



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 AM UTC

PDB ID : 5C93 / pdb_00005c93
Title : Histidine kinase with ATP
Authors : Cai, Y.
Deposited on : 2015-06-26
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 : 4-5-2 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

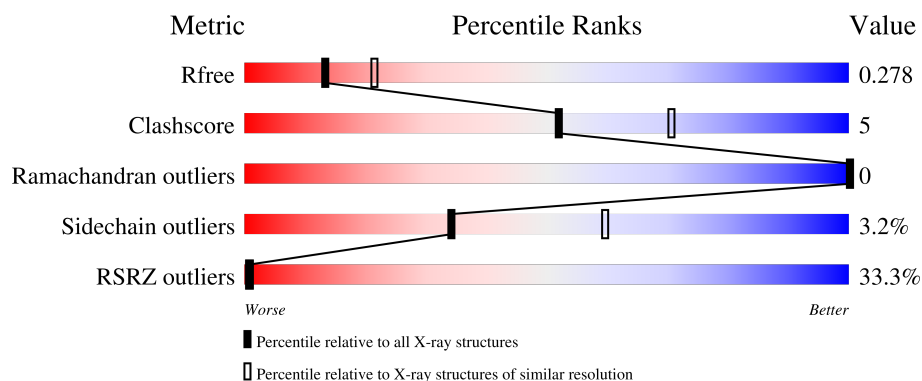
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (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	255	30% 80% 11% 8%
1	B	255	29% 73% 14% 13%

2 Entry composition [i](#)

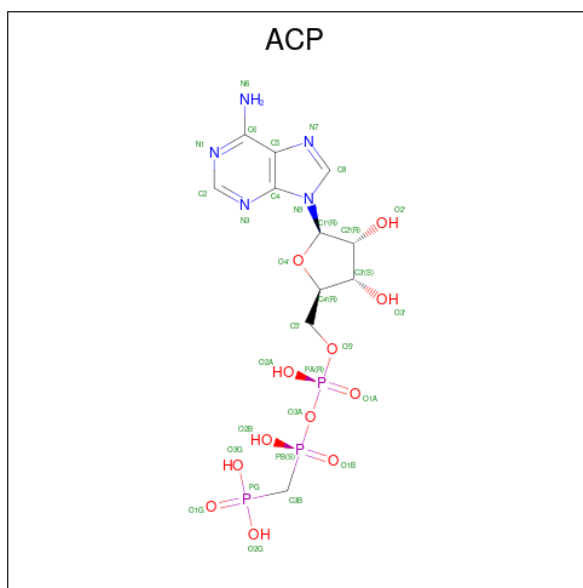
There are 4 unique types of molecules in this entry. The entry contains 3754 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	1	0
			1891	1193	325	364	9			
1	B	221	Total	C	N	O	S	0	0	0
			1775	1125	305	337	8			

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

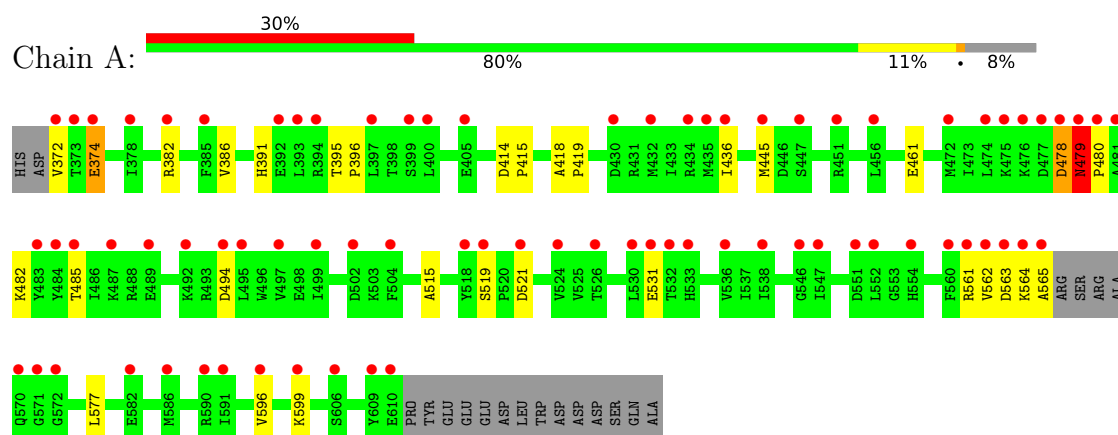
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	4	Total	O	0	0
			4	4		

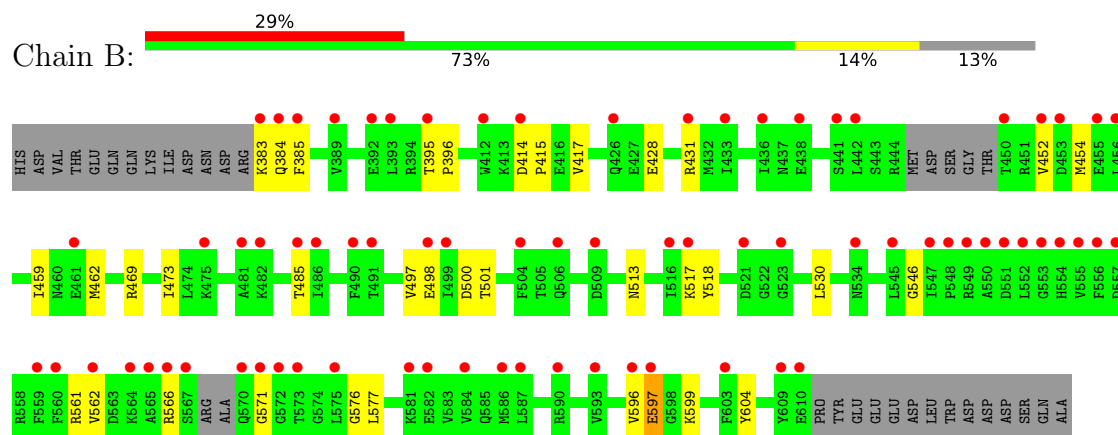
3 Residue-property plots

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: Histidine kinase



● Molecule 1: Histidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.65Å 97.76Å 117.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.01 – 2.52 37.01 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.0 (37.01-2.52) 86.4 (37.01-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.274 0.234 , 0.278	Depositor DCC
R_{free} test set	1040 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3754	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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, ACP

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	0.31	0/1926	0.97	8/2599 (0.3%)
1	B	0.30	0/1805	0.77	1/2434 (0.0%)
All	All	0.31	0/3731	0.88	9/5033 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ASP	N-CA-C	-23.09	71.77	109.40
1	A	479	ASN	N-CA-C	-12.90	81.30	109.81
1	A	478	ASP	CB-CA-C	-8.66	92.83	109.37
1	A	564	LYS	CB-CA-C	7.14	120.66	110.24
1	A	564	LYS	N-CA-C	-7.10	95.92	108.13
1	A	479	ASN	N-CA-CB	-6.33	99.10	110.37
1	A	562	VAL	CB-CA-C	5.26	119.91	111.29
1	B	384	GLN	N-CA-C	-5.06	105.89	111.71
1	A	565	ALA	N-CA-CB	5.05	117.98	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1891	0	1881	17	1
1	B	1775	0	1774	23	1
2	A	31	0	14	3	0
2	B	31	0	14	6	0
3	A	15	0	0	1	0
3	B	5	0	0	1	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
All	All	3754	0	3683	38	1

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 5.

All (38) 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:561:ARG:HA	2:A:701:ACP:O3'	1.69	0.91
1:B:577:LEU:HD12	2:B:701:ACP:H5'2	1.59	0.82
1:A:577:LEU:HD12	2:A:701:ACP:H5'1	1.66	0.77
1:A:478:ASP:O	1:A:480:PRO:CD	2.37	0.73
1:A:478:ASP:O	1:A:480:PRO:N	2.23	0.71
1:A:382:ARG:HG3	1:B:383:LYS:HE3	1.74	0.70
1:B:562:VAL:HB	1:B:566:ARG:HH22	1.60	0.66
1:B:546:GLY:HA3	1:B:597:GLU:HA	1.77	0.65
1:B:395:THR:OG1	3:B:702:SO4:O4	2.14	0.65
1:A:478:ASP:O	1:A:480:PRO:HD3	1.97	0.64
1:B:518:TYR:CZ	2:B:701:ACP:H2'	2.34	0.61
1:B:518:TYR:CE2	2:B:701:ACP:H2'	2.37	0.60
1:B:576:GLY:N	2:B:701:ACP:O1A	2.36	0.59
1:B:561:ARG:HH21	1:B:571:GLY:HA3	1.68	0.56
1:B:459:ILE:HD11	1:B:497:VAL:HB	1.88	0.56
1:B:462:MET:HE2	1:B:501:THR:HG23	1.91	0.51
1:A:372:VAL:N	1:A:374:GLU:OE2	2.42	0.51
1:A:596:VAL:HB	1:A:599:LYS:HE3	1.93	0.50
1:B:513:ASN:ND2	2:B:701:ACP:O3G	2.45	0.50
1:A:561:ARG:CA	2:A:701:ACP:O3'	2.54	0.49
1:B:396:PRO:HG3	1:B:431:ARG:NH1	2.27	0.49
1:A:391[B]:HIS:NE2	3:A:702:SO4:O3	2.45	0.49
1:B:517:LYS:HD3	2:B:701:ACP:O3G	2.12	0.48
1:B:561:ARG:NH2	1:B:571:GLY:HA3	2.28	0.48
1:B:562:VAL:HB	1:B:566:ARG:NH2	2.28	0.48
1:A:386:VAL:HG13	1:B:385:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ALA:O	1:A:519:SER:OG	2.26	0.46
1:B:599:LYS:HA	1:B:599:LYS:HD3	1.51	0.45
1:B:469:ARG:O	1:B:473:ILE:HG13	2.16	0.45
1:A:478:ASP:O	1:A:479:ASN:C	2.57	0.43
1:B:414:ASP:HB3	1:B:417:VAL:HG22	2.00	0.43
1:A:414:ASP:HA	1:A:415:PRO:HD3	1.87	0.42
1:B:452:VAL:HG23	1:B:500:ASP:HB2	2.00	0.42
1:A:395:THR:HB	1:A:396:PRO:HD3	2.01	0.42
1:A:482:LYS:HG3	1:A:521:ASP:HA	2.02	0.41
1:A:418:ALA:HB3	1:A:419:PRO:HD3	2.02	0.41
1:B:414:ASP:HA	1:B:415:PRO:HD3	1.85	0.41
1:B:454:MET:HE3	1:B:498:GLU:HB3	2.02	0.41

All (1) 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)
1:A:461:GLU:OE1	1:B:604:TYR:OH[4_445]	2.11	0.09

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	232/255 (91%)	223 (96%)	9 (4%)	0	100	100
1	B	215/255 (84%)	211 (98%)	4 (2%)	0	100	100
All	All	447/510 (88%)	434 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	212/229 (93%)	204 (96%)	8 (4%)	29	53
1	B	198/229 (86%)	193 (98%)	5 (2%)	42	67
All	All	410/458 (90%)	397 (97%)	13 (3%)	34	60

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

Mol	Chain	Res	Type
1	A	374	GLU
1	A	436	ILE
1	A	445	MET
1	A	479	ASN
1	A	485	THR
1	A	494	ASP
1	A	531	GLU
1	A	563	ASP
1	B	428	GLU
1	B	485	THR
1	B	530	LEU
1	B	596	VAL
1	B	597	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	ASN
1	B	391	HIS
1	B	479	ASN
1	B	535	GLN

5.3.3 RNA ⓘ

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](#)

6 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	$\# Z > 2$
3	SO4	A	704	-	4,4,4	0.25	0	6,6,6	0.09	0
2	ACP	A	701	-	31,33,33	2.11	10 (32%)	47,52,52	1.85	10 (21%)
3	SO4	A	702	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	703	-	4,4,4	0.23	0	6,6,6	0.07	0
2	ACP	B	701	-	31,33,33	2.10	10 (32%)	47,52,52	1.85	10 (21%)
3	SO4	B	702	-	4,4,4	0.25	0	6,6,6	0.06	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	ACP	A	701	-	-	0/19/38/38	0/3/3/3
2	ACP	B	701	-	-	3/19/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ACP	PG-O1G	5.53	1.61	1.50
2	A	701	ACP	PG-O1G	5.53	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ACP	C5-C4	4.75	1.47	1.39
2	B	701	ACP	C5-C4	4.70	1.47	1.39
2	B	701	ACP	PB-O1B	4.21	1.61	1.51
2	A	701	ACP	PB-O1B	4.19	1.61	1.51
2	A	701	ACP	PB-O2B	-3.27	1.48	1.56
2	B	701	ACP	PB-O2B	-3.26	1.48	1.56
2	B	701	ACP	PG-O3G	2.92	1.61	1.55
2	A	701	ACP	PG-O2G	-2.91	1.48	1.55
2	A	701	ACP	PG-O3G	2.91	1.61	1.55
2	B	701	ACP	PG-O2G	-2.90	1.48	1.55
2	B	701	ACP	PB-O3A	2.82	1.61	1.58
2	A	701	ACP	C5-C6	2.75	1.48	1.41
2	B	701	ACP	C5-C6	2.75	1.48	1.41
2	A	701	ACP	PB-O3A	2.71	1.61	1.58
2	A	701	ACP	C8-N7	2.38	1.36	1.31
2	B	701	ACP	C8-N7	2.31	1.36	1.31
2	A	701	ACP	C5-N7	-2.24	1.35	1.39
2	B	701	ACP	C5-N7	-2.20	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ACP	C5-C4-N3	-5.86	118.65	126.72
2	B	701	ACP	C5-C4-N3	-5.82	118.70	126.72
2	A	701	ACP	N3-C4-N9	4.61	135.01	127.17
2	B	701	ACP	N3-C4-N9	4.57	134.94	127.17
2	A	701	ACP	C2-N3-C4	3.71	120.89	111.83
2	B	701	ACP	C2-N3-C4	3.68	120.82	111.83
2	B	701	ACP	PB-O3A-PA	-3.65	120.45	132.37
2	A	701	ACP	PB-O3A-PA	-3.64	120.51	132.37
2	B	701	ACP	C4-C5-N7	-3.51	106.57	110.58
2	A	701	ACP	C4-C5-N7	-3.49	106.60	110.58
2	A	701	ACP	N3-C2-N1	-3.22	123.72	128.58
2	B	701	ACP	N3-C2-N1	-3.20	123.74	128.58
2	A	701	ACP	C4-N9-C8	2.58	108.45	105.74
2	B	701	ACP	C3'-C2'-C1'	2.56	106.31	101.46
2	A	701	ACP	C5-N7-C8	2.56	107.47	103.45
2	A	701	ACP	C3'-C2'-C1'	2.55	106.29	101.46
2	B	701	ACP	C5-N7-C8	2.55	107.45	103.45
2	B	701	ACP	C4-N9-C8	2.54	108.41	105.74
2	B	701	ACP	C6-C5-N7	2.09	136.11	132.09
2	A	701	ACP	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

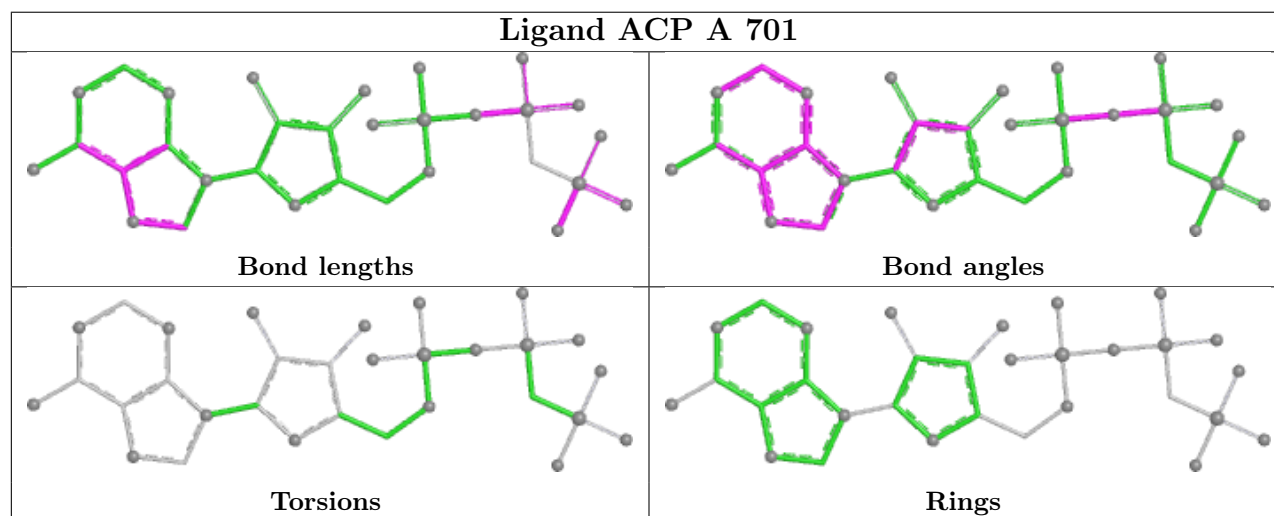
Mol	Chain	Res	Type	Atoms
2	B	701	ACP	C5'-O5'-PA-O1A
2	B	701	ACP	C5'-O5'-PA-O2A
2	B	701	ACP	C5'-O5'-PA-O3A

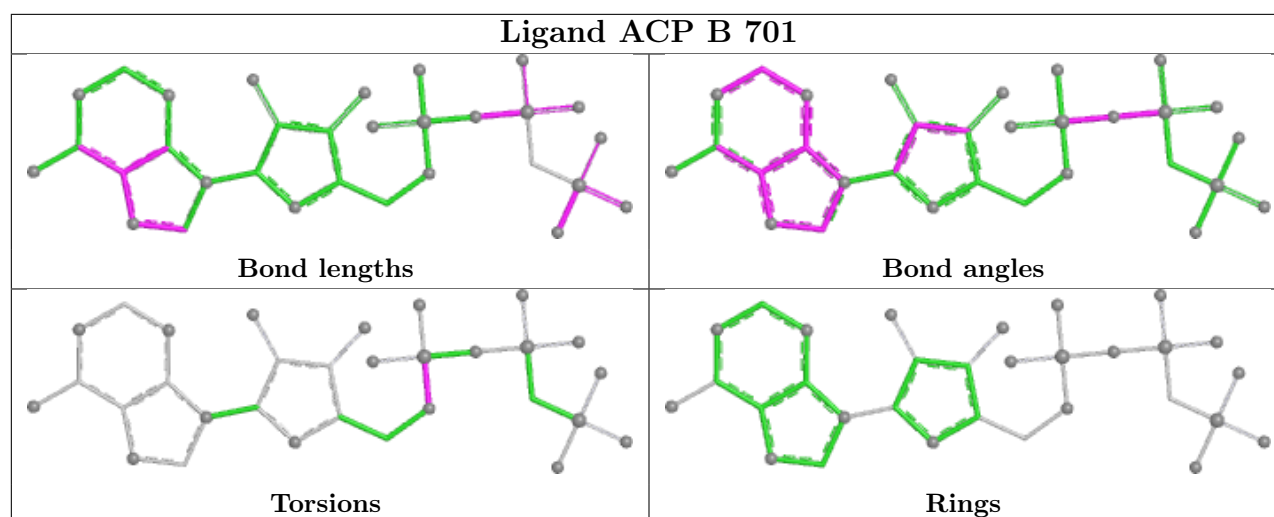
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ACP	3	0
3	A	702	SO4	1	0
2	B	701	ACP	6	0
3	B	702	SO4	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	235/255 (92%)	1.77	77 (32%)  	36, 66, 103, 162	1 (0%)
1	B	221/255 (86%)	1.77	75 (33%)  	49, 72, 111, 134	0
All	All	456/510 (89%)	1.77	152 (33%)  	36, 69, 110, 162	1 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	562	VAL	6.4
1	B	570	GLN	5.8
1	A	373	THR	5.5
1	A	372	VAL	5.1
1	B	385	PHE	5.0
1	A	565	ALA	4.8
1	B	450	THR	4.8
1	B	565	ALA	4.1
1	B	482	LYS	4.1
1	B	550	ALA	3.9
1	A	599	LYS	3.9
1	B	499	ILE	3.8
1	B	384	GLN	3.7
1	B	596	VAL	3.6
1	A	571	GLY	3.6
1	A	478	ASP	3.6
1	A	378	ILE	3.6
1	B	572	GLY	3.6
1	A	532	THR	3.5
1	A	394	ARG	3.5
1	A	563	ASP	3.5
1	A	519	SER	3.5
1	B	523	GLY	3.5
1	A	564	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	475	LYS	3.4
1	B	566	ARG	3.4
1	B	504	PHE	3.4
1	B	452	VAL	3.4
1	B	547	ILE	3.3
1	B	509	ASP	3.3
1	B	552	LEU	3.3
1	A	610	GLU	3.2
1	A	481	ALA	3.2
1	A	494	ASP	3.2
1	A	521	ASP	3.2
1	B	567	SER	3.1
1	B	442	LEU	3.1
1	A	477	ASP	3.1
1	A	484	TYR	3.0
1	B	590	ARG	3.0
1	A	572	GLY	3.0
1	A	476	LYS	3.0
1	A	479	ASN	2.9
1	B	575	LEU	2.9
1	A	385	PHE	2.9
1	A	502	ASP	2.9
1	A	487	LYS	2.9
1	B	559	PHE	2.9
1	A	499	ILE	2.8
1	B	392	GLU	2.8
1	B	498	GLU	2.8
1	B	438	GLU	2.8
1	A	474	LEU	2.7
1	A	495	LEU	2.7
1	A	570	GLN	2.7
1	B	584	VAL	2.7
1	A	400	LEU	2.7
1	A	606	SER	2.7
1	B	545	LEU	2.7
1	B	481	ALA	2.7
1	B	453	ASP	2.7
1	A	504	PHE	2.7
1	A	489	GLU	2.6
1	B	582	GLU	2.6
1	A	551	ASP	2.6
1	A	392	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	497	VAL	2.6
1	A	560	PHE	2.6
1	B	610	GLU	2.6
1	A	485	THR	2.6
1	B	485	THR	2.6
1	A	609	TYR	2.6
1	B	556	PHE	2.6
1	B	587	LEU	2.6
1	A	591	ILE	2.5
1	B	516	ILE	2.5
1	B	426	GLN	2.5
1	B	562	VAL	2.5
1	B	564	LYS	2.5
1	B	549	ARG	2.5
1	A	456	LEU	2.5
1	A	533	HIS	2.5
1	B	456	LEU	2.5
1	A	434	ARG	2.5
1	B	571	GLY	2.4
1	A	518	TYR	2.4
1	B	486	ILE	2.4
1	A	552	LEU	2.4
1	A	590	ARG	2.4
1	A	399	SER	2.4
1	A	393	LEU	2.4
1	A	530	LEU	2.4
1	A	524	VAL	2.4
1	A	547	ILE	2.4
1	B	551	ASP	2.4
1	A	546	GLY	2.3
1	B	414	ASP	2.3
1	A	445	MET	2.3
1	A	430	ASP	2.3
1	B	521	ASP	2.3
1	B	431	ARG	2.3
1	B	436	ILE	2.3
1	A	432	MET	2.3
1	B	490	PHE	2.3
1	B	389	VAL	2.3
1	B	609	TYR	2.3
1	B	597	GLU	2.3
1	A	382	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	561	ARG	2.3
1	B	554	HIS	2.2
1	B	581	LYS	2.2
1	B	455	GLU	2.2
1	B	461	GLU	2.2
1	B	555	VAL	2.2
1	A	492	LYS	2.2
1	B	553	GLY	2.2
1	B	412	TRP	2.2
1	A	374	GLU	2.2
1	A	480	PRO	2.2
1	B	573	THR	2.2
1	B	433	ILE	2.2
1	A	405	GLU	2.2
1	B	548	PRO	2.2
1	B	557	ASP	2.2
1	A	596	VAL	2.1
1	B	506	GLN	2.1
1	B	534	ASN	2.1
1	B	586	MET	2.1
1	B	393	LEU	2.1
1	A	483	TYR	2.1
1	A	531	GLU	2.1
1	A	582	GLU	2.1
1	B	441	SER	2.1
1	B	517	LYS	2.1
1	B	491	THR	2.1
1	B	475	LYS	2.1
1	A	472	MET	2.1
1	A	447	SER	2.1
1	B	603	PHE	2.1
1	A	451	ARG	2.1
1	A	526	THR	2.1
1	A	586	MET	2.1
1	A	536	VAL	2.0
1	B	593	VAL	2.0
1	A	436	ILE	2.0
1	B	395	THR	2.0
1	B	560	PHE	2.0
1	A	397	LEU	2.0
1	B	383	LYS	2.0
1	A	538	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	435	MET	2.0
1	A	554	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

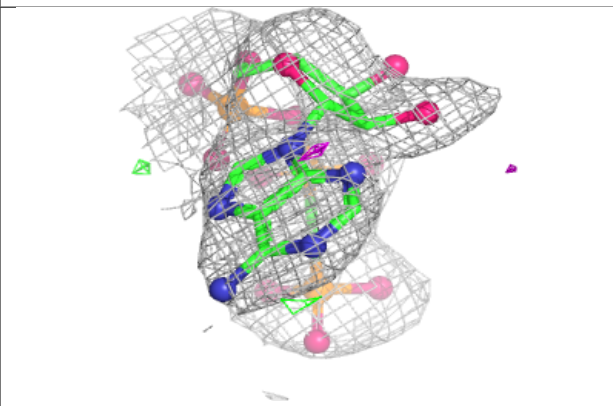
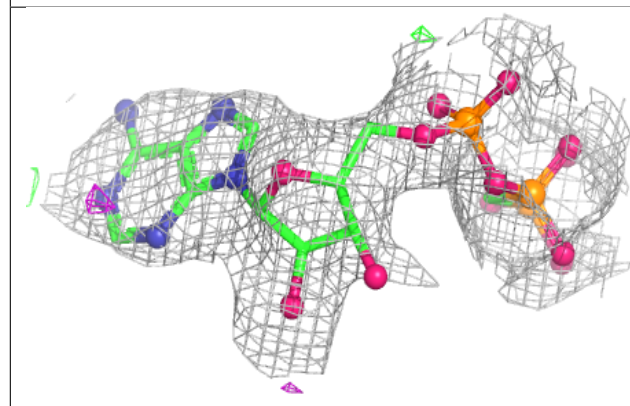
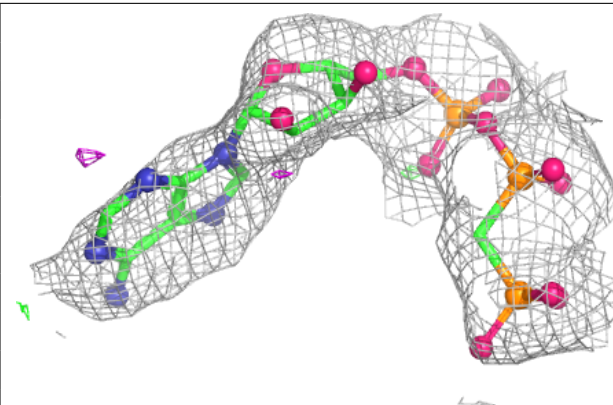
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	702	5/5	0.47	0.24	179,182,184,184	0
3	SO4	A	702	5/5	0.65	0.18	164,164,164,166	0
3	SO4	A	704	5/5	0.69	0.17	123,130,133,135	0
3	SO4	A	703	5/5	0.78	0.14	79,89,97,97	0
2	ACP	B	701	31/31	0.81	0.15	60,91,116,167	0
2	ACP	A	701	31/31	0.82	0.15	52,67,119,155	0

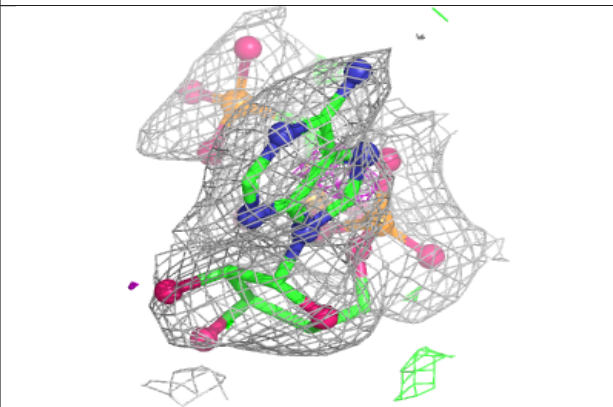
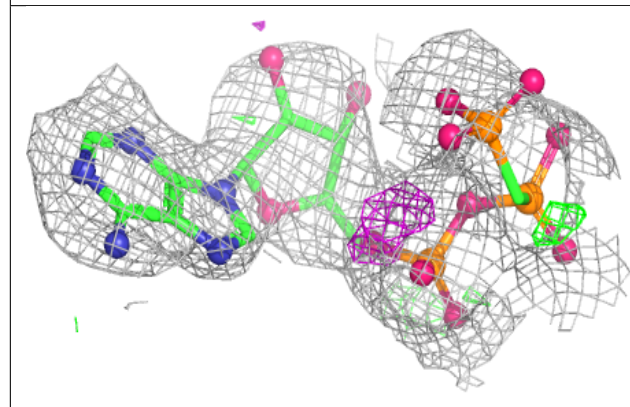
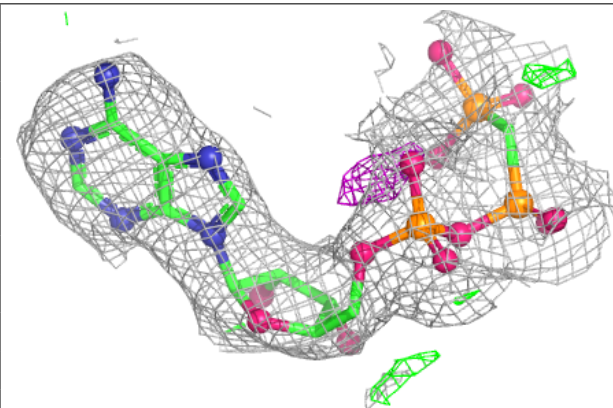
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP B 701:

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

**Electron density around ACP A 701:**

$2mF_o-DF_c$ (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.