEU
1	A	168	LEU
1	A	181	ARG
1	A	186	ASP
1	A	194	VAL
1	A	206	ASN
1	A	207	LYS

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Mol	Chain	Res	Type
1	A	212	GLN
1	A	216	LYS
1	A	229	ASN
1	A	235	SER
1	A	241	VAL
1	A	249	THR
1	A	293	LEU
1	A	304	GLU
1	A	305	ARG
1	A	309	VAL
1	A	312	ARG
1	A	313	GLU
1	A	315	LYS
1	A	317	THR
1	A	329	ARG
1	A	343	LEU
1	A	359	ILE
1	A	360	LEU
1	B	17	LYS
1	B	40	ILE
1	B	52	VAL
1	B	53	ARG
1	B	63	ARG
1	B	70	MET
1	B	76	THR
1	B	83	ARG
1	B	93	VAL
1	B	130	VAL
1	B	132	LEU
1	B	136	ILE
1	B	146	LYS
1	B	168	LEU
1	B	177	ASP
1	B	183	GLN
1	B	184	MET
1	B	194	VAL
1	B	203	THR
1	B	207	LYS
1	B	220	LYS
1	B	242	THR
1	B	256	VAL
1	B	290	GLN

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Mol	Chain	Res	Type
1	B	298	VAL
1	B	302	LEU
1	B	305	ARG
1	B	315	LYS
1	B	320	LEU
1	B	329	ARG
1	B	333	ILE
1	B	343	LEU
1	B	362	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	205	HIS
1	A	206	ASN
1	B	18	ASN
1	B	38	HIS
1	B	141	HIS
1	B	183	GLN
1	B	212	GLN
1	B	244	HIS

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 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
3	NO3	A	2001	-	1,3,3	3.48	1 (100%)	0,3,3	-	-
4	ADP	A	2601	2	28,29,29	1.58	6 (21%)	43,45,45	1.84	9 (20%)
3	NO3	A	2000	-	1,3,3	3.12	1 (100%)	0,3,3	-	-
4	ADP	B	2600	2	28,29,29	1.38	3 (10%)	43,45,45	1.94	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
4	ADP	A	2601	2	-	1/16/32/32	0/3/3/3
4	ADP	B	2600	2	-	2/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2601	ADP	C5-C4	5.16	1.48	1.39
4	B	2600	ADP	C5-C4	4.53	1.47	1.39
3	A	2001	NO3	O1-N	3.48	1.41	1.24
3	A	2000	NO3	O1-N	3.12	1.39	1.24
4	A	2601	ADP	PA-O3A	2.76	1.62	1.59
4	A	2601	ADP	C5-N7	-2.59	1.34	1.39
4	A	2601	ADP	C8-N7	2.53	1.36	1.31
4	A	2601	ADP	C5-C6	2.51	1.48	1.41
4	B	2600	ADP	C5-N7	-2.35	1.34	1.39
4	A	2601	ADP	C4-N9	-2.32	1.32	1.37
4	B	2600	ADP	C5-C6	2.10	1.46	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2600	ADP	C5-C4-N3	-5.85	118.66	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2601	ADP	C5-C4-N3	-5.84	118.67	126.72
4	B	2600	ADP	N3-C4-N9	5.60	136.69	127.17
4	A	2601	ADP	N3-C4-N9	4.86	135.43	127.17
4	B	2600	ADP	C2-N3-C4	3.61	120.65	111.83
4	B	2600	ADP	C4-N9-C8	3.60	109.52	105.74
4	A	2601	ADP	C4-C5-N7	-3.54	106.53	110.58
4	B	2600	ADP	N3-C2-N1	-3.51	123.27	128.58
4	A	2601	ADP	C4-N9-C8	3.39	109.30	105.74
4	A	2601	ADP	C2-N3-C4	2.91	118.95	111.83
4	A	2601	ADP	O3'-C3'-C4'	-2.69	103.35	111.08
4	A	2601	ADP	C5-N7-C8	2.60	107.54	103.45
4	B	2600	ADP	N6-C6-N1	2.55	124.05	118.38
4	B	2600	ADP	C4-C5-N7	-2.35	107.89	110.58
4	A	2601	ADP	N9-C8-N7	-2.27	110.72	113.94
4	B	2600	ADP	C1'-N9-C8	-2.21	122.18	127.09
4	B	2600	ADP	C5-N7-C8	2.10	106.74	103.45
4	A	2601	ADP	O3B-PB-O2B	2.02	115.37	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2601	ADP	PA-O3A-PB-O2B
4	B	2600	ADP	PA-O3A-PB-O3B
4	B	2600	ADP	PA-O3A-PB-O1B

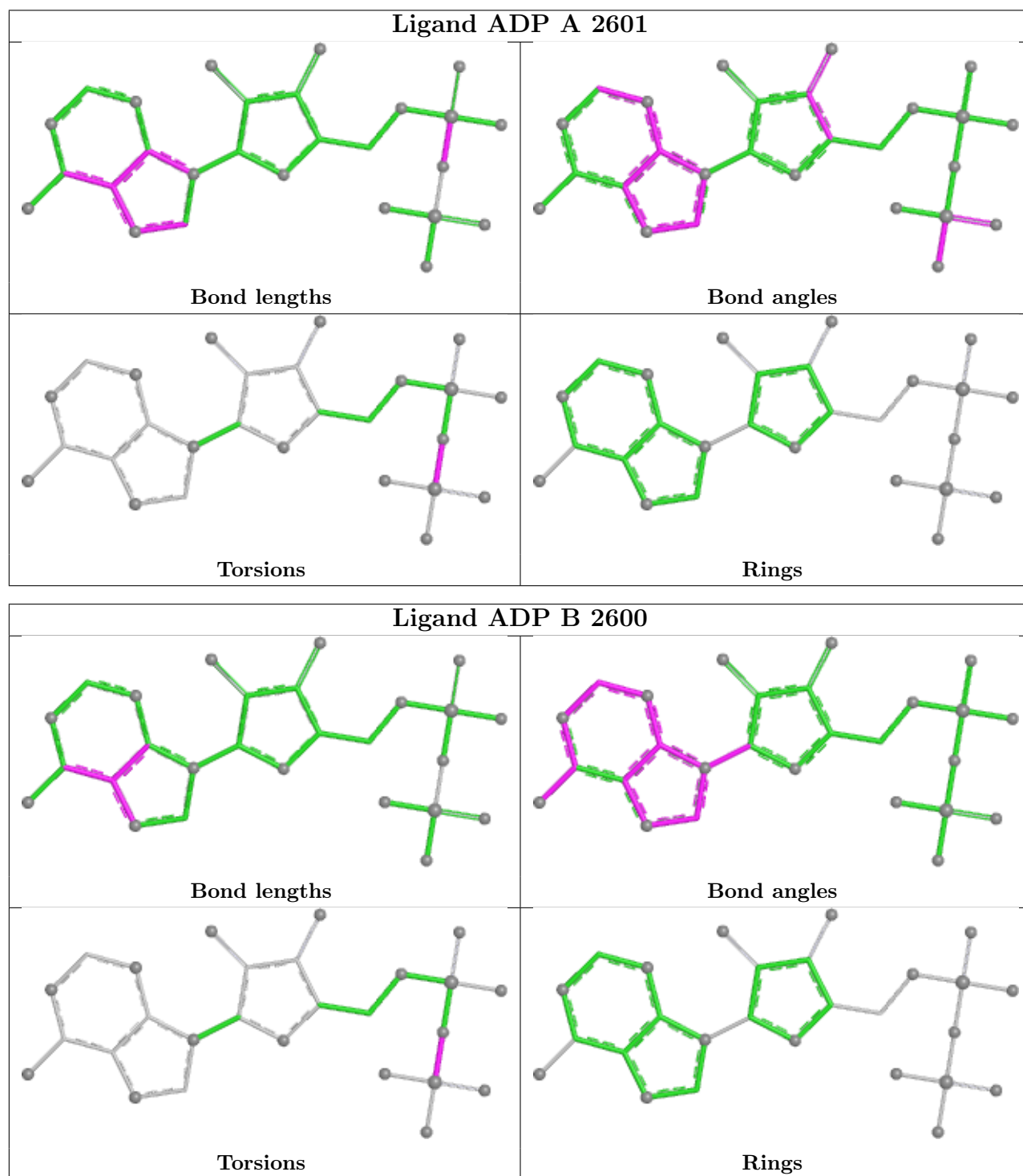
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	NO3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	327/368 (88%)	-0.43	4 (1%)	76 68	7, 24, 56, 81	1 (0%)
1	B	321/368 (87%)	-0.58	2 (0%)	85 80	10, 21, 46, 63	0
All	All	648/736 (88%)	-0.51	6 (0%)	81 74	7, 22, 54, 81	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	3.2
1	A	125	TYR	2.5
1	A	188	PRO	2.5
1	A	178	VAL	2.5
1	B	289	ASN	2.4
1	B	273	GLY	2.2

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](#)

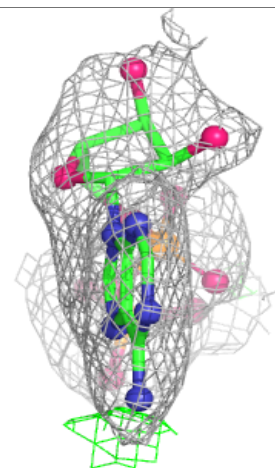
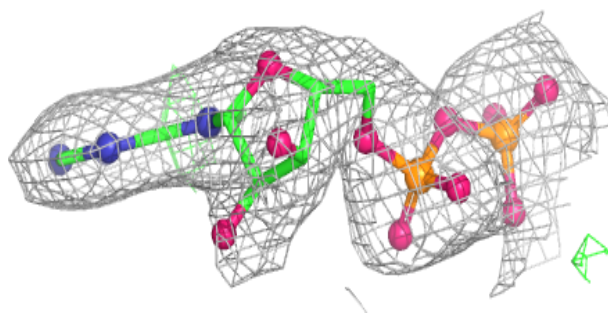
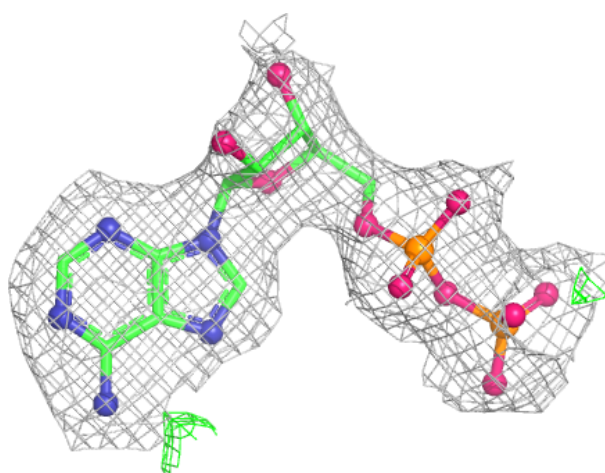
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NO3	A	2001	4/4	0.84	0.13	36,38,43,45	0
3	NO3	A	2000	4/4	0.98	0.07	15,17,19,22	0
4	ADP	A	2601	27/27	0.98	0.05	7,9,16,22	0
4	ADP	B	2600	27/27	0.98	0.05	10,13,17,18	0
2	MG	A	1365	1/1	0.99	0.11	30,30,30,30	0
2	MG	B	1365	1/1	0.99	0.12	30,30,30,30	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.

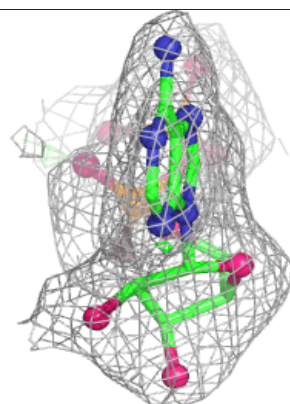
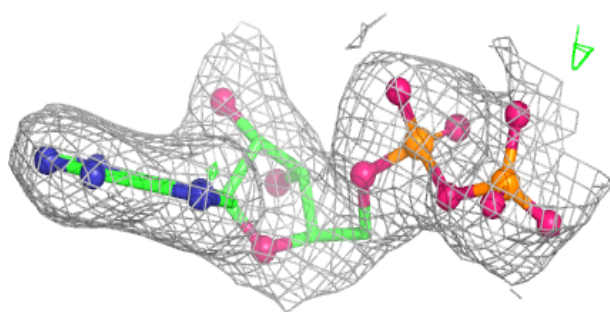
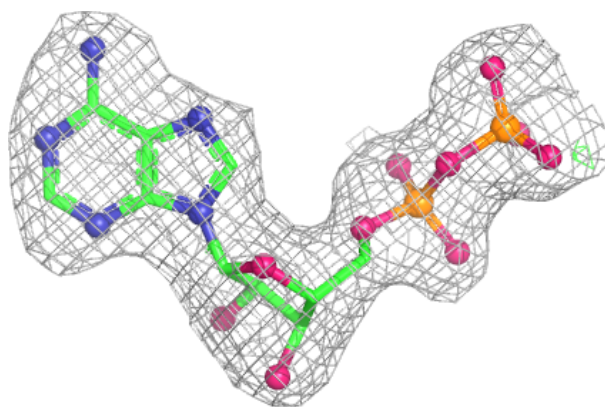
Electron density around ADP A 2601:

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 2600:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.