



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:17 AM UTC

PDB ID : 2XE8 / pdb_00002xe8
Title : The complete reaction cycle of human phosphoglycerate kinase: The open ternary complex with 3PG and AMP-PNP
Authors : Cliff, M.J.; Baxter, N.J.; Blackburn, G.M.; Merli, A.; Vas, M.; Waltho, J.P.; Bowler, M.W.
Deposited on : 2010-05-11
Resolution : 1.79 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

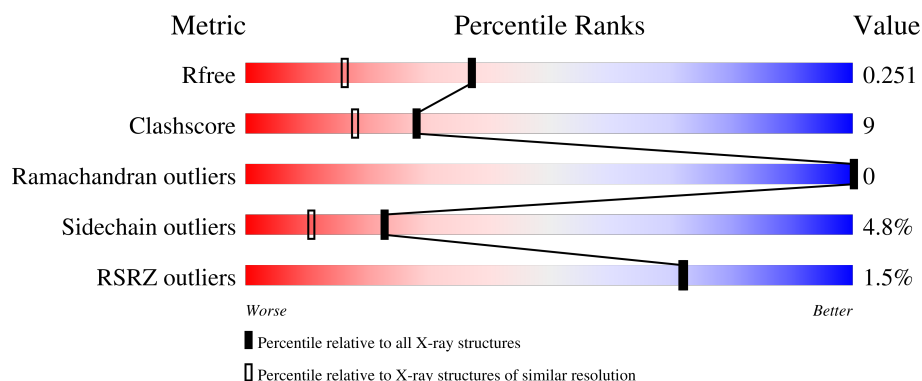
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	417	

2 Entry composition [i](#)

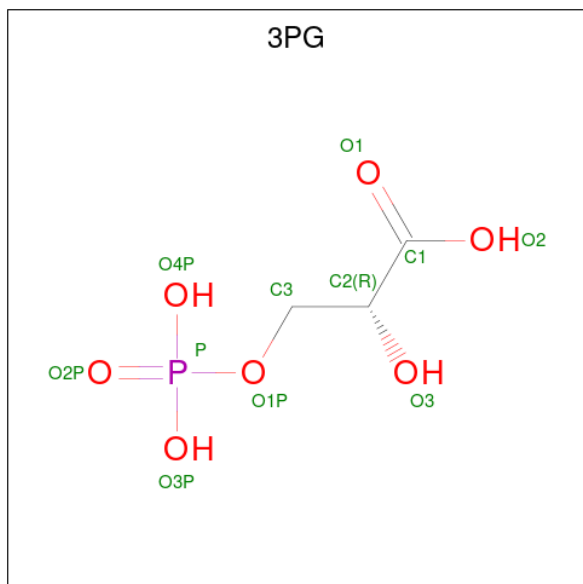
There are 4 unique types of molecules in this entry. The entry contains 3296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOGLYCERATE KINASE 1.

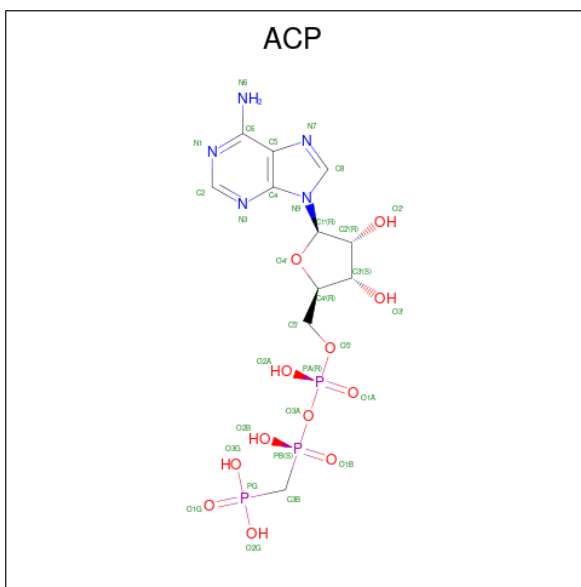
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3114	1973	533	588	20	0	3	0

- Molecule 2 is 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	11	3	7	1	0	0

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

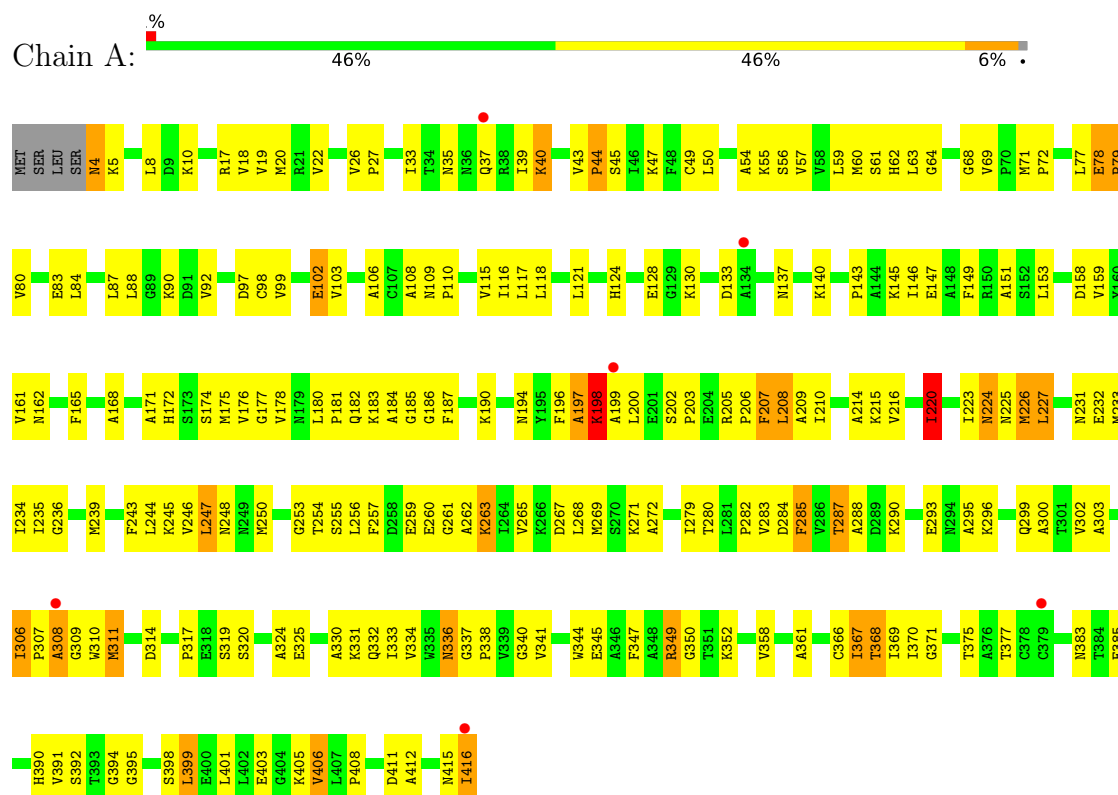
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	140	Total O 140 140	0	0

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: PHOSPHOGLYCERATE KINASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	59.32Å 71.17Å 91.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.79 20.00 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-1.79) 98.1 (20.00-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.198 , 0.243 0.206 , 0.251	Depositor DCC
R_{free} test set	1842 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3296	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: 3PG, 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	2.36	182/3169 (5.7%)	1.15	8/4273 (0.2%)

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306[A]	ILE	N-CA	-17.84	1.30	1.46
1	A	306[B]	ILE	N-CA	-17.84	1.30	1.46
1	A	19	VAL	C-O	-9.04	1.14	1.24
1	A	20	MET	C-O	-9.02	1.13	1.24
1	A	306[A]	ILE	CA-C	8.44	1.59	1.53
1	A	306[B]	ILE	CA-C	8.44	1.59	1.53
1	A	333	ILE	C-O	-8.36	1.15	1.24
1	A	224	ASN	C-O	-8.26	1.14	1.24
1	A	399	LEU	C-O	-8.21	1.14	1.24
1	A	45	SER	C-O	-8.09	1.14	1.24
1	A	257	PHE	C-O	-8.08	1.14	1.23
1	A	331	LYS	C-N	-7.91	1.23	1.33
1	A	18	VAL	C-O	-7.91	1.15	1.24
1	A	55	LYS	C-O	-7.88	1.14	1.24
1	A	57	VAL	C-O	-7.84	1.15	1.24
1	A	161	VAL	C-O	-7.82	1.16	1.24
1	A	319	SER	C-O	-7.74	1.15	1.24
1	A	60	MET	C-O	-7.73	1.14	1.23
1	A	130	LYS	C-O	-7.72	1.15	1.23
1	A	26	VAL	C-O	-7.52	1.15	1.24
1	A	63	LEU	C-O	-7.51	1.15	1.23
1	A	337	GLY	C-O	-7.49	1.13	1.24
1	A	225	ASN	C-O	-7.43	1.15	1.24
1	A	116	ILE	C-O	-7.38	1.16	1.24
1	A	368[A]	THR	N-CA	-7.34	1.37	1.46
1	A	368[B]	THR	N-CA	-7.34	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	GLY	C-O	-7.33	1.16	1.23
1	A	153	LEU	C-O	-7.30	1.15	1.24
1	A	367	ILE	C-O	-7.27	1.15	1.23
1	A	302	VAL	C-O	-7.26	1.15	1.24
1	A	235	ILE	C-O	-7.22	1.16	1.24
1	A	22	VAL	C-O	-7.22	1.16	1.23
1	A	80	VAL	C-O	-7.19	1.15	1.24
1	A	118	LEU	C-O	-7.06	1.14	1.23
1	A	303	ALA	CA-CB	-7.03	1.42	1.53
1	A	84	LEU	C-O	-6.90	1.15	1.24
1	A	287	THR	C-O	-6.90	1.15	1.23
1	A	334	VAL	C-O	-6.88	1.16	1.24
1	A	182	GLN	C-O	-6.85	1.15	1.24
1	A	61	SER	C-O	-6.85	1.15	1.23
1	A	151	ALA	CA-CB	-6.83	1.42	1.53
1	A	243	PHE	C-O	-6.83	1.16	1.24
1	A	49	CYS	C-O	-6.80	1.16	1.24
1	A	186	GLY	C-O	-6.77	1.15	1.23
1	A	177	GLY	C-O	-6.73	1.19	1.24
1	A	282	PRO	C-O	-6.70	1.16	1.23
1	A	246	VAL	C-O	-6.66	1.16	1.24
1	A	87	LEU	C-O	-6.65	1.16	1.24
1	A	412	ALA	C-O	-6.62	1.15	1.24
1	A	103	VAL	C-O	-6.60	1.16	1.24
1	A	262	ALA	C-O	-6.57	1.15	1.24
1	A	185	GLY	C-O	-6.53	1.17	1.23
1	A	140	LYS	C-O	-6.49	1.16	1.24
1	A	391	VAL	C-O	-6.48	1.17	1.24
1	A	245	LYS	C-O	-6.46	1.16	1.24
1	A	178	VAL	C-O	-6.46	1.17	1.24
1	A	110	PRO	C-O	-6.42	1.16	1.23
1	A	33	ILE	C-O	-6.39	1.17	1.24
1	A	293	GLU	C-O	-6.37	1.16	1.24
1	A	262	ALA	CA-CB	-6.37	1.42	1.53
1	A	121	LEU	C-O	-6.35	1.16	1.24
1	A	92	VAL	C-O	-6.35	1.17	1.24
1	A	187	PHE	C-O	-6.34	1.16	1.24
1	A	78	GLU	C-O	-6.33	1.18	1.24
1	A	208	LEU	C-O	-6.33	1.16	1.24
1	A	202	SER	C-O	-6.31	1.17	1.23
1	A	115	VAL	C-O	-6.28	1.17	1.24
1	A	311	MET	C-O	-6.24	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	VAL	CA-CB	-6.22	1.46	1.54
1	A	392	SER	C-O	-6.19	1.16	1.23
1	A	406	VAL	C-O	-6.19	1.16	1.24
1	A	256	LEU	C-O	-6.13	1.16	1.23
1	A	68	GLY	C-O	-6.13	1.15	1.23
1	A	285	PHE	C-O	-6.12	1.16	1.23
1	A	271	LYS	C-O	-6.12	1.17	1.24
1	A	295	ALA	CA-CB	-6.07	1.43	1.53
1	A	183	LYS	C-O	-6.07	1.17	1.24
1	A	390	HIS	C-O	-6.07	1.17	1.23
1	A	279	ILE	C-O	-6.06	1.17	1.24
1	A	369	ILE	C-O	-6.06	1.17	1.24
1	A	137	ASN	C-O	-6.03	1.16	1.23
1	A	165	PHE	C-O	-6.03	1.17	1.24
1	A	197	ALA	CA-CB	-6.00	1.43	1.53
1	A	145	LYS	C-O	-6.00	1.17	1.24
1	A	83	GLU	C-O	-5.98	1.17	1.24
1	A	210	ILE	C-O	-5.97	1.17	1.24
1	A	361	ALA	C-O	-5.95	1.17	1.24
1	A	317	PRO	C-O	-5.90	1.16	1.24
1	A	175	MET	C-O	-5.89	1.16	1.24
1	A	176	VAL	C-O	-5.89	1.17	1.24
1	A	239	MET	C-O	-5.88	1.16	1.24
1	A	314	ASP	C-O	-5.86	1.16	1.23
1	A	233	MET	C-O	-5.86	1.17	1.23
1	A	146	ILE	C-O	-5.85	1.17	1.24
1	A	377	THR	C-O	-5.85	1.17	1.24
1	A	69	VAL	C-O	-5.84	1.17	1.24
1	A	8	LEU	C-O	-5.83	1.17	1.24
1	A	250	MET	C-O	-5.83	1.16	1.23
1	A	190	LYS	C-O	-5.83	1.17	1.24
1	A	99	VAL	C-O	-5.80	1.16	1.23
1	A	102	GLU	C-O	-5.80	1.17	1.24
1	A	401	LEU	C-O	-5.80	1.17	1.24
1	A	39	ILE	C-O	-5.79	1.17	1.24
1	A	295	ALA	C-O	-5.76	1.16	1.23
1	A	159	VAL	C-O	-5.75	1.17	1.23
1	A	236	GLY	C-O	-5.75	1.16	1.23
1	A	336	ASN	C-O	-5.74	1.17	1.23
1	A	117	LEU	C-O	-5.73	1.17	1.24
1	A	59	LEU	C-O	-5.71	1.17	1.24
1	A	27	PRO	C-O	-5.66	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	LYS	C-O	-5.66	1.16	1.23
1	A	253	GLY	C-O	-5.66	1.16	1.24
1	A	227	LEU	C-O	-5.65	1.16	1.24
1	A	395	GLY	C-O	-5.64	1.16	1.23
1	A	209	ALA	C-O	-5.63	1.17	1.24
1	A	207	PHE	C-O	-5.63	1.17	1.24
1	A	184	ALA	CA-CB	-5.62	1.43	1.53
1	A	255	SER	C-O	-5.60	1.16	1.23
1	A	220	ILE	C-O	-5.60	1.17	1.24
1	A	88	LEU	C-O	-5.58	1.16	1.24
1	A	172	HIS	C-O	-5.57	1.16	1.23
1	A	143	PRO	C-O	-5.56	1.17	1.24
1	A	50	LEU	C-O	-5.55	1.17	1.24
1	A	162	ASN	C-O	-5.55	1.17	1.24
1	A	288	ALA	C-O	-5.54	1.17	1.23
1	A	62	HIS	C-O	-5.53	1.16	1.23
1	A	338	PRO	C-O	-5.52	1.17	1.23
1	A	79	PRO	C-O	-5.50	1.17	1.24
1	A	341	VAL	C-O	-5.47	1.17	1.24
1	A	366	CYS	C-O	-5.47	1.17	1.23
1	A	361	ALA	CA-CB	-5.46	1.44	1.53
1	A	226	MET	SD-CE	-5.45	1.66	1.79
1	A	54	ALA	C-O	-5.45	1.17	1.23
1	A	320	SER	C-O	-5.44	1.17	1.24
1	A	347	PHE	C-O	-5.42	1.16	1.24
1	A	232	GLU	C-O	-5.42	1.17	1.23
1	A	72	PRO	C-O	-5.40	1.17	1.24
1	A	106	ALA	C-O	-5.40	1.17	1.24
1	A	35	ASN	C-O	-5.38	1.18	1.23
1	A	375	THR	C-O	-5.36	1.17	1.24
1	A	71	MET	C-O	-5.36	1.17	1.23
1	A	168	ALA	C-O	-5.34	1.17	1.24
1	A	350	GLY	C-O	-5.33	1.17	1.23
1	A	272	ALA	CA-CB	-5.32	1.45	1.53
1	A	47	LYS	C-O	-5.32	1.17	1.24
1	A	56	SER	C-O	-5.31	1.17	1.23
1	A	44	PRO	C-O	-5.30	1.17	1.24
1	A	194	ASN	C-O	-5.30	1.18	1.24
1	A	283	VAL	C-O	-5.29	1.18	1.24
1	A	280	THR	C-O	-5.27	1.17	1.24
1	A	147	GLU	C-O	-5.26	1.18	1.24
1	A	352	LYS	C-O	-5.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	ARG	C-O	-5.25	1.17	1.24
1	A	98	CYS	C-O	-5.25	1.17	1.24
1	A	345	GLU	C-O	-5.25	1.18	1.24
1	A	330	ALA	C-O	-5.24	1.17	1.23
1	A	324	ALA	C-O	-5.23	1.18	1.24
1	A	367	ILE	CG1-CD1	-5.21	1.31	1.51
1	A	174	SER	C-O	-5.21	1.17	1.24
1	A	158	ASP	C-O	-5.21	1.17	1.24
1	A	108	ALA	C-O	-5.19	1.18	1.24
1	A	290	LYS	C-O	-5.19	1.17	1.23
1	A	149	PHE	C-O	-5.18	1.18	1.24
1	A	296	LYS	C-O	-5.18	1.17	1.23
1	A	128	GLU	C-O	-5.16	1.17	1.24
1	A	403	GLU	C-O	-5.16	1.17	1.24
1	A	90	LYS	C-O	-5.15	1.17	1.23
1	A	40	LYS	C-O	-5.14	1.17	1.24
1	A	234	ILE	C-O	-5.14	1.18	1.24
1	A	261	GLY	C-O	-5.13	1.17	1.23
1	A	268	LEU	C-O	-5.09	1.18	1.24
1	A	77	LEU	C-O	-5.07	1.17	1.24
1	A	408	PRO	C-O	-5.07	1.18	1.24
1	A	223	ILE	C-O	-5.06	1.18	1.24
1	A	325	GLU	C-O	-5.05	1.18	1.24
1	A	267	ASP	C-O	-5.04	1.18	1.24
1	A	344	TRP	C-O	-5.04	1.18	1.24
1	A	180	LEU	C-O	-5.02	1.16	1.24
1	A	109	ASN	C-O	-5.02	1.17	1.24
1	A	64	GLY	C-O	-5.02	1.16	1.23
1	A	171	ALA	CA-CB	-5.01	1.46	1.52
1	A	308	ALA	C-O	-5.00	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ALA	N-CA-C	9.16	121.04	111.14
1	A	247	LEU	N-CA-C	8.11	120.20	111.36
1	A	198	LYS	N-CA-C	-7.24	103.39	111.28
1	A	371	GLY	N-CA-C	-5.78	105.14	112.54
1	A	367	ILE	CB-CA-C	-5.43	104.35	111.25
1	A	246	VAL	N-CA-C	5.35	115.56	110.53
1	A	37	GLN	N-CA-C	-5.21	105.61	111.28
1	A	310	TRP	N-CA-C	-5.09	104.15	110.41

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	3114	0	3200	56	0
2	A	11	0	4	0	0
3	A	31	0	14	1	0
4	A	140	0	0	6	0
All	All	3296	0	3218	57	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 9.

All (57) 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:349:ARG:HG3	4:A:2121:HOH:O	1.16	1.32
1:A:207:PHE:H	1:A:231:ASN:HD22	1.16	0.92
1:A:254:THR:HG23	1:A:309:GLY:HA3	1.55	0.88
1:A:358:VAL:CG1	1:A:368[A]:THR:HG21	2.05	0.86
1:A:349:ARG:CG	4:A:2121:HOH:O	1.88	0.81
1:A:216:VAL:O	1:A:220:ILE:HD13	1.84	0.76
1:A:307:PRO:O	1:A:308:ALA:HB3	1.88	0.73
1:A:216:VAL:O	1:A:220:ILE:CD1	2.38	0.72
1:A:226:MET:HA	1:A:226:MET:HE2	1.75	0.69
1:A:40:LYS:HZ2	1:A:40:LYS:HB3	1.59	0.65
1:A:406:VAL:CG1	1:A:411:ASP:OD2	2.48	0.62
1:A:367:ILE:HD13	4:A:2129:HOH:O	2.01	0.61
1:A:358:VAL:HG12	1:A:368[A]:THR:HG21	1.84	0.60
1:A:254:THR:HG23	1:A:309:GLY:CA	2.30	0.60
1:A:349:ARG:HH11	1:A:349:ARG:HB2	1.66	0.59
1:A:200:LEU:CD2	1:A:226:MET:HE1	2.32	0.59
1:A:78:GLU:HB3	1:A:79:PRO:HD3	1.83	0.59
1:A:247:LEU:HD11	1:A:269:MET:HG3	1.85	0.59
1:A:311:MET:HE3	4:A:2106:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:VAL:HG13	1:A:368[A]:THR:HG21	1.84	0.58
1:A:358:VAL:CG1	1:A:368[A]:THR:CG2	2.80	0.57
1:A:205:ARG:HA	1:A:206:PRO:C	2.30	0.57
1:A:40:LYS:HB3	1:A:40:LYS:NZ	2.21	0.56
1:A:269:MET:HA	1:A:269:MET:HE2	1.86	0.56
1:A:220:ILE:HD13	1:A:220:ILE:N	2.23	0.53
1:A:216:VAL:HG12	1:A:220:ILE:HD11	1.90	0.53
1:A:199:ALA:HA	1:A:332[A]:GLN:OE1	2.08	0.53
3:A:1418:ACP:O2B	3:A:1418:ACP:O1A	2.26	0.53
1:A:349:ARG:HH11	1:A:349:ARG:CB	2.23	0.52
1:A:5:LYS:HD3	1:A:415:ASN:HD22	1.74	0.51
1:A:260:GLU:HA	1:A:263:LYS:HD2	1.91	0.51
1:A:40:LYS:NZ	1:A:40:LYS:CB	2.65	0.51
1:A:287:THR:HG22	1:A:306[A]:ILE:HD12	1.93	0.50
1:A:4:ASN:N	1:A:416:ILE:HG22	2.26	0.50
1:A:336:ASN:OD1	1:A:399:LEU:HD21	2.12	0.49
1:A:406:VAL:HG11	1:A:411:ASP:OD2	2.13	0.49
1:A:349:ARG:HB2	1:A:349:ARG:NH1	2.27	0.48
1:A:220:ILE:CD1	1:A:220:ILE:N	2.76	0.48
1:A:200:LEU:HD21	1:A:226:MET:HE1	1.94	0.48
1:A:181:PRO:HD2	4:A:2067:HOH:O	2.12	0.48
1:A:358:VAL:HG13	1:A:368[A]:THR:CG2	2.43	0.48
1:A:394:GLY:O	1:A:398:SER:HB3	2.15	0.47
1:A:383:ASN:CG	1:A:383:ASN:O	2.58	0.46
1:A:308:ALA:HA	1:A:309:GLY:HA2	1.53	0.46
1:A:4:ASN:C	1:A:4:ASN:ND2	2.74	0.45
1:A:244:LEU:HD23	1:A:248:ASN:HD22	1.81	0.45
1:A:43:VAL:N	1:A:44:PRO:CD	2.80	0.44
1:A:416:ILE:HD13	1:A:416:ILE:HA	1.84	0.44
1:A:197:ALA:O	1:A:198:LYS:C	2.59	0.43
1:A:284:ASP:C	1:A:285:PHE:CG	2.97	0.42
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.83	0.42
1:A:203:PRO:HA	1:A:332[A]:GLN:HE22	1.84	0.42
1:A:300:ALA:HB3	1:A:306[A]:ILE:HD13	2.02	0.42
1:A:97:ASP:OD1	1:A:124:HIS:HE1	2.02	0.42
1:A:196:PHE:CZ	1:A:398:SER:HB2	2.55	0.42
1:A:133:ASP:OD1	1:A:133:ASP:C	2.63	0.41
1:A:181:PRO:HG2	4:A:2067:HOH:O	2.21	0.41

There are no symmetry-related clashes.

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	414/417 (99%)	410 (99%)	4 (1%)	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	335/336 (100%)	319 (95%)	16 (5%)	23	11

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	10	LYS
1	A	102	GLU
1	A	198	LYS
1	A	208	LEU
1	A	215	LYS
1	A	220	ILE
1	A	224	ASN
1	A	259	GLU
1	A	263	LYS
1	A	265	VAL
1	A	299	GLN
1	A	349	ARG

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Mol	Chain	Res	Type
1	A	370	ILE
1	A	385	GLU
1	A	416	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	137	ASN
1	A	221	GLN
1	A	231	ASN
1	A	248	ASN
1	A	275	ASN
1	A	415	ASN

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](#)

2 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	ACP	A	1418	-	31,33,33	3.07	8 (25%)	47,52,52	2.47	21 (44%)
2	3PG	A	1417	-	9,10,10	0.68	0	11,14,14	2.42	4 (36%)

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
3	ACP	A	1418	-	-	7/19/38/38	0/3/3/3
2	3PG	A	1417	-	-	4/10/10/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1418	ACP	PB-O3A	8.80	1.68	1.58
3	A	1418	ACP	PG-O1G	8.51	1.67	1.50
3	A	1418	ACP	PB-O1B	6.80	1.67	1.51
3	A	1418	ACP	PG-O2G	4.79	1.65	1.55
3	A	1418	ACP	C5-N7	-4.23	1.31	1.39
3	A	1418	ACP	PA-O1A	3.86	1.64	1.50
3	A	1418	ACP	C4-N9	-3.07	1.31	1.37
3	A	1418	ACP	C8-N9	-2.04	1.34	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1418	ACP	N3-C2-N1	-7.35	117.45	128.58
2	A	1417	3PG	O2-C1-C2	6.01	125.46	112.74
3	A	1418	ACP	PB-O3A-PA	-5.90	113.10	132.37
3	A	1418	ACP	O3G-PG-C3B	4.31	116.86	106.40
3	A	1418	ACP	C2-N3-C4	4.02	121.65	111.83
3	A	1418	ACP	N9-C8-N7	-3.98	108.29	113.94
3	A	1418	ACP	C5-C4-N3	-3.78	121.51	126.72
3	A	1418	ACP	C5-N7-C8	3.37	108.75	103.45
3	A	1418	ACP	C2-N1-C6	3.37	124.26	118.73
2	A	1417	3PG	O2-C1-O1	-3.35	116.47	124.08
3	A	1418	ACP	C4-C5-N7	-3.30	106.81	110.58
3	A	1418	ACP	C4'-O4'-C1'	-3.18	102.44	109.47
3	A	1418	ACP	O2A-PA-O3A	2.92	115.17	107.27
3	A	1418	ACP	C4-N9-C8	2.73	108.60	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1418	ACP	O2G-PG-C3B	-2.57	100.17	106.40
3	A	1418	ACP	C6-C5-N7	2.42	136.76	132.09
3	A	1418	ACP	O2G-PG-O1G	-2.41	106.16	112.39
2	A	1417	3PG	O1-C1-C2	-2.38	117.84	122.60
3	A	1418	ACP	C2'-C1'-N9	-2.36	107.44	113.30
3	A	1418	ACP	N3-C4-N9	2.24	130.98	127.17
3	A	1418	ACP	O1G-PG-C3B	-2.19	106.60	111.37
3	A	1418	ACP	O2B-PB-O1B	2.18	117.04	109.95
3	A	1418	ACP	O5'-C5'-C4'	-2.10	101.84	108.99
3	A	1418	ACP	C4-N9-C1'	-2.06	121.81	126.63
2	A	1417	3PG	O4P-P-O3P	2.02	115.38	107.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1418	ACP	PB-C3B-PG-O1G
3	A	1418	ACP	PB-C3B-PG-O3G
2	A	1417	3PG	O2-C1-C2-C3
3	A	1418	ACP	PB-C3B-PG-O2G
3	A	1418	ACP	C5'-O5'-PA-O1A
3	A	1418	ACP	C5'-O5'-PA-O2A
3	A	1418	ACP	C5'-O5'-PA-O3A
2	A	1417	3PG	O1-C1-C2-O3
2	A	1417	3PG	O1-C1-C2-C3
2	A	1417	3PG	O2-C1-C2-O3
3	A	1418	ACP	PB-O3A-PA-O1A

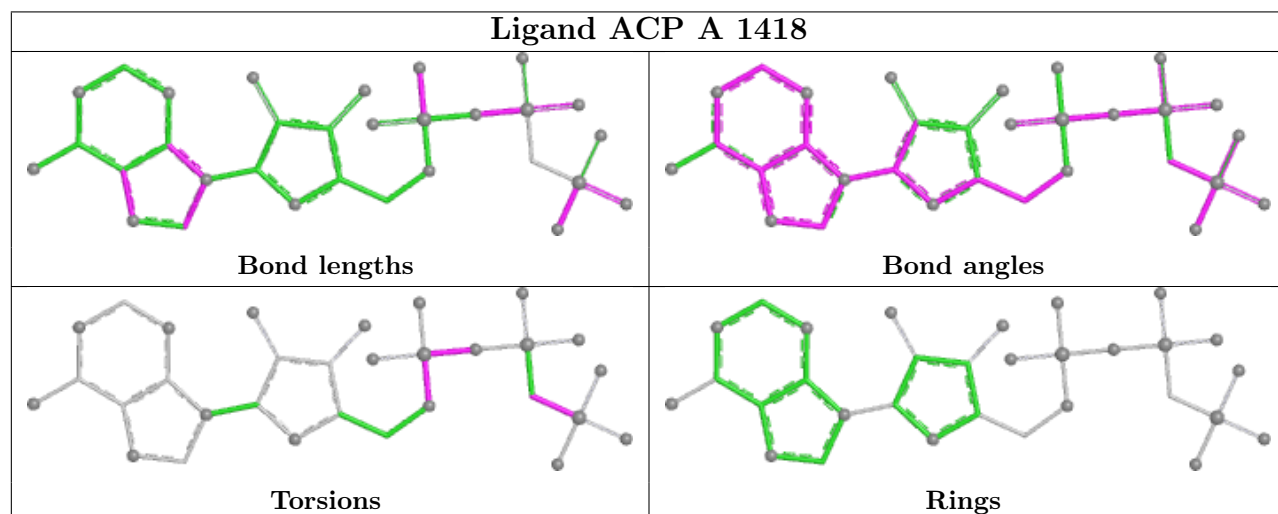
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1418	ACP	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 [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	413/417 (99%)	0.02	6 (1%) 72 72	9, 21, 33, 41	3 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	ALA	3.3
1	A	134	ALA	2.9
1	A	379	CYS	2.7
1	A	199	ALA	2.5
1	A	416	ILE	2.2
1	A	37	GLN	2.1

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](#)

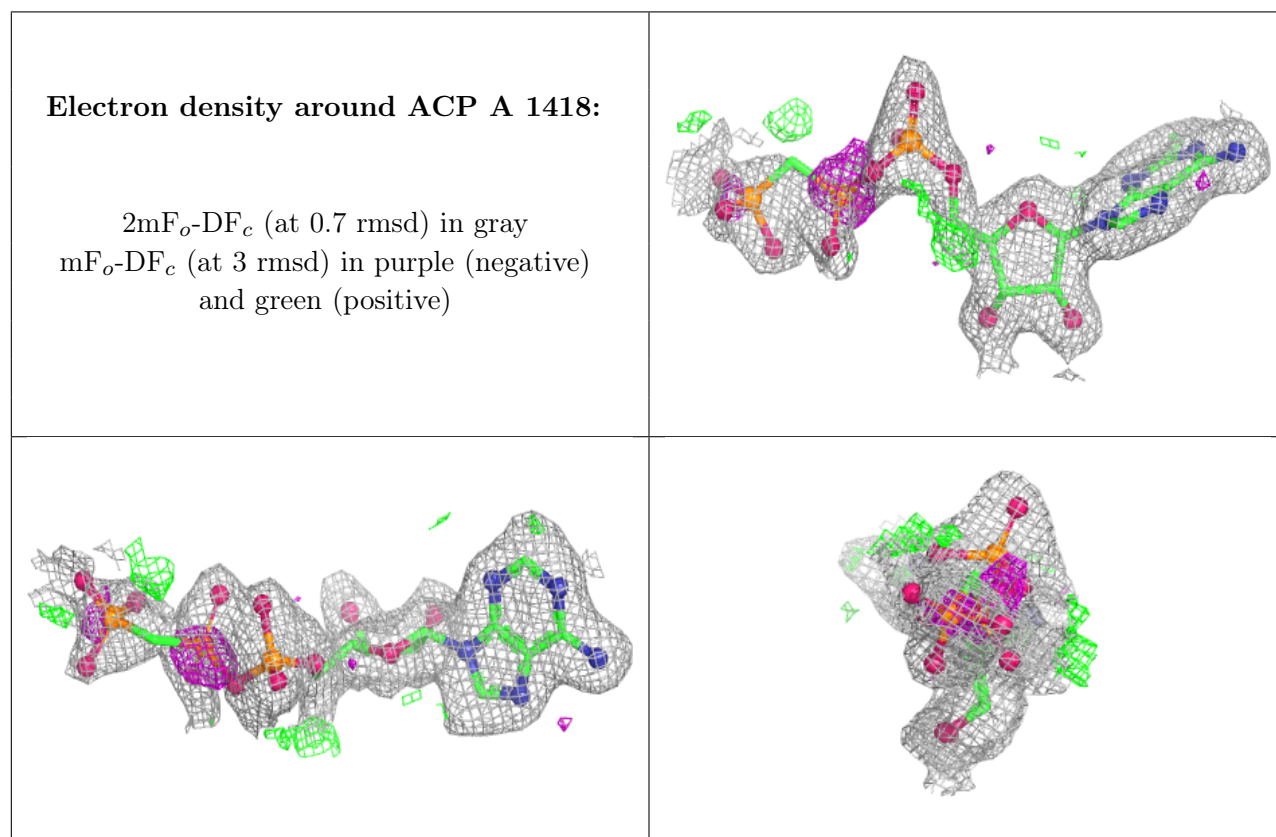
There are no oligosaccharides in this entry.

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	ACP	A	1418	31/31	0.88	0.10	15,28,54,55	0
2	3PG	A	1417	11/11	0.98	0.05	17,20,23,25	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.