



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:08 AM UTC

PDB ID : 4GWS / pdb_00004gws
Title : Crystal Structure of AMP complexes of Porcine Liver Fructose-1,6-bisphosphatase with Filled Central Cavity
Authors : Gao, Y.; Honzatko, R.B.
Deposited on : 2012-09-03
Resolution : 2.75 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

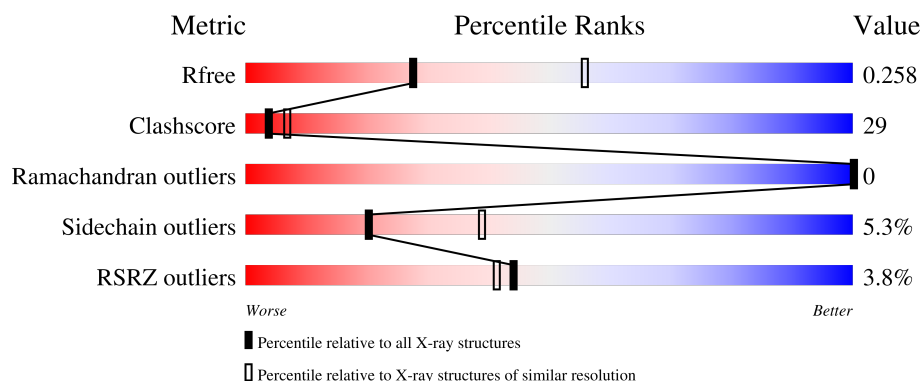
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	337	
1	B	337	

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	AMP	B	403	X	-	X	-
5	PO4	A	404	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5376 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.

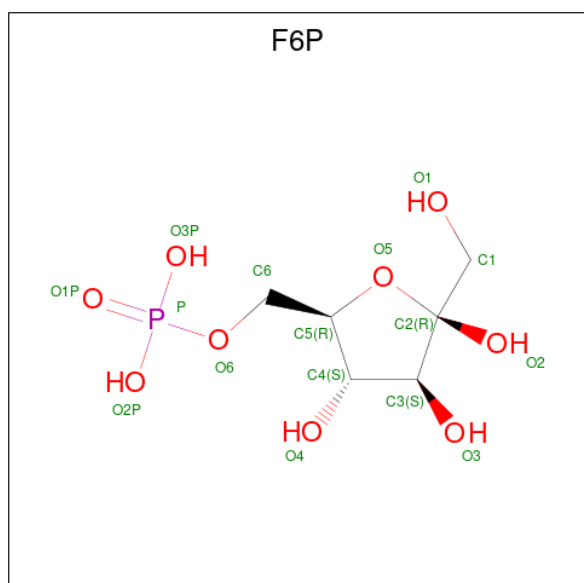
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2508	1595	425	473	15			
1	B	327	Total	C	N	O	S	0	0	0
			2508	1595	425	473	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	HIS	SER	engineered mutation	UNP P00636
A	46	ARG	THR	engineered mutation	UNP P00636
A	186	TYR	LEU	engineered mutation	UNP P00636
B	45	HIS	SER	engineered mutation	UNP P00636
B	46	ARG	THR	engineered mutation	UNP P00636
B	186	TYR	LEU	engineered mutation	UNP P00636

- Molecule 2 is 6-O-phosphono-beta-D-fructofuranose (CCD ID: F6P) (formula: $C_6H_{13}O_9P$).

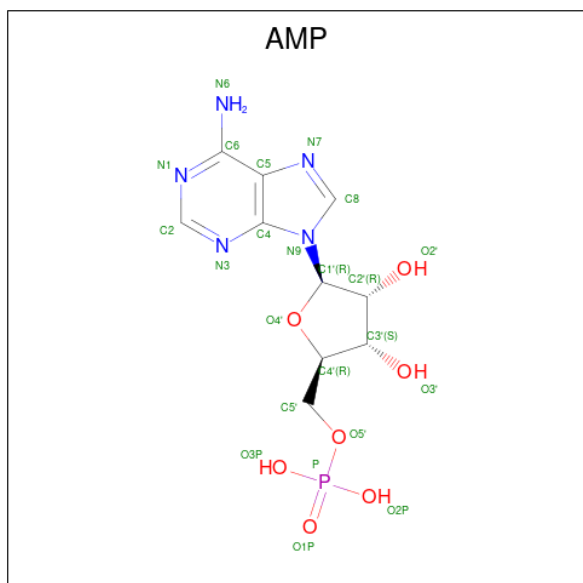


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

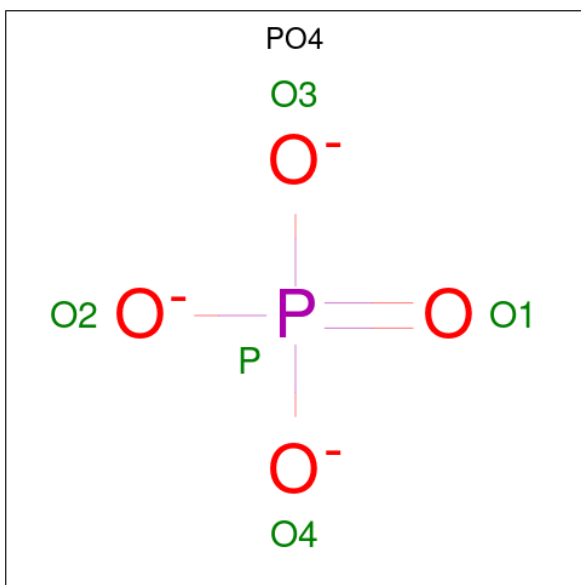
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	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	B	1	Total	O	P	0	0
			5	4	1		

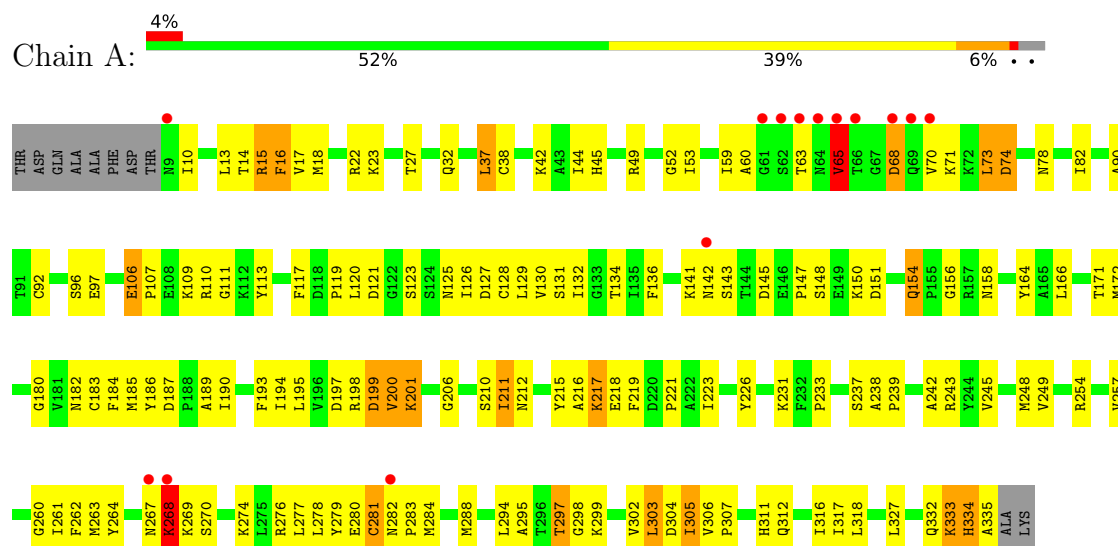
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total	O	0	0
			112	112		
6	B	158	Total	O	0	0
			158	158		

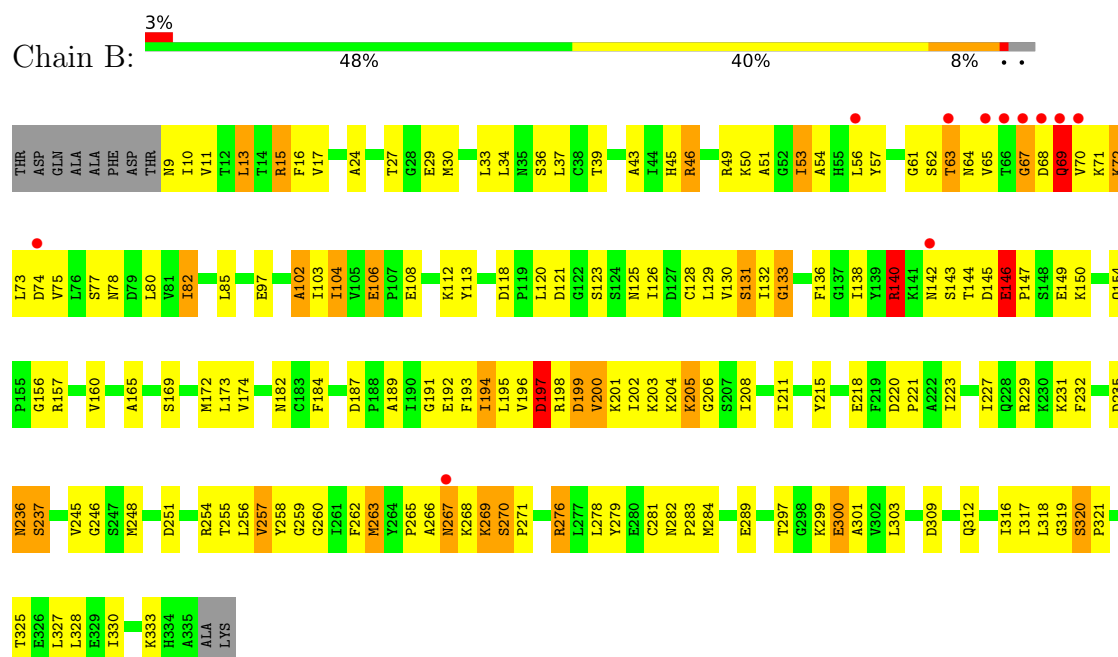
3 Residue-property plots [i](#)

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: Fructose-1,6-bisphosphatase 1



• Molecule 1: Fructose-1,6-bisphosphatase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.24Å 164.28Å 79.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.19 – 2.75 31.19 – 2.75	Depositor EDS
% Data completeness (in resolution range)	81.9 (31.19-2.75) 81.8 (31.19-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.200 , 0.262 0.198 , 0.258	Depositor DCC
R_{free} test set	896 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5376	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.32% 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: AMP, F6P, MG, 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	1.38	25/2552 (1.0%)	1.17	20/3452 (0.6%)
1	B	1.34	23/2552 (0.9%)	1.22	28/3452 (0.8%)
All	All	1.36	48/5104 (0.9%)	1.20	48/6904 (0.7%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	GLY	C-O	-8.93	1.15	1.23
1	A	215	TYR	C-O	-7.71	1.14	1.24
1	B	191	GLY	C-O	-7.63	1.15	1.24
1	B	208	ILE	C-O	-7.59	1.16	1.24
1	B	270	SER	C-O	-7.51	1.18	1.25
1	A	268	LYS	N-CA	-7.23	1.36	1.46
1	A	306	VAL	CA-C	-7.23	1.47	1.53
1	A	281	CYS	CB-SG	-6.71	1.59	1.81
1	A	305	ILE	C-O	-6.64	1.17	1.24
1	A	281	CYS	C-O	-6.59	1.16	1.24
1	B	132	ILE	C-O	-6.56	1.15	1.23
1	A	262	PHE	C-O	-6.41	1.16	1.24
1	A	197	ASP	C-O	-6.38	1.16	1.23
1	B	192	GLU	C-O	-6.37	1.15	1.23
1	B	197	ASP	C-O	-6.21	1.17	1.23
1	B	266	ALA	CA-CB	-6.20	1.43	1.53
1	B	205	LYS	C-O	-6.15	1.16	1.23
1	A	199	ASP	CA-C	-6.08	1.45	1.53
1	B	300	GLU	C-O	-6.05	1.16	1.23
1	B	140	ARG	C-O	-6.04	1.16	1.23
1	B	281	CYS	CB-SG	-5.98	1.61	1.81
1	A	278	LEU	C-O	-5.93	1.17	1.24
1	A	233	PRO	C-O	-5.86	1.18	1.24
1	A	304	ASP	C-O	-5.86	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	PHE	C-O	-5.78	1.17	1.24
1	B	263	MET	C-O	-5.75	1.17	1.24
1	B	320	SER	C-O	-5.74	1.16	1.24
1	B	319	GLY	C-O	-5.72	1.16	1.23
1	A	17	VAL	C-O	-5.71	1.17	1.24
1	A	14	THR	C-O	-5.70	1.17	1.24
1	B	262	PHE	C-O	-5.68	1.17	1.24
1	A	210	SER	C-O	-5.66	1.17	1.24
1	B	189	ALA	CA-CB	-5.51	1.44	1.53
1	A	151	ASP	C-O	-5.50	1.17	1.24
1	A	237	SER	C-O	-5.48	1.16	1.23
1	A	190	ILE	C-O	-5.36	1.16	1.24
1	B	199	ASP	CA-C	-5.36	1.46	1.53
1	A	199	ASP	C-N	-5.28	1.27	1.33
1	B	281	CYS	C-O	-5.27	1.17	1.24
1	B	265	PRO	C-O	-5.24	1.17	1.24
1	B	278	LEU	C-O	-5.24	1.18	1.24
1	A	60	ALA	CA-CB	-5.20	1.44	1.53
1	B	131	SER	C-O	-5.15	1.17	1.23
1	A	201	LYS	N-CA	5.09	1.52	1.46
1	A	305	ILE	CA-C	-5.08	1.46	1.52
1	A	312	GLN	C-O	-5.08	1.17	1.23
1	A	303	LEU	C-O	-5.07	1.17	1.24
1	B	301	ALA	CA-CB	-5.05	1.45	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	THR	N-CA-C	-11.67	99.26	114.31
1	A	278	LEU	N-CA-C	9.28	121.47	111.36
1	B	278	LEU	N-CA-C	9.10	120.97	111.14
1	B	69	GLN	N-CA-C	8.72	122.94	108.73
1	B	68	ASP	N-CA-C	-8.36	102.99	113.02
1	A	306	VAL	N-CA-C	-8.18	99.50	107.76
1	A	334	HIS	N-CA-C	-8.09	102.97	112.92
1	A	180	GLY	N-CA-C	7.24	119.95	111.63
1	A	65	VAL	N-CA-C	7.14	118.42	107.78
1	A	68	ASP	O-C-N	6.96	129.24	122.07
1	A	231	LYS	N-CA-C	6.78	118.75	111.36
1	B	333	LYS	N-CA-C	6.41	118.06	111.14
1	B	160	VAL	CB-CA-C	-6.35	105.47	111.06
1	B	301	ALA	CA-C-N	6.23	128.99	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	ALA	C-N-CA	6.23	128.99	120.46
1	A	127	ASP	N-CA-C	6.18	118.81	111.71
1	A	264	TYR	CA-C-N	6.14	126.60	120.52
1	A	264	TYR	C-N-CA	6.14	126.60	120.52
1	A	154	GLN	N-CA-C	-6.09	100.94	110.14
1	B	200	VAL	N-CA-C	5.94	117.08	109.30
1	B	237	SER	N-CA-CB	-5.80	102.43	110.38
1	A	257	VAL	N-CA-C	5.79	116.57	110.72
1	B	270	SER	CA-C-N	5.77	125.14	118.85
1	B	270	SER	C-N-CA	5.77	125.14	118.85
1	B	297	THR	N-CA-C	-5.77	106.20	113.18
1	B	67	GLY	N-CA-C	5.75	121.98	112.66
1	B	236	ASN	CA-C-N	5.64	131.67	121.06
1	B	236	ASN	C-N-CA	5.64	131.67	121.06
1	A	37	LEU	N-CA-C	-5.63	105.29	111.82
1	B	69	GLN	CB-CA-C	-5.58	101.14	110.19
1	A	68	ASP	N-CA-C	5.57	117.03	111.07
1	A	74	ASP	N-CA-C	5.48	117.34	111.36
1	B	263	MET	N-CA-C	5.35	117.80	108.76
1	B	199	ASP	N-CA-CB	5.34	119.61	111.70
1	B	215	TYR	N-CA-C	-5.33	106.36	112.92
1	B	146	GLU	N-CA-C	-5.23	103.00	109.64
1	B	138	ILE	N-CA-C	5.17	115.35	108.11
1	B	281	CYS	N-CA-C	5.16	116.99	111.36
1	A	15	ARG	N-CA-C	5.12	116.86	111.28
1	B	102	ALA	N-CA-C	-5.10	103.42	110.35
1	A	281	CYS	N-CA-C	5.09	116.91	111.36
1	A	200	VAL	N-CA-C	5.08	116.94	109.63
1	A	297	THR	N-CA-C	-5.07	107.10	113.28
1	B	191	GLY	N-CA-C	5.04	122.84	113.76
1	B	205	LYS	CA-C-N	5.03	126.05	121.82
1	B	205	LYS	C-N-CA	5.03	126.05	121.82
1	B	267	ASN	O-C-N	-5.00	117.11	123.17
1	A	298	GLY	N-CA-C	-5.00	107.94	113.79

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	2508	0	2558	134	0
1	B	2508	0	2558	172	0
2	A	16	0	11	1	0
2	B	16	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	12	1	0
4	B	23	0	10	11	0
5	A	5	0	0	2	0
5	B	5	0	0	1	0
6	A	112	0	0	7	0
6	B	158	0	0	15	0
All	All	5376	0	5160	294	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 29.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLN:O	1:B:69:GLN:HG2	1.54	1.08
1:A:13:LEU:HD21	1:A:38:CYS:SG	1.99	1.02
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.24	1.01
1:B:235:ASP:OD1	1:B:237:SER:HB2	1.62	1.00
1:B:218:GLU:HG3	6:B:616:HOH:O	1.63	0.97
1:A:121:ASP:HA	5:A:404:PO4:O2	1.65	0.96
1:B:113:TYR:OH	4:B:403:AMP:H5'2	1.65	0.96
1:B:64:ASN:ND2	1:B:65:VAL:HG23	1.82	0.94
1:B:64:ASN:HD22	1:B:65:VAL:HG23	1.31	0.94
1:B:15:ARG:HD3	6:B:522:HOH:O	1.70	0.91
1:A:218:GLU:OE1	1:A:269:LYS:HD3	1.71	0.90
1:A:13:LEU:CD2	1:A:38:CYS:SG	2.60	0.90
1:B:268:LYS:HG2	1:B:269:LYS:N	1.88	0.89
1:A:97:GLU:HB2	1:A:279:TYR:CE1	2.08	0.88
1:A:123:SER:HA	1:A:126:ILE:HG13	1.55	0.87
1:A:267:ASN:OD1	1:A:270:SER:HB2	1.75	0.86
1:B:106:GLU:CD	1:B:106:GLU:H	1.84	0.86
4:B:403:AMP:O5'	4:B:403:AMP:O3'	1.94	0.85
1:A:110:ARG:HD3	1:A:147:PRO:HG3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:THR:HG22	1:B:144:THR:O	1.76	0.85
1:B:268:LYS:HG2	1:B:269:LYS:H	1.43	0.84
1:B:29:GLU:OE1	1:B:112:LYS:HG2	1.75	0.83
1:B:202:ILE:HD12	1:B:256:LEU:HA	1.60	0.83
1:B:268:LYS:CG	1:B:269:LYS:N	2.41	0.83
1:B:269:LYS:HD2	1:B:269:LYS:O	1.81	0.81
1:B:121:ASP:HA	5:B:404:PO4:O4	1.82	0.79
1:B:269:LYS:C	1:B:269:LYS:CD	2.55	0.79
1:B:236:ASN:O	1:B:236:ASN:OD1	2.00	0.79
1:A:186:TYR:HB2	1:A:193:PHE:CE1	2.19	0.78
1:B:45:HIS:CE1	1:B:49:ARG:HE	2.01	0.78
1:A:332:GLN:HG3	6:A:603:HOH:O	1.84	0.78
1:B:108:GLU:HG2	6:B:625:HOH:O	1.82	0.78
1:B:267:ASN:O	1:B:270:SER:C	2.29	0.76
1:B:218:GLU:CD	1:B:268:LYS:HD2	2.11	0.76
1:A:217:LYS:HG3	1:B:232:PHE:CD1	2.21	0.75
1:A:123:SER:HA	1:A:126:ILE:CG1	2.17	0.75
1:B:144:THR:O	1:B:144:THR:CG2	2.35	0.73
1:B:269:LYS:HD2	1:B:269:LYS:C	2.13	0.73
1:A:276:ARG:NH1	1:A:311:HIS:O	2.21	0.73
1:B:269:LYS:O	1:B:269:LYS:CD	2.37	0.72
1:B:321:PRO:O	1:B:325:THR:HG23	1.90	0.72
1:B:73:LEU:HG	1:B:120:LEU:HD21	1.71	0.72
1:A:282:ASN:HB2	1:A:283:PRO:HD3	1.71	0.71
1:B:69:GLN:O	1:B:69:GLN:CG	2.30	0.71
1:B:248:MET:HE2	1:B:284:MET:HG3	1.73	0.71
1:A:217:LYS:HG3	1:B:232:PHE:CE1	2.25	0.71
1:A:110:ARG:NH1	1:A:147:PRO:HG2	2.07	0.70
1:B:72:LYS:HE2	1:B:74:ASP:OD1	1.91	0.70
1:B:102:ALA:HB2	1:B:149:GLU:HG2	1.74	0.70
1:A:110:ARG:NH1	1:A:147:PRO:CG	2.55	0.69
1:A:130:VAL:CG1	1:A:131:SER:N	2.56	0.69
1:B:204:LYS:HD3	6:B:546:HOH:O	1.94	0.67
1:A:96:SER:HB2	1:A:117:PHE:CZ	2.30	0.66
1:B:218:GLU:OE1	1:B:268:LYS:HB3	1.95	0.66
1:B:251:ASP:OD1	1:B:254:ARG:NH2	2.25	0.66
1:B:218:GLU:OE1	1:B:268:LYS:HD2	1.96	0.66
1:A:333:LYS:O	1:A:333:LYS:HG2	1.96	0.65
1:B:74:ASP:HB2	6:B:601:HOH:O	1.96	0.65
1:A:110:ARG:HH11	1:A:147:PRO:CG	2.10	0.65
1:B:211:ILE:HD12	1:B:263:MET:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:CB	1:A:283:PRO:HD3	2.27	0.64
1:A:130:VAL:HG12	1:A:131:SER:N	2.12	0.64
1:B:123:SER:HA	1:B:126:ILE:HG13	1.78	0.64
1:B:62:SER:HA	1:B:64:ASN:OD1	1.97	0.64
1:A:277:LEU:HA	1:A:281:CYS:HB2	1.79	0.64
1:A:106:GLU:CD	1:A:106:GLU:H	2.06	0.64
1:B:143:SER:OG	1:B:144:THR:N	2.30	0.63
1:B:77:SER:OG	1:B:120:LEU:HD22	1.98	0.63
1:B:113:TYR:HH	4:B:403:AMP:H5'2	1.62	0.63
1:B:268:LYS:O	1:B:271:PRO:HD3	1.99	0.63
1:A:15:ARG:HH11	1:A:15:ARG:CG	2.04	0.63
1:B:140:ARG:HH11	4:B:403:AMP:H5'1	1.62	0.63
1:A:15:ARG:HG3	1:A:15:ARG:NH1	1.99	0.63
1:B:104:ILE:HD13	1:B:104:ILE:N	2.13	0.62
1:B:140:ARG:NH1	4:B:403:AMP:H5'1	2.15	0.62
1:B:13:LEU:HD23	1:B:184:PHE:CG	2.34	0.62
1:A:267:ASN:O	1:A:270:SER:N	2.21	0.62
1:B:72:LYS:HB2	1:B:72:LYS:NZ	2.15	0.62
1:A:128:CYS:O	1:A:129:LEU:HB2	2.00	0.61
1:A:195:LEU:HD21	1:A:198:ARG:HG3	1.82	0.61
1:A:73:LEU:HG	1:A:120:LEU:HD21	1.81	0.61
1:A:123:SER:CA	1:A:126:ILE:HG13	2.30	0.60
1:B:16:PHE:CZ	1:B:182:ASN:ND2	2.68	0.60
1:A:267:ASN:O	1:A:269:LYS:N	2.34	0.60
1:A:63:THR:HG23	1:A:63:THR:O	2.01	0.60
1:B:173:LEU:HD23	1:B:173:LEU:C	2.27	0.60
1:A:37:LEU:HD21	1:A:136:PHE:CD2	2.36	0.60
1:B:318:LEU:C	1:B:318:LEU:HD12	2.28	0.59
1:B:11:VAL:HG13	1:B:15:ARG:HG2	1.84	0.58
1:A:37:LEU:HD21	1:A:136:PHE:CE2	2.37	0.58
1:A:45:HIS:CE1	1:A:171:THR:OG1	2.57	0.58
1:B:229:ARG:NH1	1:B:330:ILE:HD11	2.17	0.58
1:B:16:PHE:CE2	1:B:182:ASN:ND2	2.72	0.58
1:B:78:ASN:O	1:B:82:ILE:HG13	2.03	0.58
1:B:27:THR:N	4:B:403:AMP:O1P	2.33	0.57
1:A:334:HIS:O	1:A:335:ALA:C	2.45	0.57
1:A:73:LEU:HG	1:A:120:LEU:CD2	2.33	0.57
1:B:9:ASN:HA	6:B:502:HOH:O	2.04	0.57
1:A:156:GLY:HA3	1:A:303:LEU:HD22	1.86	0.57
1:A:221:PRO:HB2	1:A:334:HIS:CE1	2.40	0.56
1:A:45:HIS:CE1	1:A:49:ARG:HE	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:NZ	1:A:145:ASP:O	2.36	0.56
1:A:189:ALA:HB2	1:B:51:ALA:HB1	1.87	0.56
1:B:37:LEU:HD21	1:B:136:PHE:CZ	2.40	0.56
1:B:103:ILE:C	1:B:104:ILE:HD13	2.31	0.56
1:A:15:ARG:CG	1:A:15:ARG:NH1	2.62	0.56
1:A:16:PHE:CZ	1:A:182:ASN:ND2	2.74	0.56
1:A:53:ILE:HG22	1:B:187:ASP:HB2	1.87	0.56
1:B:316:ILE:HD11	1:B:318:LEU:HD23	1.86	0.56
1:A:154:GLN:HE21	1:A:158:ASN:HD22	1.54	0.56
1:B:130:VAL:HG12	1:B:131:SER:N	2.21	0.56
1:B:63:THR:HG22	1:B:63:THR:O	2.05	0.55
1:B:194:ILE:O	1:B:196:VAL:HG13	2.06	0.55
1:A:261:ILE:HD11	1:A:317:ILE:HG23	1.89	0.55
1:A:70:VAL:HG22	1:A:71:LYS:N	2.21	0.55
1:A:123:SER:HA	1:A:126:ILE:CD1	2.36	0.55
1:A:274:LYS:HE2	2:A:401:F6P:H12	1.88	0.54
1:B:142:ASN:HB2	6:B:598:HOH:O	2.07	0.54
1:A:49:ARG:NH1	1:B:169:SER:HA	2.23	0.54
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.88	0.54
1:B:130:VAL:CG1	1:B:131:SER:N	2.70	0.54
1:A:13:LEU:HD23	1:A:38:CYS:SG	2.43	0.54
1:B:223:ILE:O	1:B:227:ILE:HG12	2.07	0.54
1:B:282:ASN:HB2	1:B:283:PRO:HD3	1.89	0.54
1:A:218:GLU:HB2	1:A:267:ASN:HB2	1.89	0.54
1:B:146:GLU:HG2	6:B:614:HOH:O	2.07	0.53
1:B:218:GLU:CD	1:B:268:LYS:CD	2.81	0.53
1:B:276:ARG:HG2	1:B:279:TYR:CE1	2.43	0.53
1:A:10:ILE:HD12	1:B:57:TYR:O	2.08	0.53
1:B:70:VAL:HG22	1:B:71:LYS:H	1.72	0.53
1:B:112:LYS:NZ	4:B:403:AMP:O3P	2.36	0.53
1:A:120:LEU:HD11	1:A:132:ILE:HD12	1.91	0.53
1:B:128:CYS:O	1:B:129:LEU:HB2	2.08	0.52
1:A:194:ILE:HD11	1:B:54:ALA:HB2	1.91	0.52
1:B:82:ILE:HD13	1:B:103:ILE:HD13	1.91	0.52
1:A:254:ARG:HD2	6:A:516:HOH:O	2.09	0.52
1:B:150:LYS:HB2	6:B:584:HOH:O	2.08	0.52
1:B:267:ASN:O	1:B:268:LYS:C	2.47	0.52
1:A:129:LEU:HD11	1:B:172:MET:HB2	1.92	0.52
1:B:246:GLY:O	2:B:401:F6P:H4	2.09	0.52
1:A:45:HIS:ND1	1:A:171:THR:OG1	2.41	0.52
1:A:23:LYS:NZ	6:A:584:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.45	0.51
1:A:242:ALA:O	1:A:243:ARG:HG2	2.10	0.51
1:B:13:LEU:HD23	1:B:184:PHE:CD2	2.45	0.51
1:A:90:ALA:O	1:A:113:TYR:HB2	2.11	0.51
1:A:45:HIS:CE1	1:A:171:THR:HG1	2.27	0.51
1:A:18:MET:O	1:A:22:ARG:HG3	2.11	0.51
1:A:68:ASP:HA	6:A:607:HOH:O	2.11	0.51
1:B:73:LEU:HG	1:B:120:LEU:CD2	2.40	0.51
1:B:316:ILE:CD1	1:B:318:LEU:HD23	2.41	0.51
1:A:226:TYR:CG	1:A:327:LEU:HD13	2.46	0.50
1:B:197:ASP:OD1	1:B:200:VAL:HG22	2.11	0.50
1:A:276:ARG:NH1	1:A:311:HIS:HB3	2.26	0.50
1:A:110:ARG:HH11	1:A:147:PRO:CD	2.24	0.50
1:A:318:LEU:HD12	1:A:318:LEU:C	2.36	0.50
1:B:70:VAL:HA	6:B:624:HOH:O	2.11	0.50
1:B:102:ALA:CB	1:B:149:GLU:HG2	2.41	0.50
1:B:70:VAL:HG22	1:B:71:LYS:N	2.27	0.50
1:B:267:ASN:C	1:B:267:ASN:OD1	2.55	0.49
1:B:125:ASN:HB3	1:B:130:VAL:HB	1.94	0.49
1:A:211:ILE:HB	1:A:263:MET:HB2	1.94	0.49
1:B:198:ARG:HD2	6:B:526:HOH:O	2.11	0.49
1:B:37:LEU:HD21	1:B:136:PHE:CE2	2.48	0.49
1:B:146:GLU:OE2	1:B:147:PRO:HD2	2.13	0.49
1:A:42:LYS:O	1:A:45:HIS:HB3	2.12	0.49
1:A:267:ASN:O	1:A:268:LYS:C	2.54	0.48
1:A:78:ASN:ND2	1:A:82:ILE:HD11	2.28	0.48
1:A:211:ILE:HG12	1:A:212:ASN:N	2.28	0.48
1:A:27:THR:HG23	6:A:554:HOH:O	2.12	0.48
1:A:248:MET:HE2	1:A:284:MET:HG3	1.94	0.48
1:A:130:VAL:CG1	1:A:131:SER:H	2.25	0.48
1:A:282:ASN:CB	1:A:283:PRO:CD	2.90	0.48
1:A:52:GLY:HA2	6:B:510:HOH:O	2.12	0.48
1:A:113:TYR:OH	4:A:403:AMP:H5'2	2.14	0.48
1:A:148:SER:OG	1:A:150:LYS:HG2	2.13	0.48
1:A:117:PHE:CE2	1:A:119:PRO:HG3	2.49	0.47
1:A:200:VAL:O	1:A:201:LYS:HD3	2.14	0.47
1:B:13:LEU:HD23	1:B:184:PHE:CD1	2.49	0.47
1:B:24:ALA:HB1	4:B:403:AMP:O2'	2.13	0.47
1:B:130:VAL:CG1	1:B:131:SER:H	2.27	0.47
1:B:33:LEU:O	1:B:36:SER:HB2	2.14	0.47
1:A:277:LEU:HD23	1:A:307:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:SER:OG	1:B:145:ASP:N	2.35	0.47
1:B:220:ASP:HB2	1:B:221:PRO:HD2	1.97	0.47
1:A:97:GLU:O	1:A:97:GLU:HG2	2.14	0.47
1:A:172:MET:SD	1:A:183:CYS:HB3	2.54	0.47
1:A:129:LEU:CD1	1:B:172:MET:HB2	2.45	0.46
1:A:187:ASP:OD1	1:A:189:ALA:HB3	2.15	0.46
1:A:267:ASN:OD1	1:A:267:ASN:O	2.34	0.46
1:B:276:ARG:HG2	1:B:279:TYR:CZ	2.51	0.46
1:B:106:GLU:OE2	1:B:106:GLU:N	2.38	0.46
1:A:206:GLY:HA3	1:A:260:GLY:N	2.31	0.46
1:B:123:SER:HA	1:B:126:ILE:CG1	2.46	0.46
1:A:32:GLN:HA	1:A:32:GLN:OE1	2.15	0.46
1:B:74:ASP:OD1	1:B:75:VAL:N	2.49	0.46
1:B:123:SER:HA	1:B:126:ILE:CD1	2.46	0.46
1:B:195:LEU:CD2	1:B:198:ARG:NH1	2.79	0.46
1:A:134:THR:O	1:A:164:TYR:HA	2.16	0.46
1:A:269:LYS:N	1:A:269:LYS:HD2	2.31	0.46
1:A:65:VAL:O	1:A:65:VAL:HG12	2.16	0.46
1:A:217:LYS:HB3	1:A:218:GLU:OE2	2.17	0.45
1:A:117:PHE:HE2	1:A:119:PRO:HG3	1.80	0.45
1:A:130:VAL:HG13	1:A:131:SER:H	1.80	0.45
1:B:282:ASN:ND2	6:B:517:HOH:O	2.37	0.45
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.71	0.45
1:A:10:ILE:HD12	1:B:57:TYR:C	2.41	0.45
1:B:263:MET:HB3	1:B:317:ILE:CD1	2.47	0.45
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.68	0.45
1:B:187:ASP:C	1:B:187:ASP:OD1	2.59	0.45
1:B:227:ILE:HG22	1:B:231:LYS:HE3	1.99	0.45
1:A:107:PRO:HG3	1:A:110:ARG:NH2	2.31	0.45
1:B:140:ARG:HH12	4:B:403:AMP:C4'	2.28	0.45
1:A:70:VAL:CG2	1:A:71:LYS:N	2.80	0.45
1:B:195:LEU:HD21	1:B:198:ARG:HG3	1.99	0.45
1:B:133:GLY:CA	1:B:165:ALA:O	2.65	0.44
1:B:46:ARG:HE	1:B:46:ARG:HB3	1.48	0.44
1:A:142:ASN:OD1	1:A:143:SER:N	2.49	0.44
1:A:226:TYR:HB2	1:A:327:LEU:CD1	2.47	0.44
1:B:203:LYS:HE3	1:B:258:TYR:O	2.17	0.44
1:B:317:ILE:HG21	1:B:327:LEU:HD23	1.98	0.44
1:A:218:GLU:HB3	1:A:268:LYS:H	1.83	0.44
1:A:282:ASN:OD1	6:A:507:HOH:O	2.21	0.44
1:A:106:GLU:OE1	1:A:109:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:HG13	1:B:245:VAL:HG22	1.99	0.44
1:A:288:MET:HG3	1:A:318:LEU:HB2	1.99	0.44
1:B:142:ASN:CG	1:B:154:GLN:NE2	2.76	0.44
1:B:200:VAL:O	1:B:201:LYS:HD3	2.18	0.44
1:B:236:ASN:OD1	1:B:236:ASN:C	2.57	0.44
1:B:206:GLY:HA3	1:B:260:GLY:N	2.33	0.44
1:A:186:TYR:HB2	1:A:193:PHE:HE1	1.77	0.43
1:B:276:ARG:HG2	1:B:279:TYR:OH	2.17	0.43
1:A:123:SER:HA	1:A:126:ILE:HD11	1.99	0.43
1:A:154:GLN:HE21	1:A:158:ASN:ND2	2.17	0.43
1:B:199:ASP:OD2	1:B:199:ASP:C	2.59	0.43
1:A:185:MET:HE3	1:B:50:LYS:HZ2	1.83	0.43
1:B:97:GLU:OE1	1:B:118:ASP:OD2	2.37	0.43
1:B:43:ALA:HB1	1:B:80:LEU:HD13	2.01	0.43
1:B:299:LYS:C	1:B:300:GLU:HG3	2.42	0.43
1:B:45:HIS:O	1:B:49:ARG:HD3	2.18	0.43
1:A:295:ALA:HB3	6:A:530:HOH:O	2.19	0.43
1:A:297:THR:HG21	1:A:305:ILE:HD11	2.00	0.42
1:B:142:ASN:HB2	1:B:154:GLN:NE2	2.33	0.42
1:B:220:ASP:HB2	1:B:221:PRO:CD	2.49	0.42
1:B:267:ASN:O	1:B:270:SER:O	2.37	0.42
1:B:63:THR:O	1:B:63:THR:CG2	2.68	0.42
1:B:198:ARG:HD2	1:B:198:ARG:HH11	1.69	0.42
1:B:267:ASN:O	1:B:270:SER:N	2.53	0.42
1:B:320:SER:HA	1:B:321:PRO:HD3	1.93	0.42
1:B:269:LYS:O	1:B:269:LYS:HD3	2.19	0.42
1:A:44:ILE:O	1:A:45:HIS:C	2.62	0.42
1:A:110:ARG:NH1	1:A:147:PRO:HD2	2.35	0.42
1:A:184:PHE:HB3	1:A:193:PHE:HB3	2.01	0.42
1:A:238:ALA:HA	1:A:239:PRO:HD3	1.65	0.42
1:B:312:GLN:NE2	6:B:590:HOH:O	2.20	0.42
1:B:157:ARG:NH2	1:B:289:GLU:OE2	2.53	0.42
1:B:43:ALA:CB	1:B:80:LEU:HD13	2.49	0.42
1:B:184:PHE:CD1	1:B:184:PHE:N	2.87	0.42
1:A:110:ARG:NH1	1:A:147:PRO:CD	2.83	0.42
1:A:125:ASN:HB3	1:A:130:VAL:HB	2.02	0.41
1:A:125:ASN:CG	1:A:130:VAL:HG11	2.45	0.41
1:B:65:VAL:C	1:B:67:GLY:H	2.28	0.41
1:B:202:ILE:HD11	1:B:255:THR:O	2.20	0.41
1:B:268:LYS:O	1:B:269:LYS:C	2.62	0.41
1:B:203:LYS:CE	1:B:258:TYR:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:NH1	4:B:403:AMP:C5'	2.82	0.41
1:B:65:VAL:C	1:B:67:GLY:N	2.77	0.41
1:B:235:ASP:O	1:B:236:ASN:HB3	2.19	0.41
1:A:294:LEU:O	1:A:318:LEU:HA	2.20	0.41
1:B:53:ILE:HA	1:B:56:LEU:HD13	2.02	0.41
1:B:61:GLY:O	1:B:64:ASN:OD1	2.38	0.41
1:B:282:ASN:CB	1:B:283:PRO:HD3	2.51	0.41
1:A:302:VAL:HG21	1:A:316:ILE:HD12	2.01	0.41
1:B:37:LEU:HD21	1:B:136:PHE:CE1	2.55	0.41
1:B:71:LYS:N	6:B:624:HOH:O	2.53	0.41
1:B:173:LEU:HD23	1:B:174:VAL:N	2.34	0.41
1:B:156:GLY:HA3	1:B:303:LEU:HD22	2.02	0.41
1:A:59:ILE:HB	1:B:10:ILE:HD13	2.03	0.41
1:A:68:ASP:OD1	1:A:68:ASP:O	2.38	0.41
1:B:30:MET:HE2	1:B:34:LEU:HD11	2.03	0.41
1:A:97:GLU:OE1	5:A:404:PO4:O3	2.38	0.41
1:A:92:CYS:HB3	1:A:111:GLY:O	2.20	0.40
1:A:123:SER:O	1:A:126:ILE:HG13	2.21	0.40
1:B:30:MET:O	1:B:30:MET:HG2	2.20	0.40
1:B:255:THR:O	1:B:259:GLY:HA2	2.20	0.40
1:B:13:LEU:HB2	1:B:193:PHE:HB2	2.03	0.40
1:B:113:TYR:OH	4:B:403:AMP:C5'	2.52	0.40
1:B:309:ASP:O	1:B:312:GLN:HB2	2.21	0.40
1:B:257:VAL:HG12	1:B:258:TYR:CD2	2.56	0.40
1:A:198:ARG:O	1:A:199:ASP:C	2.64	0.40
1:A:277:LEU:O	1:A:282:ASN:N	2.51	0.40
1:B:13:LEU:O	1:B:17:VAL:HG22	2.21	0.40
1:B:227:ILE:CG2	1:B:231:LYS:HE3	2.51	0.40
1:B:229:ARG:NH2	1:B:330:ILE:HD12	2.36	0.40

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	325/337 (96%)	316 (97%)	9 (3%)	0	100	100
1	B	325/337 (96%)	320 (98%)	5 (2%)	0	100	100
All	All	650/674 (96%)	636 (98%)	14 (2%)	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	272/279 (98%)	261 (96%)	11 (4%)	28	50
1	B	272/279 (98%)	254 (93%)	18 (7%)	15	29
All	All	544/558 (98%)	515 (95%)	29 (5%)	20	39

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	73	LEU
1	A	74	ASP
1	A	106	GLU
1	A	211	ILE
1	A	217	LYS
1	A	223	ILE
1	A	268	LYS
1	A	280	GLU
1	A	299	LYS
1	A	333	LYS
1	B	13	LEU
1	B	15	ARG
1	B	39	THR
1	B	46	ARG
1	B	53	ILE
1	B	69	GLN
1	B	72	LYS

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Mol	Chain	Res	Type
1	B	82	ILE
1	B	104	ILE
1	B	106	GLU
1	B	140	ARG
1	B	146	GLU
1	B	194	ILE
1	B	197	ASP
1	B	205	LYS
1	B	257	VAL
1	B	269	LYS
1	B	276	ARG

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	154	GLN
1	B	154	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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
2	F6P	A	401	3	15,16,16	0.94	1 (6%)	16,25,25	0.88	0
2	F6P	B	401	3	15,16,16	0.70	0	16,25,25	0.97	2 (12%)
5	PO4	A	404	3	4,4,4	1.46	1 (25%)	6,6,6	0.83	0
4	AMP	B	403	-	25,25,25	1.47	3 (12%)	37,38,38	3.23	14 (37%)
4	AMP	A	403	-	25,25,25	1.36	2 (8%)	37,38,38	1.50	7 (18%)
5	PO4	B	404	3	4,4,4	1.19	0	6,6,6	0.66	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
4	AMP	A	403	-	-	2/10/26/26	0/3/3/3
4	AMP	B	403	-	2/2/5/5	2/10/26/26	0/3/3/3
2	F6P	A	401	3	-	3/9/28/28	0/1/1/1
2	F6P	B	401	3	-	7/9/28/28	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	AMP	C5-C4	4.47	1.47	1.39
4	A	403	AMP	C5-C4	4.43	1.47	1.39
4	A	403	AMP	C5-C6	2.41	1.47	1.41
4	B	403	AMP	C5-N7	-2.29	1.34	1.39
2	A	401	F6P	O2-C2	2.27	1.44	1.40
5	A	404	PO4	P-O2	-2.09	1.48	1.54
4	B	403	AMP	C5-C6	2.07	1.46	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	AMP	C4'-O4'-C1'	-9.99	87.40	109.47
4	B	403	AMP	O4'-C4'-C5'	6.74	130.91	109.33
4	B	403	AMP	C2'-C1'-N9	6.50	129.44	113.30
4	B	403	AMP	O4'-C1'-N9	5.31	118.28	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	AMP	N3-C4-N9	4.97	135.62	127.17
4	B	403	AMP	C5-C4-N3	-4.88	120.00	126.72
4	B	403	AMP	O3'-C3'-C4'	-4.47	98.24	111.08
4	A	403	AMP	C5-C4-N3	-4.20	120.94	126.72
4	B	403	AMP	C1'-N9-C8	-3.90	118.44	127.09
4	A	403	AMP	N3-C4-N9	3.63	133.33	127.17
4	B	403	AMP	O4'-C4'-C3'	3.19	111.48	105.15
4	B	403	AMP	C4-N9-C8	3.14	109.04	105.74
4	A	403	AMP	C2-N1-C6	2.74	123.23	118.73
4	B	403	AMP	C3'-C2'-C1'	-2.70	96.36	101.46
4	B	403	AMP	C2-N3-C4	2.69	118.39	111.83
4	A	403	AMP	C2-N3-C4	2.48	117.89	111.83
4	B	403	AMP	O4'-C1'-C2'	2.46	111.89	106.62
4	A	403	AMP	C4-C5-N7	-2.43	107.81	110.58
4	A	403	AMP	N3-C2-N1	-2.37	125.00	128.58
2	B	401	F6P	O2-C2-O5	-2.36	104.78	109.33
4	A	403	AMP	O3P-P-O2P	2.29	116.39	107.80
4	B	403	AMP	C4-N9-C1'	2.28	131.95	126.63
2	B	401	F6P	O3P-P-O2P	2.05	115.50	107.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	403	AMP	C1'
4	B	403	AMP	C4'

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	F6P	C6-O6-P-O2P
2	A	401	F6P	C6-O6-P-O3P
2	B	401	F6P	O1-C1-C2-O2
2	B	401	F6P	O1-C1-C2-C3
2	B	401	F6P	C6-O6-P-O2P
2	B	401	F6P	C6-O6-P-O3P
4	A	403	AMP	O4'-C4'-C5'-O5'
4	B	403	AMP	O4'-C4'-C5'-O5'
2	B	401	F6P	O1-C1-C2-O5
4	A	403	AMP	C3'-C4'-C5'-O5'
2	A	401	F6P	C6-O6-P-O1P
2	B	401	F6P	C6-O6-P-O1P
4	B	403	AMP	O4'-C1'-N9-C8

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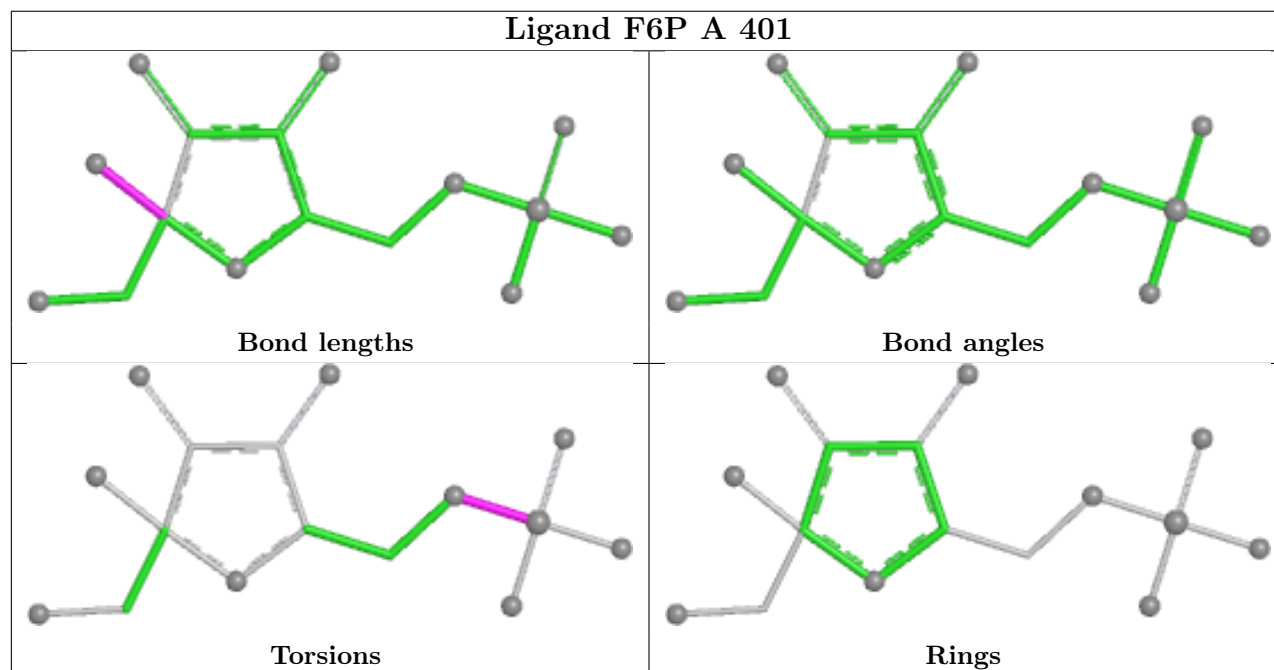
Mol	Chain	Res	Type	Atoms
2	B	401	F6P	C4-C5-C6-O6

There are no ring outliers.

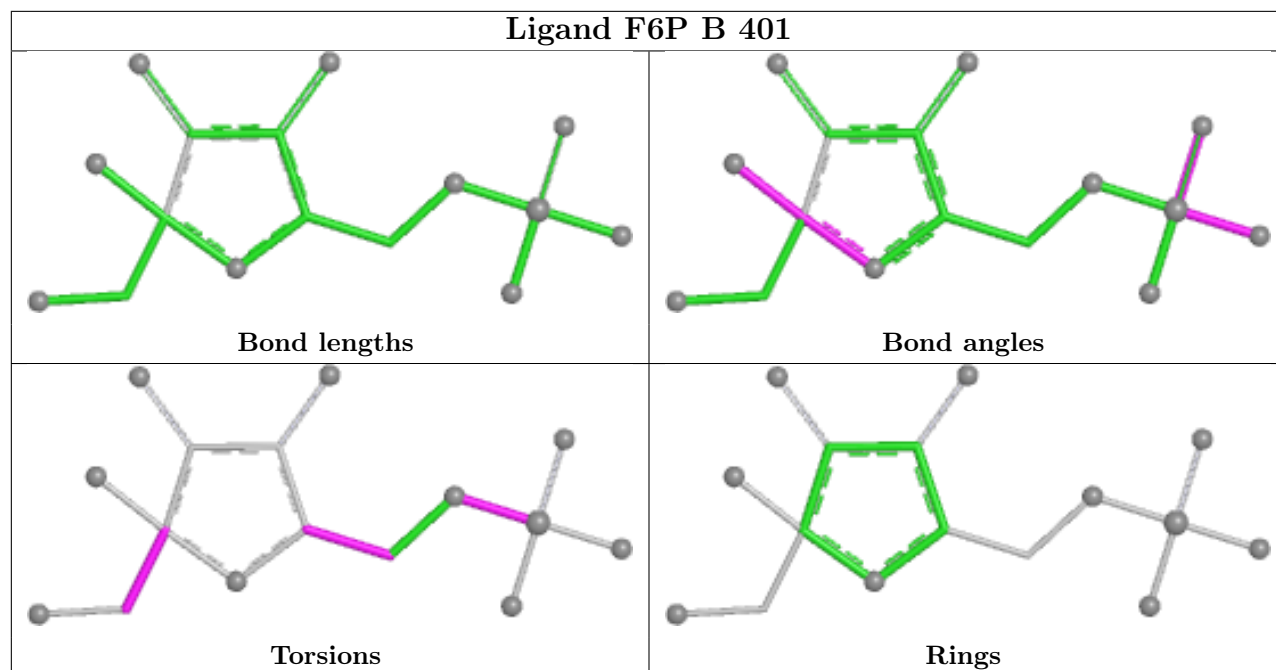
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	F6P	1	0
2	B	401	F6P	1	0
5	A	404	PO4	2	0
4	B	403	AMP	11	0
4	A	403	AMP	1	0
5	B	404	PO4	1	0

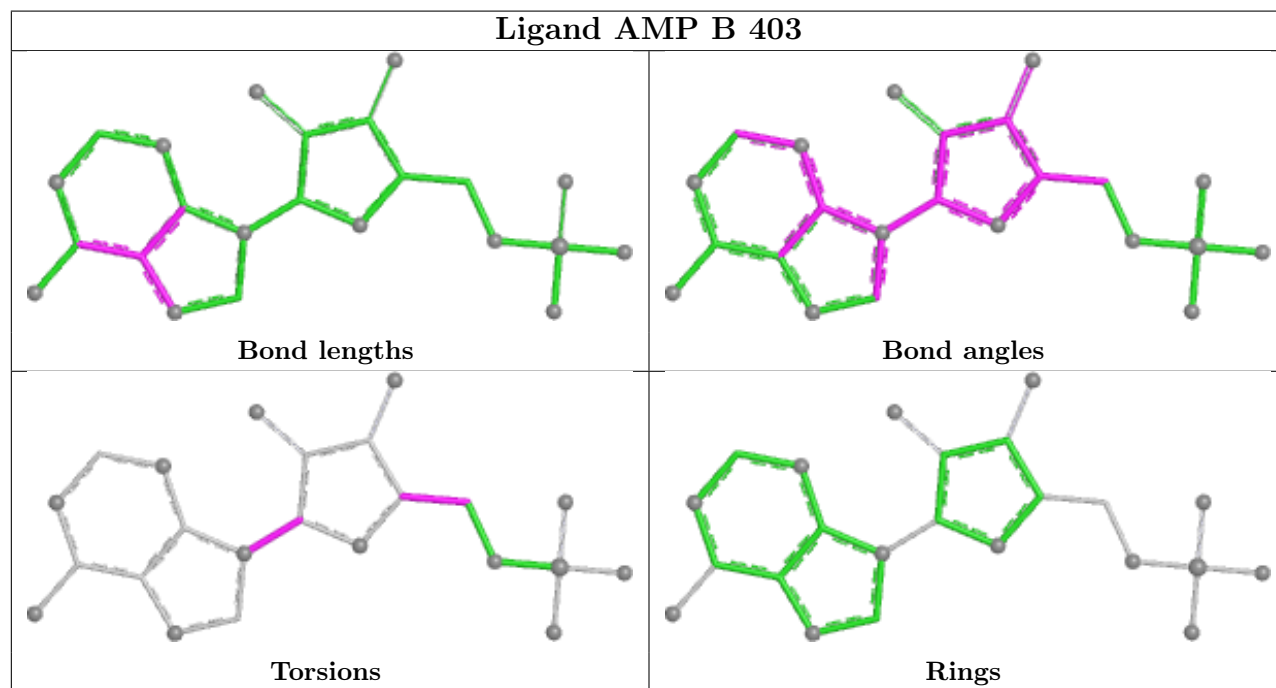
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

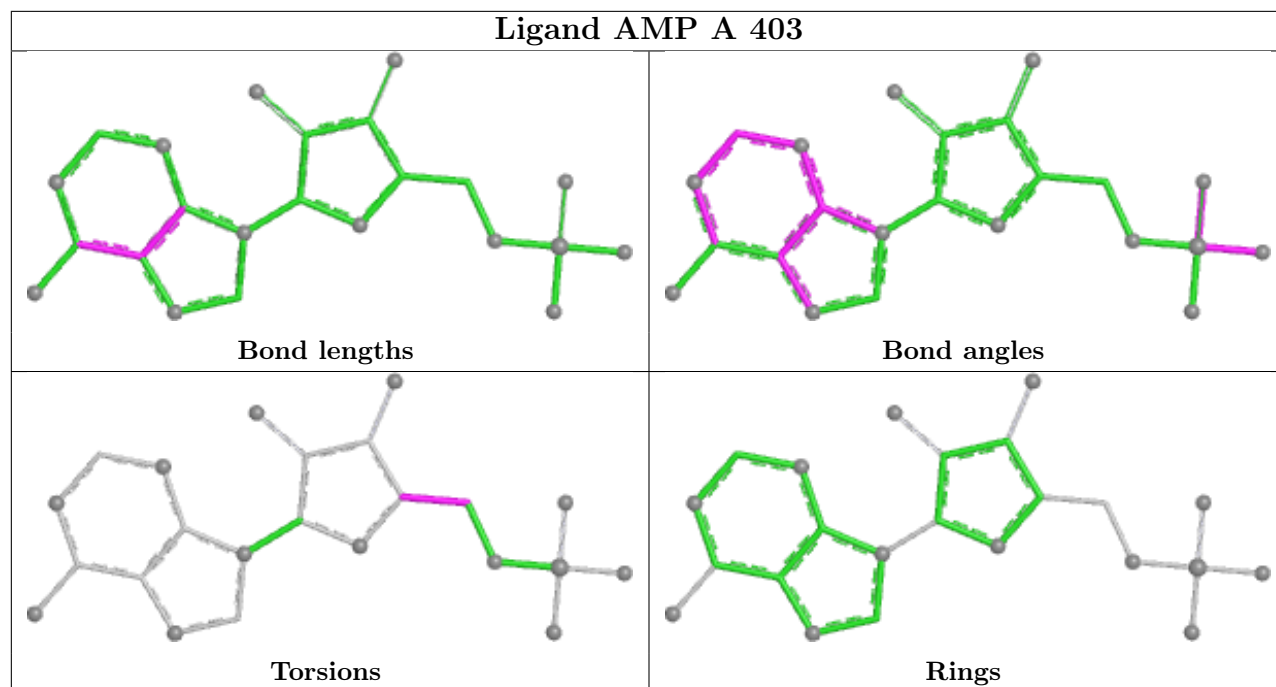


Ligand F6P B 401



Ligand AMP B 403





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	327/337 (97%)	-0.03	14 (4%) 40 38	8, 19, 41, 83	0
1	B	327/337 (97%)	-0.11	11 (3%) 48 46	4, 18, 43, 81	0
All	All	654/674 (97%)	-0.07	25 (3%) 44 41	4, 18, 43, 83	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	6.4
1	A	66	THR	6.1
1	B	66	THR	5.0
1	B	65	VAL	4.7
1	A	69	GLN	4.0
1	A	282	ASN	3.9
1	B	70	VAL	3.7
1	B	67	GLY	3.6
1	B	69	GLN	3.4
1	A	68	ASP	3.4
1	A	62	SER	3.1
1	A	267	ASN	2.8
1	B	68	ASP	2.8
1	A	142	ASN	2.6
1	A	65	VAL	2.6
1	A	63	THR	2.6
1	A	9	ASN	2.6
1	B	74	ASP	2.5
1	A	61	GLY	2.4
1	B	142	ASN	2.4
1	A	268	LYS	2.4
1	A	64	ASN	2.3
1	B	63	THR	2.3
1	B	56	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	267	ASN	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](#)

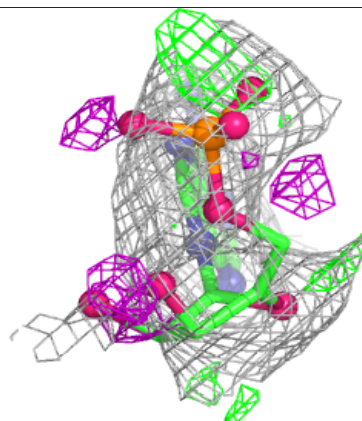
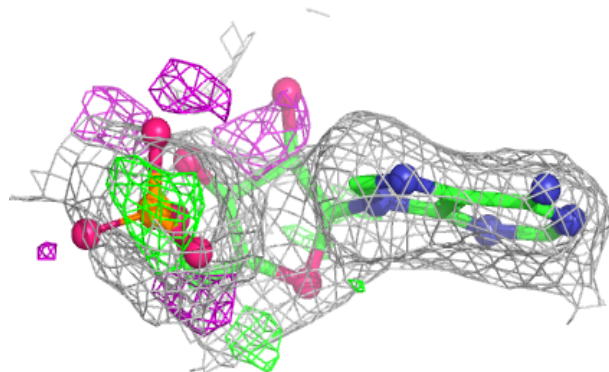
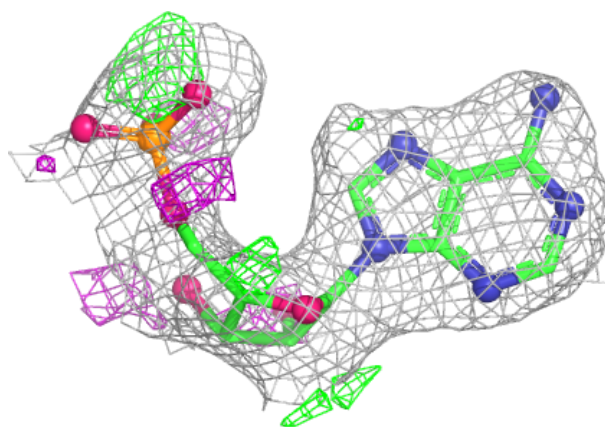
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	A	404	5/5	0.88	0.16	34,37,38,41	0
4	AMP	B	403	23/23	0.91	0.15	22,29,40,46	0
3	MG	A	402	1/1	0.94	0.09	20,20,20,20	0
3	MG	B	402	1/1	0.96	0.04	19,19,19,19	0
4	AMP	A	403	23/23	0.96	0.09	10,21,25,29	0
5	PO4	B	404	5/5	0.96	0.09	41,42,44,45	0
2	F6P	A	401	16/16	0.97	0.09	14,17,20,20	0
2	F6P	B	401	16/16	0.98	0.07	11,15,19,23	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.

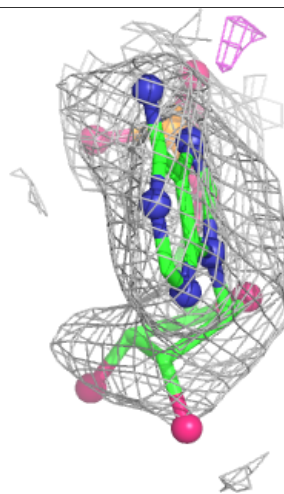
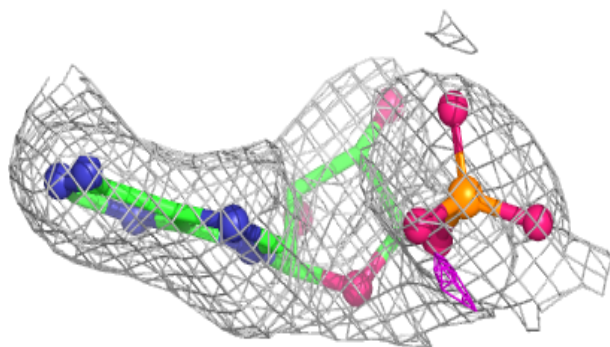
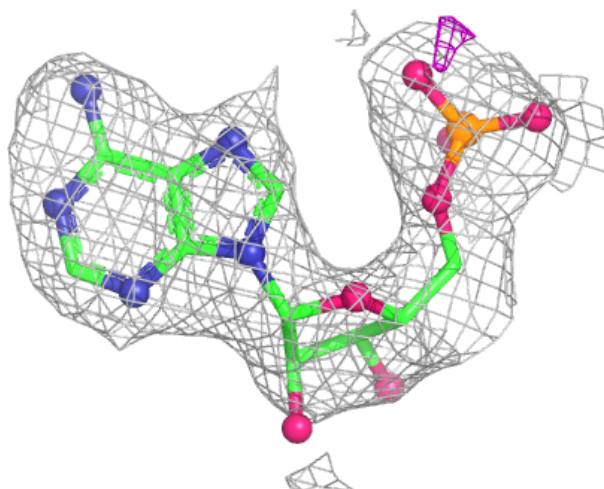
Electron density around AMP B 403:

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



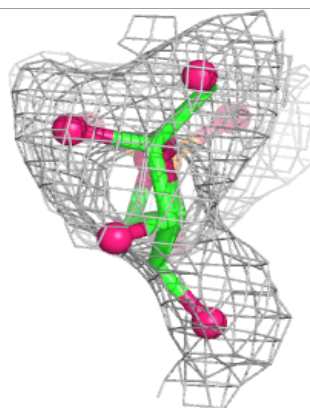
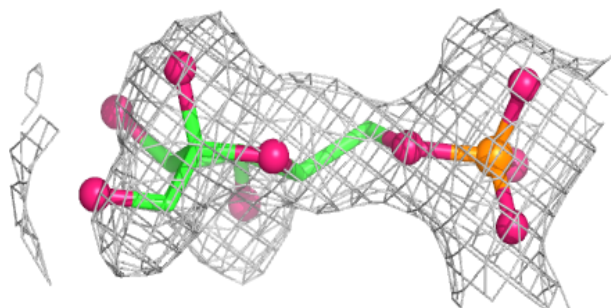
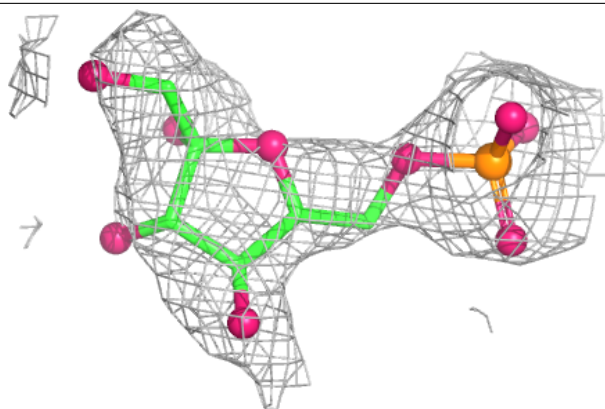
Electron density around AMP A 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

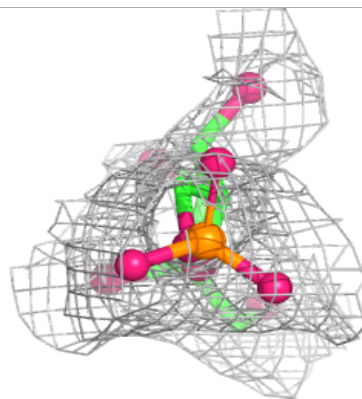
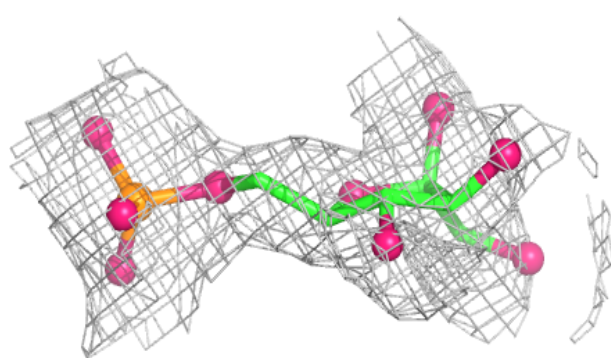
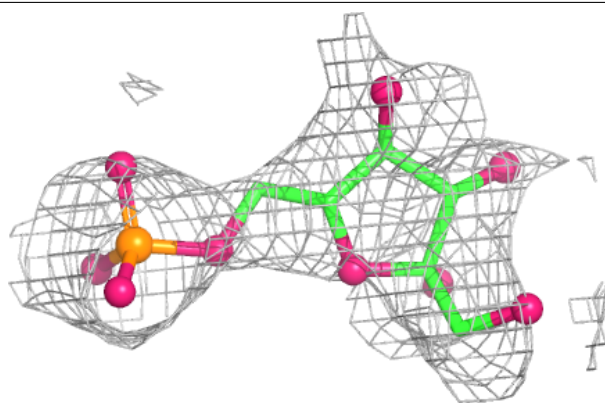


Electron density around F6P A 401:

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

**Electron density around F6P B 401:**

$2mF_o-DF_c$ (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.