



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:45 AM UTC

PDB ID : 6ASY / pdb_00006asy
Title : BiP-ATP2
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Deposited on : 2017-08-26
Resolution : 1.85 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

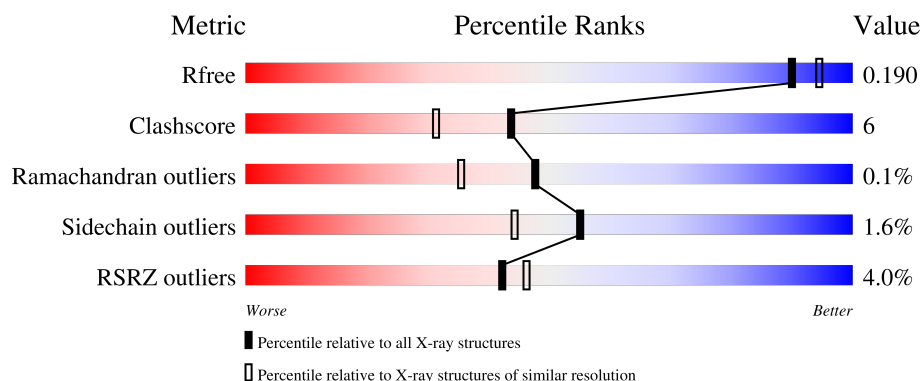
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	606	4% 88% 11%
1	B	606	3% 89% 10%

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
4	SO4	B	706	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10997 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 78 kDa glucose-regulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	11	0
			4797	3010	822	953	12			
1	B	606	Total	C	N	O	S	0	10	0
			4791	3006	821	952	12			

There are 16 discrepancies between the modelled and reference sequences:

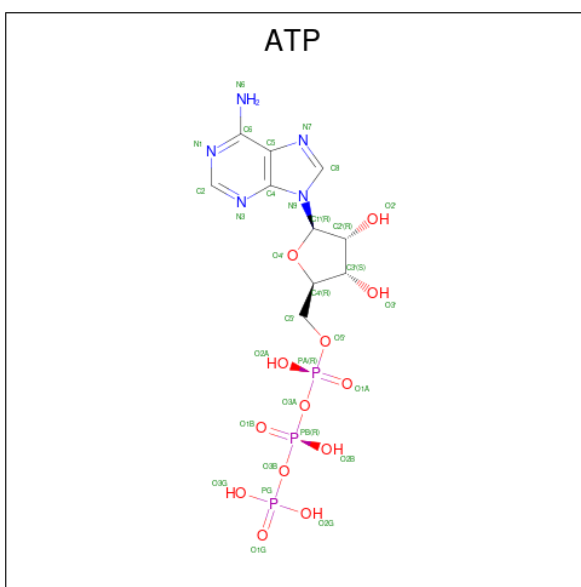
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP P11021
A	?	-	THR	deletion	UNP P11021
A	?	-	ALA	deletion	UNP P11021
A	?	-	SER	deletion	UNP P11021
A	?	-	ASP	deletion	UNP P11021
A	453	VAL	ASN	conflict	UNP P11021
A	454	GLY	GLN	conflict	UNP P11021
A	455	GLY	PRO	conflict	UNP P11021
B	24	SER	-	expression tag	UNP P11021
B	?	-	THR	deletion	UNP P11021
B	?	-	ALA	deletion	UNP P11021
B	?	-	SER	deletion	UNP P11021
B	?	-	ASP	deletion	UNP P11021
B	453	VAL	ASN	conflict	UNP P11021
B	454	GLY	GLN	conflict	UNP P11021
B	455	GLY	PRO	conflict	UNP P11021

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



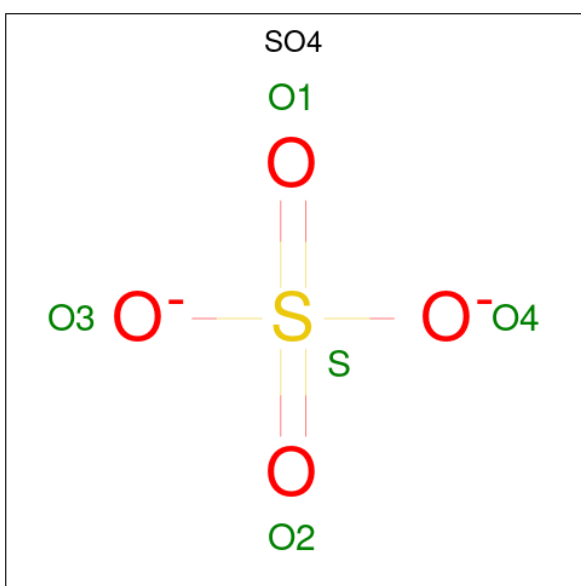
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



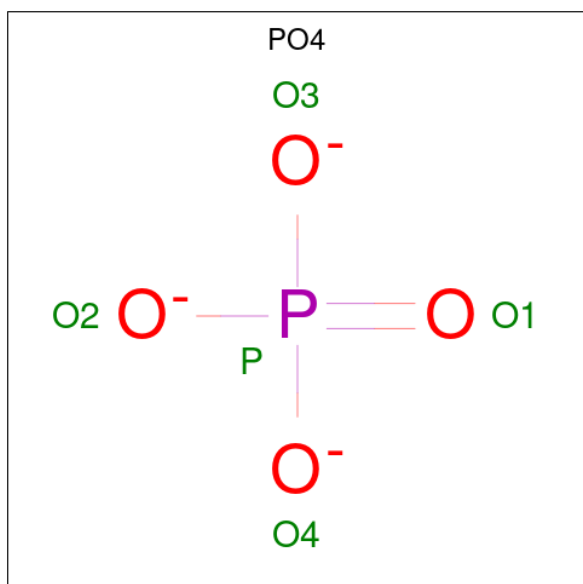
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

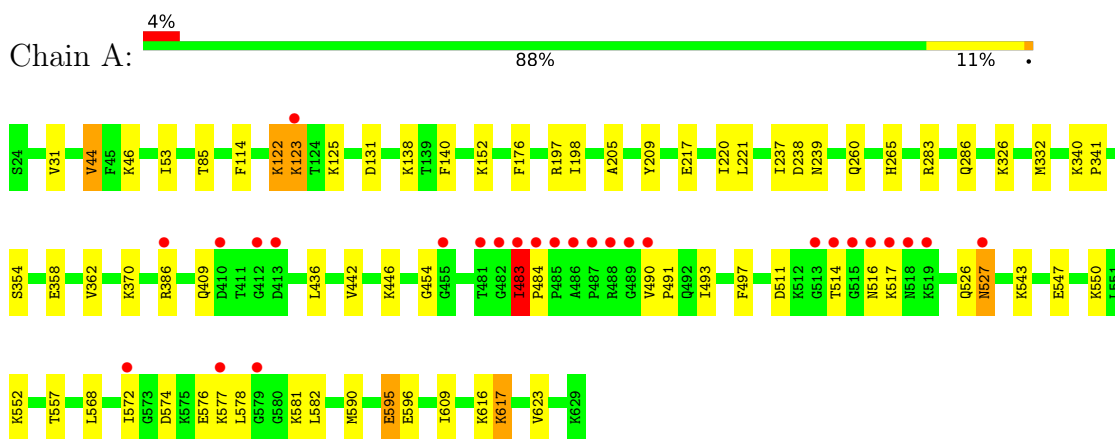
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	617	Total	O	0	0
			617	617		
6	B	592	Total	O	0	0
			592	592		

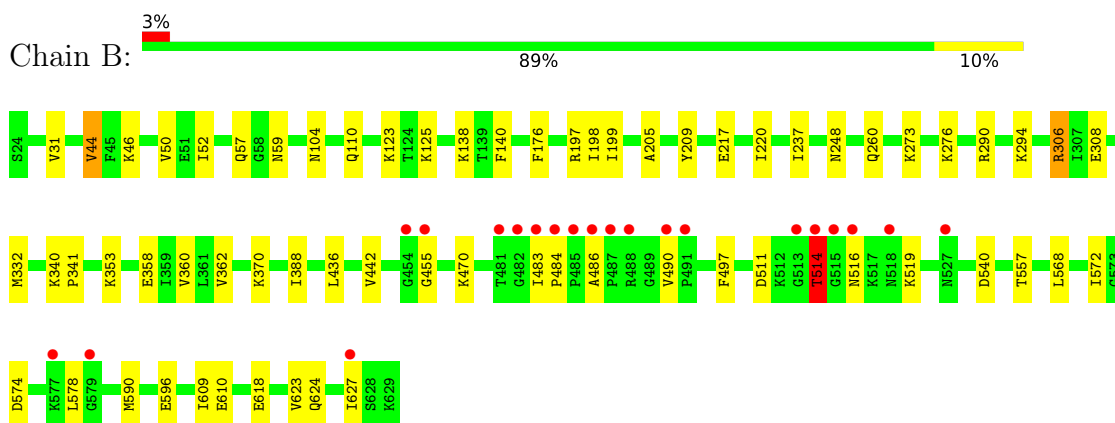
3 Residue-property plots

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

- Molecule 1: 78 kDa glucose-regulated protein



- Molecule 1: 78 kDa glucose-regulated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.83Å 75.75Å 78.79Å 62.05° 62.23° 73.42°	Depositor
Resolution (Å)	39.09 – 1.85 39.09 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.09-1.85) 97.7 (39.09-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.159 , 0.189 (Not available) , 0.190	Depositor DCC
R_{free} test set	5717 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.460 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10997	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: SO4, ATP, GOL, PO4

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	0.58	1/4864 (0.0%)	0.80	4/6564 (0.1%)
1	B	0.55	0/4858	0.77	3/6555 (0.0%)
All	All	0.57	1/9722 (0.0%)	0.78	7/13119 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	LYS	CA-C	5.84	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	486	ALA	CA-C-N	6.13	127.50	119.84
1	B	486	ALA	C-N-CA	6.13	127.50	119.84
1	A	484	PRO	CA-C-N	-5.79	113.62	120.11
1	A	484	PRO	C-N-CA	-5.79	113.62	120.11
1	A	483	ILE	CA-C-N	5.78	126.33	120.38
1	A	483	ILE	C-N-CA	5.78	126.33	120.38
1	B	514	THR	N-CA-C	-5.17	105.73	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	526	GLN	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	4797	0	4827	67	1
1	B	4791	0	4821	49	1
2	A	30	0	40	3	0
2	B	18	0	24	3	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	20	0	0	0	0
4	B	20	0	0	2	0
5	A	30	0	0	1	0
5	B	20	0	0	0	0
6	A	617	0	0	32	1
6	B	592	0	0	23	1
All	All	10997	0	9736	120	2

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 (120) 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:574:ASP:O	6:A:801:HOH:O	1.89	0.90
1:A:483:ILE:HD11	1:A:491:PRO:HB3	1.58	0.86
1:B:260:GLN:NE2	6:B:805:HOH:O	2.09	0.85
1:A:197[B]:ARG:NH1	1:A:198:ILE:O	2.12	0.82
5:A:711:PO4:O4	6:A:802:HOH:O	1.98	0.81
1:B:197[B]:ARG:NH1	1:B:198:ILE:O	2.11	0.81
1:B:306:ARG:NH2	6:B:807:HOH:O	2.14	0.80
1:A:46:LYS:NZ	6:A:810:HOH:O	2.14	0.78
1:A:527:ASN:O	6:A:803:HOH:O	2.03	0.77
1:A:578:LEU:N	6:A:801:HOH:O	2.17	0.76
1:A:217:GLU:OE1	6:A:804:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLN:OE1	6:B:801:HOH:O	2.05	0.73
1:B:578:LEU:N	6:B:808:HOH:O	2.18	0.73
3:B:704:ATP:O1B	6:B:803:HOH:O	2.05	0.73
1:B:618:GLU:OE2	6:B:802:HOH:O	2.05	0.72
1:A:543:LYS:HE2	6:A:1339:HOH:O	1.89	0.72
1:A:595:GLU:N	1:A:595:GLU:OE1	2.25	0.70
1:B:217:GLU:OE1	6:B:804:HOH:O	2.09	0.70
1:A:220:ILE:HG13	1:A:237:ILE:HD12	1.73	0.69
1:A:582:LEU:O	6:A:806:HOH:O	2.09	0.69
1:A:123:LYS:HB2	6:A:826:HOH:O	1.91	0.69
1:B:220:ILE:HG13	1:B:237:ILE:HD12	1.74	0.68
1:B:276:LYS:NZ	6:B:806:HOH:O	2.25	0.68
1:A:239:ASN:OD1	6:A:808:HOH:O	2.13	0.66
4:B:706:SO4:O2	6:B:806:HOH:O	2.12	0.66
1:A:152:LYS:NZ	6:A:820:HOH:O	2.26	0.66
1:A:543:LYS:NZ	1:A:547:GLU:OE2	2.30	0.64
1:B:104:ASN:HB2	6:B:955:HOH:O	1.98	0.64
1:A:454:GLY:O	6:A:809:HOH:O	2.14	0.64
1:A:114:PHE:CD1	1:A:260:GLN:NE2	2.66	0.64
1:B:290:ARG:NH1	6:B:812:HOH:O	2.24	0.63
1:A:197[B]:ARG:NH1	6:A:829:HOH:O	2.32	0.61
1:B:340:LYS:HG2	6:B:856:HOH:O	2.00	0.61
1:A:446:LYS:NZ	6:A:818:HOH:O	2.23	0.61
1:A:238:ASP:OD2	6:A:811:HOH:O	2.16	0.60
1:B:332:MET:HE1	1:B:370:LYS:HG2	1.83	0.60
1:A:386:ARG:NH1	2:A:703:GOL:O3	2.36	0.58
1:A:616:LYS:HD2	6:A:1093:HOH:O	2.03	0.57
2:A:702:GOL:O1	6:A:812:HOH:O	2.17	0.57
1:A:332:MET:HE1	1:A:370:LYS:HG2	1.86	0.57
1:B:514:THR:HG22	1:B:516:ASN:H	1.69	0.56
1:A:596:GLU:HG2	6:A:813:HOH:O	2.05	0.56
1:A:514:THR:HG23	1:A:516:ASN:N	2.21	0.55
1:B:46:LYS:NZ	6:B:827:HOH:O	2.38	0.55
1:B:31:VAL:HG12	1:B:44[B]:VAL:HG22	1.89	0.55
1:B:572:ILE:HD11	1:B:590:MET:HE3	1.89	0.55
1:A:511:ASP:HB3	1:A:514:THR:HG22	1.90	0.53
1:A:514:THR:CG2	1:A:516:ASN:HB3	2.38	0.53
1:B:59:ASN:HA	2:B:701:GOL:H32	1.90	0.53
1:A:514:THR:HG23	1:A:516:ASN:H	1.73	0.53
1:A:454:GLY:HA2	1:A:483:ILE:HD13	1.90	0.52
1:A:574:ASP:HA	6:A:822:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HG12	1:A:44[B]:VAL:HG22	1.93	0.51
1:A:596:GLU:OE2	6:A:813:HOH:O	2.18	0.51
1:A:552:LYS:NZ	6:A:839:HOH:O	2.44	0.50
1:A:557:THR:HG21	1:A:609:ILE:HD11	1.94	0.50
1:B:197[B]:ARG:NE	6:B:809:HOH:O	2.18	0.50
1:A:514:THR:HG23	1:A:516:ASN:HB3	1.92	0.50
1:B:557:THR:HG21	1:B:609:ILE:HD11	1.95	0.49
1:B:340:LYS:HB2	1:B:341:PRO:HD3	1.94	0.49
1:A:197[A]:ARG:NH1	6:A:805:HOH:O	2.21	0.49
1:B:568:LEU:HD13	1:B:623:VAL:HG21	1.95	0.48
1:B:353:LYS:HZ3	2:B:703:GOL:H32	1.78	0.48
1:B:511:ASP:HB3	1:B:514:THR:HB	1.95	0.48
1:A:572:ILE:HD11	1:A:590:MET:HE3	1.94	0.48
1:A:197[A]:ARG:HD2	6:A:805:HOH:O	2.13	0.47
1:B:574:ASP:HB3	6:B:808:HOH:O	2.14	0.47
1:A:265:HIS:CE1	1:A:326:LYS:HE2	2.49	0.47
1:A:386:ARG:H	2:A:703:GOL:H12	1.80	0.47
1:A:568:LEU:HD13	1:A:623:VAL:HG21	1.97	0.46
1:B:353:LYS:NZ	2:B:703:GOL:H32	2.31	0.46
1:A:574:ASP:OD1	1:A:576:GLU:HG2	2.15	0.46
1:A:578:LEU:HD12	1:A:581:LYS:HD3	1.97	0.46
1:B:125:LYS:HB3	6:B:1274:HOH:O	2.15	0.46
1:B:442[B]:VAL:HG12	6:B:1145:HOH:O	2.15	0.46
1:A:442[B]:VAL:HG12	6:A:1146:HOH:O	2.15	0.46
3:A:706:ATP:O1B	6:A:815:HOH:O	2.20	0.46
1:A:340:LYS:HB2	1:A:341:PRO:HD3	1.97	0.46
1:B:294[A]:LYS:NZ	6:B:850:HOH:O	2.48	0.46
1:A:122:LYS:HB3	1:A:122:LYS:HE3	1.77	0.45
1:B:455:GLY:O	1:B:483:ILE:HD12	2.17	0.45
1:A:85:THR:O	1:A:283:ARG:NE	2.50	0.45
1:A:125:LYS:HD3	6:A:983:HOH:O	2.17	0.45
1:A:205:ALA:HB1	1:A:362:VAL:HG11	1.99	0.44
1:A:511:ASP:HB3	1:A:514:THR:CG2	2.46	0.44
1:A:409:GLN:N	6:A:814:HOH:O	2.19	0.44
1:A:131:ASP:OD2	6:A:816:HOH:O	2.21	0.44
1:A:516:ASN:OD1	1:A:517:LYS:N	2.50	0.44
1:A:617:LYS:HB2	1:A:617:LYS:HE3	1.72	0.44
1:B:209:TYR:OH	1:B:358:GLU:HG3	2.16	0.44
1:B:436:LEU:HD21	1:B:497:PHE:CD1	2.53	0.44
1:A:386:ARG:NH1	1:B:50:VAL:O	2.43	0.44
1:A:354:SER:OG	6:A:817:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ASP:HB3	6:A:801:HOH:O	2.17	0.43
1:B:514:THR:CG2	1:B:516:ASN:HB2	2.49	0.43
1:A:209:TYR:OH	1:A:358:GLU:HG3	2.17	0.43
1:B:273:LYS:HB2	1:B:273:LYS:HE3	1.77	0.43
1:B:123:LYS:N	6:B:853:HOH:O	2.52	0.43
1:B:197[B]:ARG:NH1	1:B:199:ILE:HA	2.34	0.42
1:B:248:ASN:ND2	6:B:847:HOH:O	2.48	0.42
1:B:470:LYS:HE3	1:B:470:LYS:HB2	1.81	0.42
1:B:138:LYS:HG2	1:B:140:PHE:CZ	2.55	0.42
1:B:483:ILE:HA	1:B:484:PRO:HD3	1.91	0.42
1:A:483:ILE:HD12	1:A:493:ILE:HG12	2.01	0.42
1:B:205:ALA:HB1	1:B:362:VAL:HG11	2.02	0.41
1:B:540:ASP:HB3	6:B:1301:HOH:O	2.20	0.41
1:A:138:LYS:HG2	1:A:140:PHE:CZ	2.55	0.41
1:A:286:GLN:HG2	6:A:1077:HOH:O	2.20	0.41
1:B:360:VAL:HG13	1:B:388:ILE:HD13	2.02	0.41
1:B:624:GLN:OE1	1:B:627:ILE:HD11	2.20	0.41
4:B:706:SO4:O2	6:B:810:HOH:O	2.19	0.41
1:A:436:LEU:HD21	1:A:497:PHE:CD1	2.56	0.41
1:A:550:LYS:HA	1:A:550:LYS:HD2	1.78	0.41
1:B:220:ILE:HD12	1:B:358:GLU:HB2	2.03	0.41
1:B:596:GLU:HG2	6:B:838:HOH:O	2.19	0.41
1:A:386:ARG:NH2	1:B:52:ILE:HG12	2.36	0.41
1:B:306:ARG:HG2	1:B:308:GLU:OE1	2.20	0.41
1:A:44[A]:VAL:HG22	1:A:53:ILE:HD11	2.02	0.40
1:A:260:GLN:HA	1:A:260:GLN:OE1	2.22	0.40
1:A:125:LYS:NZ	6:A:864:HOH:O	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1154:HOH:O	6:B:1087:HOH:O[1_545]	2.09	0.11
1:A:517:LYS:NZ	1:B:57:GLN:OE1[1_455]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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	615/606 (102%)	600 (98%)	14 (2%)	1 (0%)	43	31
1	B	614/606 (101%)	596 (97%)	18 (3%)	0	100	100
All	All	1229/1212 (101%)	1196 (97%)	32 (3%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	LYS

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	520/519 (100%)	510 (98%)	10 (2%)	50	38
1	B	526/519 (101%)	518 (98%)	8 (2%)	57	47
All	All	1046/1038 (101%)	1028 (98%)	18 (2%)	55	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44[A]	VAL
1	A	44[B]	VAL
1	A	122	LYS
1	A	176	PHE
1	A	221	LEU

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Mol	Chain	Res	Type
1	A	483	ILE
1	A	490	VAL
1	A	527	ASN
1	A	595	GLU
1	A	617	LYS
1	B	44[A]	VAL
1	B	44[B]	VAL
1	B	176	PHE
1	B	306	ARG
1	B	490	VAL
1	B	514	THR
1	B	519	LYS
1	B	610	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	A	527	ASN
1	B	110	GLN
1	B	380	ASN
1	B	571	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

28 ligands are modelled in this entry.

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	$\# Z > 2$
2	GOL	A	704	-	5,5,5	0.39	0	5,5,5	0.25	0
5	PO4	B	711	-	4,4,4	0.94	0	6,6,6	0.51	0
5	PO4	B	709	-	4,4,4	0.94	0	6,6,6	0.39	0
5	PO4	B	710	-	4,4,4	0.95	0	6,6,6	0.38	0
5	PO4	B	712	-	4,4,4	0.91	0	6,6,6	0.47	0
4	SO4	A	709	-	4,4,4	0.22	0	6,6,6	0.10	0
5	PO4	A	711	-	4,4,4	0.94	0	6,6,6	0.49	0
5	PO4	A	712	-	4,4,4	0.91	0	6,6,6	0.55	0
2	GOL	B	702	-	5,5,5	0.39	0	5,5,5	0.22	0
2	GOL	A	701	-	5,5,5	0.40	0	5,5,5	0.21	0
4	SO4	A	707	-	4,4,4	0.24	0	6,6,6	0.14	0
4	SO4	A	708	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	B	707	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	B	708	-	4,4,4	0.23	0	6,6,6	0.09	0
5	PO4	A	715	-	4,4,4	0.91	0	6,6,6	0.50	0
2	GOL	A	703	-	5,5,5	0.35	0	5,5,5	0.42	0
2	GOL	B	703	-	5,5,5	0.35	0	5,5,5	0.29	0
5	PO4	A	713	-	4,4,4	0.93	0	6,6,6	0.37	0
4	SO4	B	706	-	4,4,4	0.22	0	6,6,6	0.15	0
5	PO4	A	714	-	4,4,4	0.91	0	6,6,6	0.52	0
4	SO4	A	710	-	4,4,4	0.23	0	6,6,6	0.09	0
5	PO4	A	716	-	4,4,4	0.95	0	6,6,6	0.52	0
2	GOL	A	705	-	5,5,5	0.37	0	5,5,5	0.28	0
3	ATP	A	706	-	32,33,33	1.66	8 (25%)	48,52,52	1.79	11 (22%)
4	SO4	B	705	-	4,4,4	0.23	0	6,6,6	0.09	0
3	ATP	B	704	-	32,33,33	1.66	7 (21%)	48,52,52	1.80	11 (22%)
2	GOL	A	702	-	5,5,5	0.37	0	5,5,5	0.34	0
2	GOL	B	701	-	5,5,5	0.37	0	5,5,5	0.43	0

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
2	GOL	B	703	-	-	2/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-
2	GOL	A	701	-	-	4/4/4/4	-
3	ATP	A	706	-	-	4/22/38/38	0/3/3/3
3	ATP	B	704	-	-	5/22/38/38	0/3/3/3
2	GOL	A	702	-	-	2/4/4/4	-
2	GOL	B	701	-	-	4/4/4/4	-
2	GOL	A	705	-	-	4/4/4/4	-
2	GOL	A	703	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	ATP	C5-C4	4.58	1.47	1.39
3	B	704	ATP	C5-C4	4.53	1.47	1.39
3	A	706	ATP	PA-O3A	3.68	1.63	1.59
3	B	704	ATP	PA-O3A	3.64	1.63	1.59
3	B	704	ATP	PB-O3B	3.41	1.63	1.59
3	A	706	ATP	PB-O3A	3.19	1.62	1.59
3	B	704	ATP	PB-O3A	3.18	1.62	1.59
3	A	706	ATP	PB-O3B	3.18	1.62	1.59
3	B	704	ATP	C5-C6	2.60	1.48	1.41
3	B	704	ATP	C8-N7	2.56	1.36	1.31
3	A	706	ATP	C4-N9	-2.54	1.32	1.37
3	A	706	ATP	C5-C6	2.46	1.47	1.41
3	A	706	ATP	C8-N7	2.31	1.36	1.31
3	B	704	ATP	C4-N9	-2.21	1.33	1.37
3	A	706	ATP	C5-N7	-2.03	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	ATP	C5-C4-N3	-5.25	119.49	126.72
3	A	706	ATP	C5-C4-N3	-5.15	119.62	126.72
3	A	706	ATP	N3-C4-N9	4.29	134.46	127.17
3	B	704	ATP	N3-C4-N9	4.17	134.26	127.17
3	A	706	ATP	C4-N9-C8	3.54	109.45	105.74
3	B	704	ATP	C2-N3-C4	3.44	120.23	111.83
3	B	704	ATP	C4-N9-C8	3.40	109.30	105.74
3	B	704	ATP	C4-C5-N7	-3.36	106.74	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	706	ATP	C2-N3-C4	3.33	119.97	111.83
3	B	704	ATP	N3-C2-N1	-3.28	123.61	128.58
3	A	706	ATP	C4-C5-N7	-3.10	107.04	110.58
3	A	706	ATP	N3-C2-N1	-3.06	123.95	128.58
3	B	704	ATP	N9-C8-N7	-2.56	110.30	113.94
3	B	704	ATP	C5-N7-C8	2.53	107.42	103.45
3	A	706	ATP	N9-C8-N7	-2.43	110.48	113.94
3	B	704	ATP	O3A-PA-O1A	-2.37	103.58	110.70
3	A	706	ATP	C5-N7-C8	2.33	107.11	103.45
3	B	704	ATP	C6-C5-N7	2.23	136.39	132.09
3	B	704	ATP	O2A-PA-O1A	2.09	122.19	112.44
3	A	706	ATP	O2A-PA-O1A	2.08	122.13	112.44
3	A	706	ATP	C6-C5-N7	2.08	136.10	132.09
3	A	706	ATP	O3B-PG-O1G	-2.01	100.49	111.04

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-O2
2	A	701	GOL	O1-C1-C2-C3
2	A	701	GOL	C1-C2-C3-O3
2	A	701	GOL	O2-C2-C3-O3
2	A	703	GOL	O1-C1-C2-C3
2	A	703	GOL	C1-C2-C3-O3
2	A	705	GOL	O1-C1-C2-C3
3	A	706	ATP	C5'-O5'-PA-O2A
3	B	704	ATP	C5'-O5'-PA-O1A
2	A	702	GOL	O1-C1-C2-C3
2	A	704	GOL	C1-C2-C3-O3
2	A	705	GOL	C1-C2-C3-O3
2	B	701	GOL	O1-C1-C2-C3
2	B	701	GOL	C1-C2-C3-O3
2	B	703	GOL	O1-C1-C2-C3
2	A	702	GOL	O1-C1-C2-O2
2	A	703	GOL	O2-C2-C3-O3
2	B	701	GOL	O2-C2-C3-O3
2	B	703	GOL	O1-C1-C2-O2
2	A	705	GOL	O1-C1-C2-O2
2	A	705	GOL	O2-C2-C3-O3
2	B	701	GOL	O1-C1-C2-O2
2	A	703	GOL	O1-C1-C2-O2

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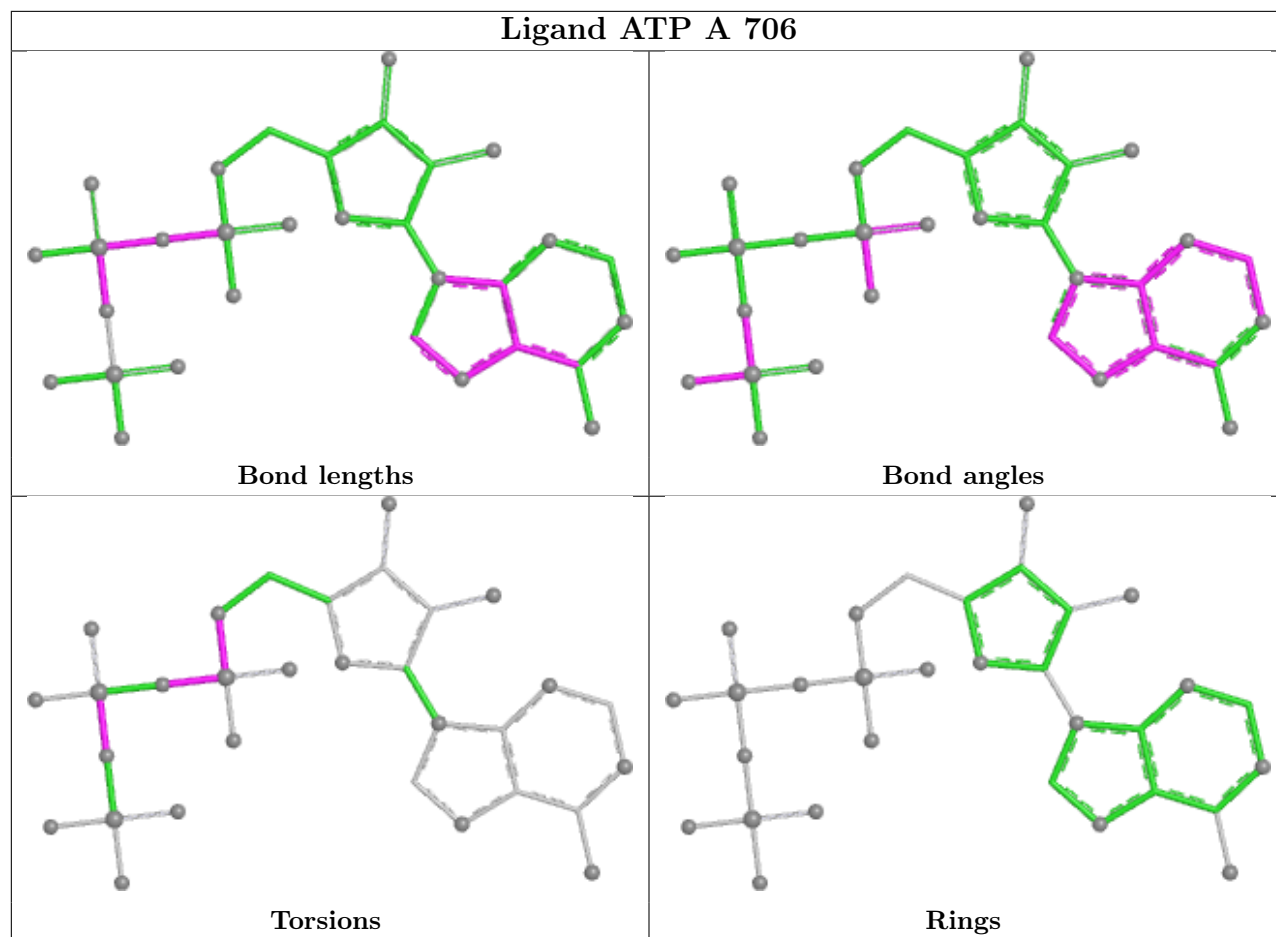
Mol	Chain	Res	Type	Atoms
2	B	702	GOL	O1-C1-C2-O2
3	B	704	ATP	PG-O3B-PB-O1B
2	B	702	GOL	C1-C2-C3-O3
3	A	706	ATP	PB-O3A-PA-O2A
3	A	706	ATP	PG-O3B-PB-O1B
2	A	704	GOL	O2-C2-C3-O3
3	B	704	ATP	PG-O3B-PB-O2B
3	A	706	ATP	PG-O3B-PB-O2B
3	B	704	ATP	PB-O3A-PA-O1A
3	B	704	ATP	PB-O3A-PA-O2A

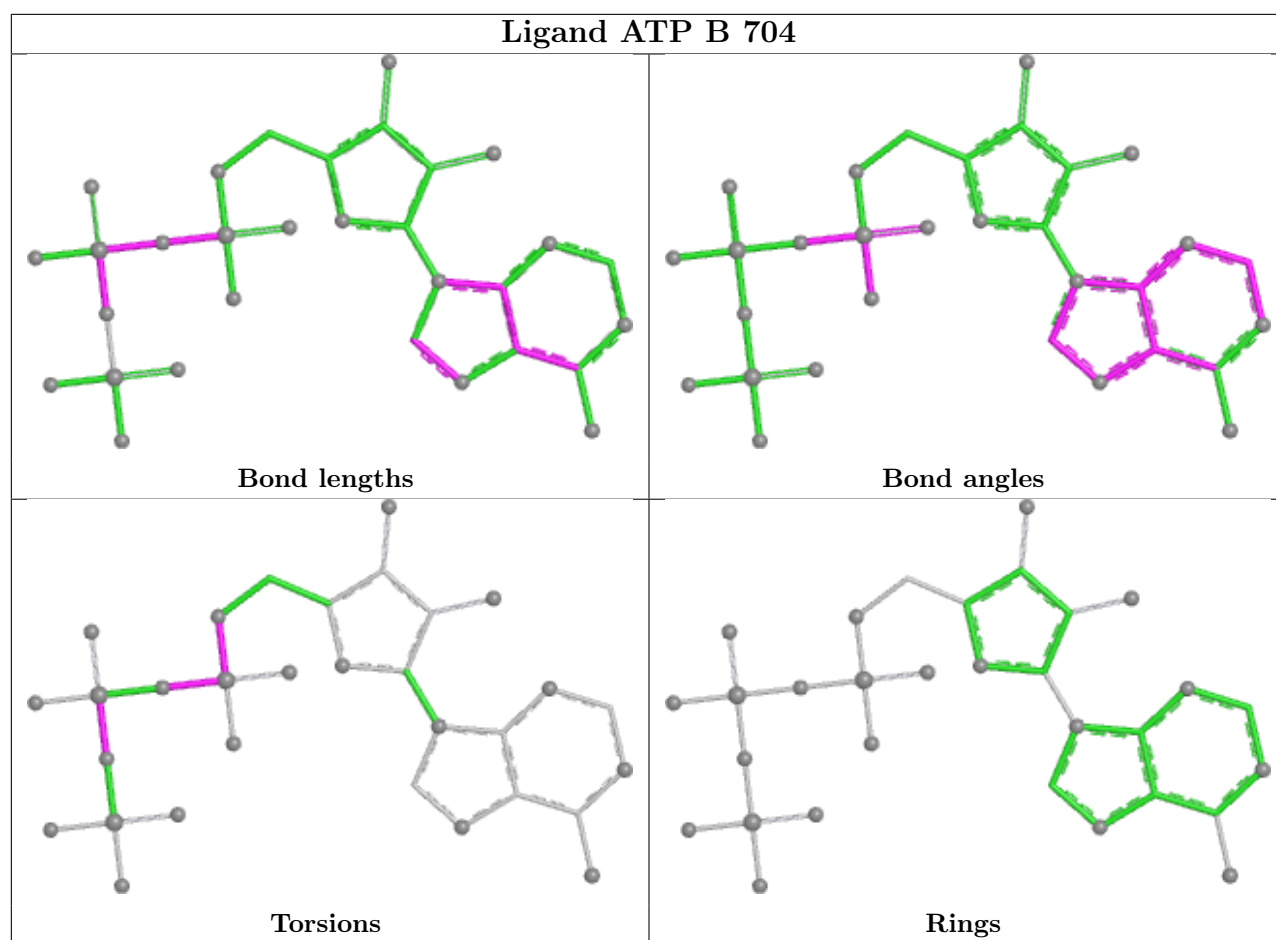
There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	711	PO4	1	0
2	A	703	GOL	2	0
2	B	703	GOL	2	0
4	B	706	SO4	2	0
3	A	706	ATP	1	0
3	B	704	ATP	1	0
2	A	702	GOL	1	0
2	B	701	GOL	1	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	606/606 (100%)	-0.16	27 (4%)	38	41	6, 24, 67, 135	11 (1%)
1	B	606/606 (100%)	-0.16	21 (3%)	47	51	6, 24, 66, 134	10 (1%)
All	All	1212/1212 (100%)	-0.16	48 (3%)	42	46	6, 24, 66, 135	21 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	PRO	5.6
1	B	483	ILE	5.4
1	B	487	PRO	4.9
1	B	490	VAL	4.9
1	A	485	PRO	4.8
1	B	485	PRO	4.7
1	A	515	GLY	4.7
1	B	486	ALA	4.4
1	B	482	GLY	4.1
1	A	483	ILE	4.0
1	A	486	ALA	4.0
1	A	482	GLY	3.9
1	B	515	GLY	3.8
1	B	514	THR	3.6
1	A	489	GLY	3.5
1	A	484	PRO	3.3
1	A	513	GLY	3.3
1	A	481	THR	3.2
1	B	484	PRO	3.2
1	A	577	LYS	3.1
1	B	579	GLY	3.0
1	A	488	ARG	3.0
1	A	517	LYS	2.9
1	B	488	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	577	LYS	2.9
1	A	490	VAL	2.8
1	A	579	GLY	2.8
1	B	454	GLY	2.8
1	A	123	LYS	2.7
1	B	518	ASN	2.7
1	B	481	THR	2.7
1	A	413	ASP	2.6
1	A	516	ASN	2.6
1	A	518	ASN	2.6
1	A	410	ASP	2.6
1	B	491	PRO	2.5
1	B	513	GLY	2.5
1	A	514	THR	2.4
1	A	386	ARG	2.3
1	A	519	LYS	2.3
1	B	455	GLY	2.2
1	A	412	GLY	2.2
1	B	527	ASN	2.2
1	A	527	ASN	2.1
1	B	516	ASN	2.1
1	B	627	ILE	2.0
1	A	572	ILE	2.0
1	A	455	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

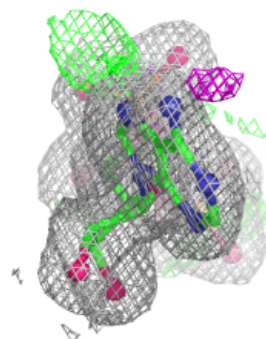
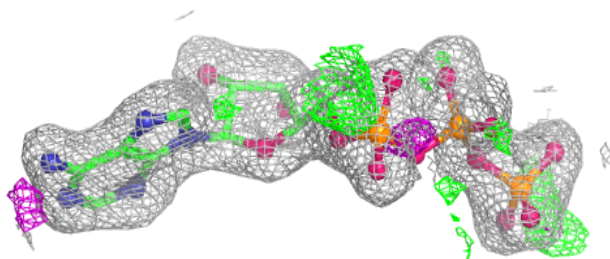
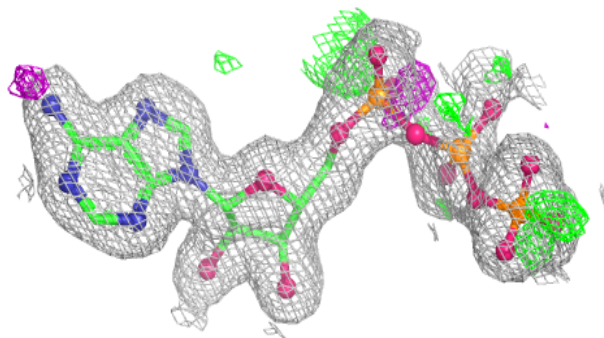
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	704	6/6	0.67	0.15	48,56,57,60	0
2	GOL	A	705	6/6	0.70	0.16	63,72,74,76	0
2	GOL	B	703	6/6	0.70	0.18	55,58,63,67	0
2	GOL	B	701	6/6	0.74	0.21	65,74,81,81	0
2	GOL	A	703	6/6	0.74	0.20	58,61,65,67	0
2	GOL	B	702	6/6	0.78	0.13	40,54,55,58	0
5	PO4	B	712	5/5	0.79	0.14	74,77,80,80	0
5	PO4	A	714	5/5	0.80	0.12	79,84,87,88	0
2	GOL	A	701	6/6	0.81	0.15	54,58,63,66	0
4	SO4	B	707	5/5	0.81	0.17	106,106,107,109	0
4	SO4	B	708	5/5	0.84	0.12	100,101,102,104	0
5	PO4	B	710	5/5	0.85	0.15	76,79,82,86	0
5	PO4	B	711	5/5	0.85	0.13	86,91,93,94	0
5	PO4	A	716	5/5	0.85	0.15	77,81,83,83	0
4	SO4	A	710	5/5	0.86	0.13	94,95,96,97	0
2	GOL	A	702	6/6	0.86	0.16	62,75,80,81	0
5	PO4	A	715	5/5	0.87	0.12	60,63,67,70	0
5	PO4	B	709	5/5	0.88	0.13	74,76,78,79	0
4	SO4	A	709	5/5	0.88	0.10	65,71,74,79	0
4	SO4	B	705	5/5	0.89	0.11	77,79,80,82	0
5	PO4	A	711	5/5	0.90	0.13	71,75,77,77	0
4	SO4	B	706	5/5	0.90	0.10	71,77,78,81	0
4	SO4	A	708	5/5	0.90	0.08	91,92,94,94	0
4	SO4	A	707	5/5	0.90	0.10	74,76,78,79	0
5	PO4	A	712	5/5	0.92	0.10	50,53,53,53	0
5	PO4	A	713	5/5	0.93	0.09	48,49,51,53	0
3	ATP	A	706	31/31	0.96	0.07	17,22,32,129	2
3	ATP	B	704	31/31	0.97	0.07	18,22,31,123	2

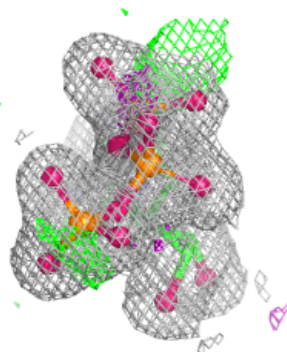
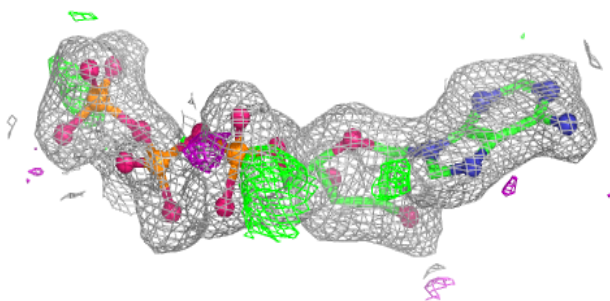
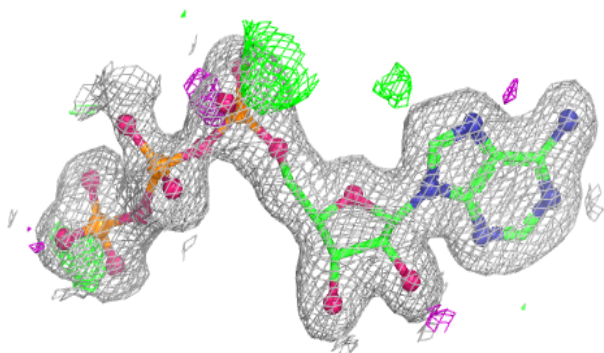
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 706:

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

**Electron density around ATP B 704:**

$2mF_o-DF_c$ (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.