



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 11:59 PM UTC

PDB ID : 1BG3 / pdb_00001bg3
Title : RAT BRAIN HEXOKINASE TYPE I COMPLEX WITH GLUCOSE AND INHIBITOR GLUCOSE-6-PHOSPHATE
Authors : Mulichak, A.M.; Garavito, R.M.
Deposited on : 1998-06-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

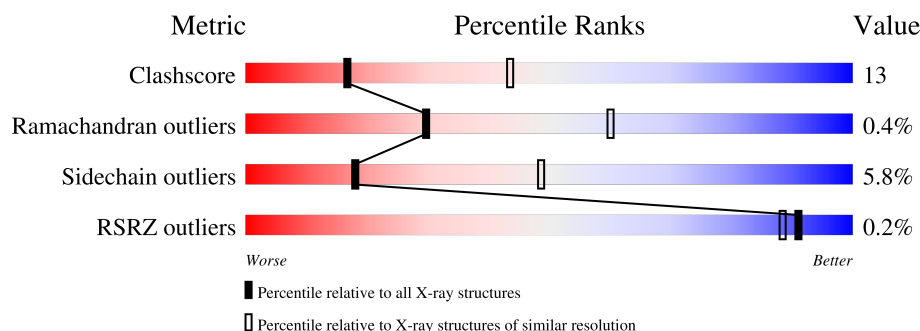
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	918	
1	B	918	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G6P	A	1002	X	-	-	-
3	G6P	A	1004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G6P	B	1002	X	-	-	-
3	G6P	B	1004	X	-	-	-

2 Entry composition [i](#)

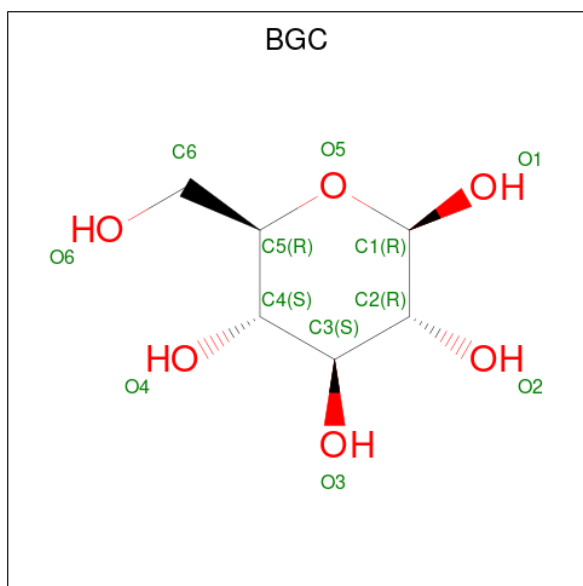
There are 5 unique types of molecules in this entry. The entry contains 13962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEXOKINASE.

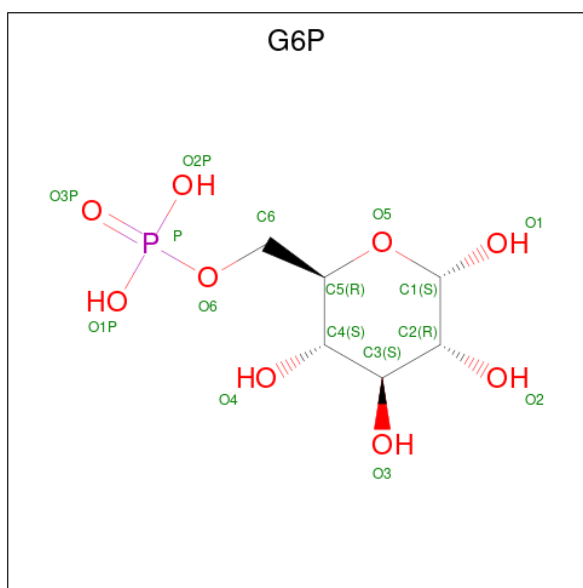
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	0	0
			6832	4304	1177	1296	55			
1	B	902	Total	C	N	O	S	0	0	0
			6783	4276	1157	1295	55			

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: $C_6H_{13}O_9P$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

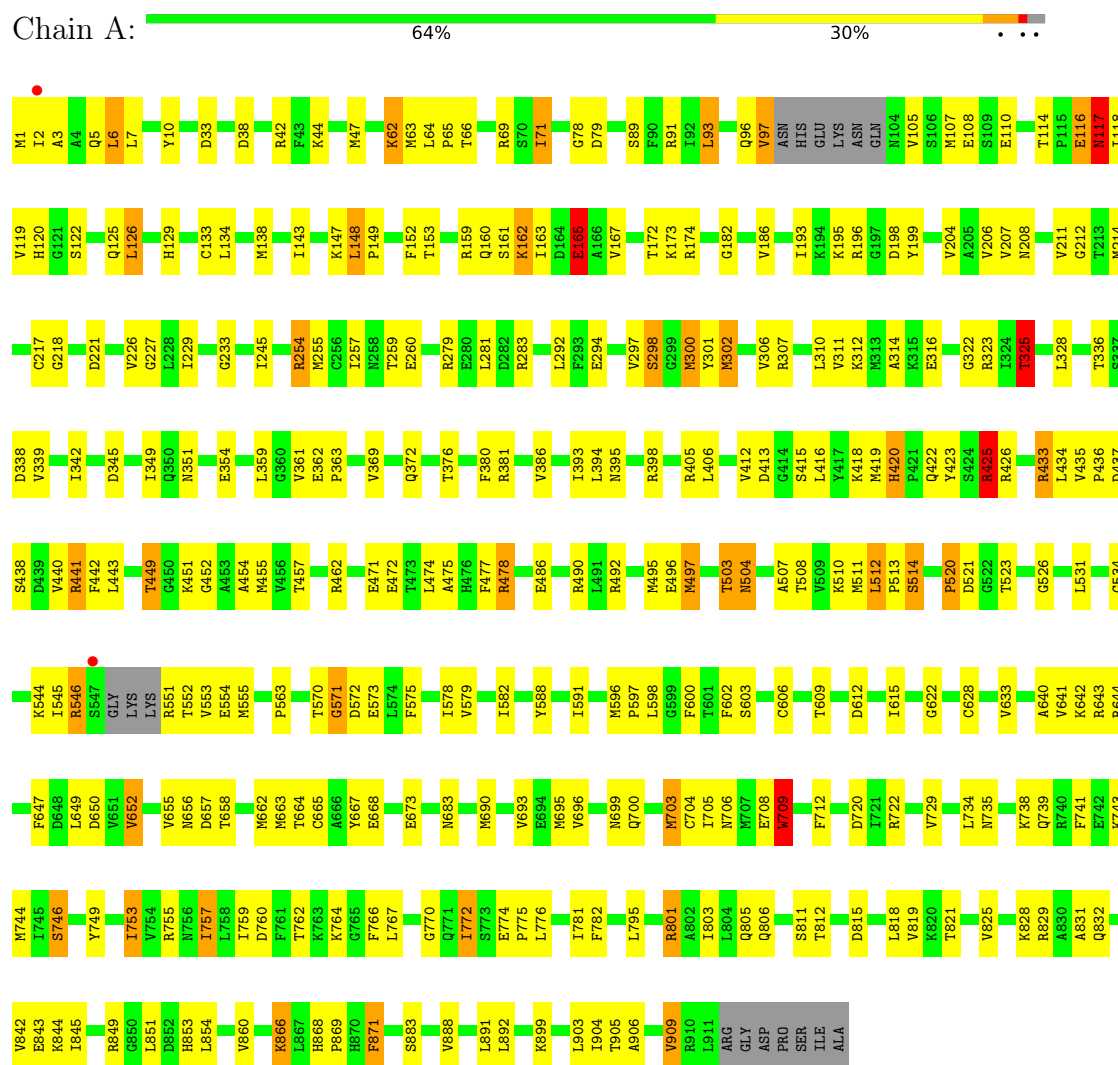
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	98	Total	O	0	0
			98	98		

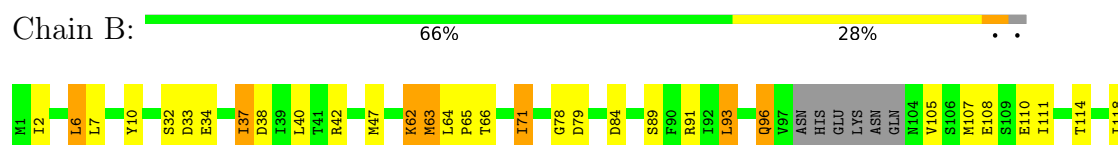
3 Residue-property plots

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: HEXOKINASE



• Molecule 1: HEXOKINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.10Å 77.10Å 137.10Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	71.0 (20.00-2.80) 70.3 (20.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.251 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13962	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: BGC, CA, G6P

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	0.76	0/6935	1.20	62/9367 (0.7%)
1	B	0.78	4/6885 (0.1%)	1.21	65/9310 (0.7%)
All	All	0.77	4/13820 (0.0%)	1.20	127/18677 (0.7%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	MET	SD-CE	-6.14	1.64	1.79
1	B	255	MET	SD-CE	-6.12	1.64	1.79
1	B	302	MET	SD-CE	-5.60	1.65	1.79
1	B	550	LYS	CA-C	5.17	1.56	1.53

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ILE	N-CA-C	-13.91	99.85	111.81
1	B	883	SER	CA-C-N	10.26	130.07	119.19
1	B	883	SER	C-N-CA	10.26	130.07	119.19
1	A	117	ASN	N-CA-C	-9.48	103.82	114.62
1	B	514	SER	N-CA-C	-9.28	94.11	109.24
1	A	514	SER	N-CA-C	-9.26	94.14	109.24
1	B	161	SER	N-CA-C	-9.07	101.78	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	883	SER	CA-C-N	8.93	128.65	119.19
1	A	883	SER	C-N-CA	8.93	128.65	119.19
1	B	300	MET	N-CA-C	-8.90	103.26	114.56
1	A	161	SER	N-CA-C	-8.23	102.83	113.12
1	B	66	THR	N-CA-C	-8.04	98.93	110.59
1	B	145	ASP	N-CA-C	8.01	122.83	112.26
1	A	300	MET	N-CA-C	-7.91	104.51	114.56
1	A	66	THR	N-CA-C	-7.79	99.30	110.59
1	A	843	GLU	N-CA-C	-7.75	102.53	110.97
1	A	302	MET	N-CA-C	7.56	119.21	110.97
1	A	420	HIS	CA-C-N	7.29	126.92	119.56
1	A	420	HIS	C-N-CA	7.29	126.92	119.56
1	A	504	ASN	N-CA-C	7.18	119.78	111.02
1	A	148	LEU	CA-C-N	7.13	126.89	119.76
1	A	148	LEU	C-N-CA	7.13	126.89	119.76
1	B	753	ILE	N-CA-C	-7.13	103.83	110.53
1	A	425	ARG	NE-CZ-NH2	-7.10	112.81	119.20
1	B	279	ARG	NE-CZ-NH2	-7.10	112.81	119.20
1	A	78	GLY	N-CA-C	7.09	119.24	112.08
1	A	292	LEU	N-CA-C	7.08	119.90	111.33
1	B	843	GLU	N-CA-C	-7.00	103.58	111.14
1	B	292	LEU	N-CA-C	7.00	119.80	111.33
1	B	302	MET	N-CA-C	7.00	119.56	111.02
1	A	279	ARG	NE-CZ-NH2	-6.97	112.93	119.20
1	B	593	GLY	CA-C-N	6.87	126.90	119.89
1	B	593	GLY	C-N-CA	6.87	126.90	119.89
1	B	165	GLU	N-CA-C	-6.86	98.65	109.50
1	A	454	ALA	N-CA-C	-6.86	103.89	111.36
1	B	420	HIS	CA-C-N	6.83	126.46	119.56
1	B	420	HIS	C-N-CA	6.83	126.46	119.56
1	B	195	LYS	N-CA-C	-6.82	103.85	111.28
1	B	358	ARG	N-CA-C	-6.80	103.89	111.71
1	B	78	GLY	N-CA-C	6.79	118.94	112.08
1	A	254	ARG	CD-NE-CZ	6.77	133.88	124.40
1	A	165	GLU	N-CA-C	-6.73	98.96	109.72
1	A	571	GLY	N-CA-C	-6.71	104.38	113.37
1	A	753	ILE	N-CA-C	-6.70	104.23	110.53
1	B	425	ARG	NE-CZ-NH2	-6.61	113.26	119.20
1	B	381	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	B	652	VAL	N-CA-C	6.58	117.36	110.72
1	B	866	LYS	N-CA-C	6.53	118.48	111.36
1	B	148	LEU	CA-C-N	6.47	126.23	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	LEU	C-N-CA	6.47	126.23	119.76
1	B	550	LYS	N-CA-C	-6.43	102.57	108.75
1	B	526	GLY	N-CA-C	6.40	118.99	111.63
1	A	381	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	A	652	VAL	N-CA-C	6.40	117.18	110.72
1	A	866	LYS	N-CA-C	6.36	118.29	111.36
1	B	512	LEU	N-CA-C	6.36	118.84	109.50
1	B	279	ARG	CD-NE-CZ	6.33	133.26	124.40
1	A	512	LEU	N-CA-C	6.31	118.77	109.50
1	B	96	GLN	N-CA-C	-6.31	97.99	108.34
1	B	609	THR	N-CA-C	-6.27	103.99	113.89
1	B	746	SER	N-CA-C	6.18	119.62	110.48
1	B	254	ARG	CB-CG-CD	-6.18	97.09	111.30
1	A	746	SER	N-CA-C	6.13	119.55	110.48
1	A	812	THR	N-CA-C	-6.08	101.19	109.95
1	A	415	SER	N-CA-C	6.05	117.57	110.97
1	A	381	ARG	CD-NE-CZ	5.98	132.77	124.40
1	B	910	ARG	N-CA-C	-5.97	104.15	112.45
1	B	449	THR	N-CA-C	5.97	117.87	111.36
1	B	622	GLY	N-CA-C	5.92	123.07	115.32
1	A	279	ARG	CD-NE-CZ	5.91	132.67	124.40
1	A	195	LYS	N-CA-C	-5.88	104.87	111.28
1	A	338	ASP	N-CA-C	-5.87	104.96	111.36
1	B	454	ALA	N-CA-C	-5.85	104.98	111.36
1	B	279	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	B	740	ARG	N-CA-C	5.84	117.31	111.07
1	B	298	SER	N-CA-C	5.79	117.77	110.24
1	A	254	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	A	5	GLN	N-CA-C	-5.77	104.89	111.07
1	A	381	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	B	254	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	A	162	LYS	N-CA-C	-5.75	101.41	109.69
1	A	298	SER	N-CA-C	5.71	117.66	110.24
1	A	609	THR	N-CA-C	-5.67	104.93	113.89
1	A	449	THR	N-CA-C	5.67	117.53	111.36
1	B	423	TYR	N-CA-C	5.66	117.92	111.02
1	B	381	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	B	254	ARG	CG-CD-NE	5.61	124.35	112.00
1	B	425	ARG	N-CA-C	5.61	117.47	111.36
1	A	254	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	B	325	THR	CA-C-N	5.55	125.16	119.56
1	B	325	THR	C-N-CA	5.55	125.16	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	CD-NE-CZ	5.53	132.15	124.40
1	B	510	LYS	N-CA-C	-5.50	101.52	110.20
1	B	66	THR	CA-C-N	-5.49	114.99	123.17
1	B	66	THR	C-N-CA	-5.49	114.99	123.17
1	A	71	ILE	CA-C-N	5.47	125.48	119.90
1	A	71	ILE	C-N-CA	5.47	125.48	119.90
1	A	441	ARG	N-CA-C	-5.47	101.66	110.14
1	A	622	GLY	N-CA-C	5.41	122.41	115.32
1	B	425	ARG	CD-NE-CZ	5.41	131.97	124.40
1	B	338	ASP	N-CA-C	-5.39	105.32	111.14
1	A	853	HIS	N-CA-C	5.37	118.19	108.69
1	B	644	ARG	N-CA-C	5.36	117.20	111.36
1	A	66	THR	CA-C-N	-5.35	115.20	123.17
1	A	66	THR	C-N-CA	-5.35	115.20	123.17
1	A	757	ILE	N-CA-C	-5.31	105.67	110.82
1	B	709	TRP	N-CA-C	5.31	119.38	113.01
1	B	796	ALA	N-CA-C	-5.30	102.63	110.48
1	A	279	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	433	ARG	N-CA-C	-5.23	105.64	112.23
1	A	843	GLU	CB-CA-C	-5.18	102.98	110.96
1	A	854	LEU	N-CA-C	5.18	117.92	109.59
1	A	325	THR	CA-C-N	5.16	124.77	119.56
1	A	325	THR	C-N-CA	5.16	124.77	119.56
1	A	709	TRP	N-CA-C	5.16	119.20	113.01
1	B	381	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	497	MET	N-CA-C	5.13	117.61	111.71
1	B	71	ILE	CA-C-N	5.13	125.13	119.90
1	B	71	ILE	C-N-CA	5.13	125.13	119.90
1	A	62	LYS	N-CA-C	5.11	118.29	111.75
1	B	504	ASN	N-CA-C	5.09	119.72	111.37
1	A	734	LEU	N-CA-C	-5.09	105.38	111.03
1	B	852	ASP	N-CA-C	-5.08	106.25	112.90
1	B	37	ILE	N-CA-C	-5.07	105.60	110.72
1	B	378	VAL	N-CA-C	5.06	115.83	110.72
1	B	62	LYS	N-CA-C	5.03	118.18	111.75
1	A	657	ASP	N-CA-C	5.01	117.48	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	ARG	Sidechain

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	6832	0	6711	196	0
1	B	6783	0	6623	153	0
2	A	24	0	23	2	0
2	B	24	0	24	1	0
3	A	32	0	22	0	0
3	B	32	0	22	0	0
4	A	1	0	0	0	0
5	A	136	0	0	6	0
5	B	98	0	0	0	0
All	All	13962	0	13425	347	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 13.

All (347) 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:361:VAL:O	1:A:363:PRO:HD3	1.62	1.00
1:B:722:ARG:HG2	1:B:744:MET:HE1	1.48	0.96
1:B:361:VAL:O	1:B:363:PRO:HD3	1.67	0.93
1:A:722:ARG:HG2	1:A:744:MET:HE1	1.49	0.92
1:A:312:LYS:O	1:A:316:GLU:HG3	1.80	0.81
1:A:162:LYS:HG3	1:A:165:GLU:HB2	1.62	0.81
1:A:849:ARG:HB2	1:A:851:LEU:HD11	1.62	0.81
1:A:69:ARG:HD3	5:A:2044:HOH:O	1.81	0.78
1:B:690:MET:HE3	1:B:703:MET:HB2	1.65	0.77
1:A:477:PHE:HB2	1:A:825:VAL:HG12	1.65	0.76
1:B:397:LEU:O	1:B:401:LYS:HG3	1.85	0.76
1:B:906:ALA:O	1:B:909:VAL:HG12	1.85	0.76
1:B:204:VAL:HG22	1:B:457:THR:HG23	1.68	0.75
1:B:477:PHE:HB2	1:B:825:VAL:HG12	1.68	0.75
1:A:520:PRO:HD3	1:A:663:MET:SD	2.27	0.74
1:B:662:MET:HE2	1:B:663:MET:HE2	1.70	0.73
1:A:212:GLY:HA3	1:A:449:THR:HG23	1.70	0.73
1:B:658:THR:HG21	1:B:683:ASN:HD22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HG13	1:A:105:VAL:HG22	1.71	0.72
1:B:212:GLY:HA3	1:B:449:THR:HG23	1.71	0.72
1:B:520:PRO:HD3	1:B:663:MET:SD	2.29	0.72
1:A:578:ILE:O	1:A:582:ILE:HG13	1.89	0.72
1:A:172:THR:HG22	1:A:173:LYS:HG3	1.70	0.72
1:A:571:GLY:HA2	1:A:628:CYS:SG	2.30	0.72
1:A:652:VAL:HB	1:A:905:THR:HG23	1.71	0.72
1:A:302:MET:HE2	1:A:336:THR:HG23	1.72	0.71
1:A:690:MET:HE3	1:A:703:MET:HB2	1.71	0.71
1:A:762:THR:O	1:A:770:GLY:HA2	1.91	0.71
1:A:2:ILE:O	1:A:6:LEU:HB2	1.91	0.70
1:A:658:THR:HG21	1:A:683:ASN:HD22	1.56	0.70
1:B:172:THR:HG22	1:B:173:LYS:HG3	1.71	0.70
1:B:302:MET:HE2	1:B:336:THR:HG23	1.73	0.70
1:B:545:ILE:O	1:B:546:ARG:HD3	1.92	0.70
1:A:665:CYS:SG	1:A:891:LEU:HD23	2.34	0.68
1:B:380:PHE:CE1	1:B:426:ARG:HB3	2.28	0.68
1:B:578:ILE:O	1:B:582:ILE:HG13	1.95	0.67
1:A:159:ARG:HB2	1:A:167:VAL:HB	1.77	0.67
1:B:89:SER:HB2	1:B:91:ARG:NH1	2.10	0.67
1:B:65:PRO:HB3	1:B:255:MET:HE1	1.77	0.67
1:A:89:SER:HB2	1:A:91:ARG:NH1	2.11	0.66
1:B:107:MET:SD	1:B:451:LYS:HB2	2.36	0.65
1:B:204:VAL:CG2	1:B:457:THR:HG23	2.25	0.65
1:A:545:ILE:O	1:A:546:ARG:HD3	1.97	0.65
1:A:118:ILE:HG23	1:A:126:LEU:HA	1.77	0.65
1:A:302:MET:HE3	1:A:339:VAL:HG11	1.77	0.65
1:A:65:PRO:HB3	1:A:255:MET:HE1	1.79	0.64
1:B:481:LYS:O	1:B:485:MET:HB2	1.96	0.64
1:A:849:ARG:HB2	1:A:851:LEU:CD1	2.25	0.64
1:A:204:VAL:HG22	1:A:457:THR:HG23	1.79	0.64
1:A:435:VAL:HG12	1:A:438:SER:OG	1.97	0.64
1:A:325:THR:HG21	1:A:359:LEU:O	1.97	0.63
1:A:662:MET:HE2	1:A:663:MET:HE2	1.78	0.63
1:A:906:ALA:O	1:A:909:VAL:HG12	1.98	0.63
1:B:571:GLY:HA2	1:B:628:CYS:SG	2.38	0.63
1:A:695:MET:HG2	5:A:2029:HOH:O	1.97	0.62
1:A:570:THR:HG22	1:A:572:ASP:H	1.65	0.62
1:B:217:CYS:HB3	1:B:443:LEU:HD23	1.81	0.62
1:A:755:ARG:HD3	1:A:781:ILE:HG22	1.81	0.62
1:B:501:LYS:HG2	1:B:695:MET:SD	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:LYS:O	1:B:832:GLN:HG3	2.01	0.61
1:B:762:THR:O	1:B:770:GLY:HA2	2.00	0.61
1:A:495:MET:HE2	1:A:844:LYS:HD3	1.83	0.61
1:B:2:ILE:O	1:B:6:LEU:HB2	2.00	0.60
1:B:325:THR:HG21	1:B:359:LEU:O	2.01	0.60
1:B:302:MET:HE3	1:B:339:VAL:HG11	1.83	0.60
1:B:866:LYS:HE3	1:B:892:LEU:HD11	1.82	0.59
1:A:204:VAL:CG2	1:A:457:THR:HG23	2.31	0.59
1:A:866:LYS:HE3	1:A:892:LEU:HD11	1.84	0.59
1:A:351:ASN:HA	1:A:354:GLU:HG2	1.84	0.59
1:A:298:SER:HB3	1:A:301:TYR:HD2	1.68	0.58
1:A:477:PHE:HB2	1:A:825:VAL:CG1	2.34	0.58
1:A:545:ILE:HG23	1:A:553:VAL:HG22	1.85	0.58
1:A:767:LEU:HD13	1:A:818:LEU:HD23	1.85	0.58
1:B:569:GLY:O	1:B:625:ALA:HA	2.04	0.58
1:B:605:PRO:HB2	1:B:617:ILE:HB	1.87	0.57
1:A:591:ILE:HG21	1:A:596:MET:SD	2.44	0.57
1:A:507:ALA:O	1:A:510:LYS:HE3	2.03	0.57
1:B:520:PRO:HG2	1:B:903:LEU:HD13	1.86	0.56
1:A:196:ARG:HG2	1:A:198:ASP:HB2	1.86	0.56
1:A:570:THR:HB	1:A:573:GLU:H	1.69	0.56
1:B:298:SER:HB3	1:B:301:TYR:HD2	1.68	0.56
1:B:542:LEU:HD13	1:B:591:ILE:CD1	2.35	0.56
1:A:107:MET:SD	1:A:451:LYS:HB2	2.45	0.56
1:B:570:THR:OG1	1:B:573:GLU:HG3	2.06	0.56
1:B:767:LEU:HD13	1:B:818:LEU:HD23	1.88	0.56
1:A:755:ARG:O	1:A:759:ILE:HG13	2.06	0.55
1:A:673:GLU:CD	1:A:849:ARG:HH22	2.14	0.55
1:B:755:ARG:HD3	1:B:781:ILE:HG22	1.87	0.55
1:A:513:PRO:HB3	1:A:703:MET:HE3	1.89	0.55
1:A:849:ARG:CB	1:A:851:LEU:HD11	2.34	0.55
1:A:652:VAL:CB	1:A:905:THR:HG23	2.37	0.55
1:B:507:ALA:O	1:B:510:LYS:HE3	2.06	0.55
1:B:114:THR:HG22	1:B:119:VAL:HG23	1.88	0.55
1:A:2:ILE:O	1:A:6:LEU:HD23	2.07	0.54
1:B:513:PRO:HB3	1:B:703:MET:HE3	1.88	0.54
1:A:712:PHE:O	1:A:741:PHE:HB2	2.07	0.54
1:B:223:GLN:OE1	1:B:441:ARG:NH2	2.40	0.54
1:B:91:ARG:HA	1:B:110:GLU:O	2.08	0.54
1:A:1:MET:C	1:A:3:ALA:H	2.15	0.54
1:B:477:PHE:HB2	1:B:825:VAL:CG1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:ARG:O	1:B:759:ILE:HG13	2.07	0.54
1:A:1:MET:C	1:A:3:ALA:N	2.64	0.54
1:A:570:THR:HG22	1:A:571:GLY:N	2.23	0.54
1:A:114:THR:HG22	1:A:119:VAL:HG23	1.90	0.54
1:B:544:LYS:HB2	1:B:554:GLU:HB3	1.90	0.53
1:A:544:LYS:HB2	1:A:554:GLU:HB3	1.91	0.53
1:B:531:LEU:HD12	1:B:600:PHE:CD1	2.44	0.53
1:B:579:VAL:HG13	1:B:647:PHE:HZ	1.73	0.53
1:B:62:LYS:HB3	1:B:64:LEU:HG	1.90	0.53
1:A:602:PHE:CE2	1:A:633:VAL:HG11	2.44	0.53
1:B:545:ILE:HD13	1:B:903:LEU:HD23	1.90	0.53
1:A:91:ARG:HA	1:A:110:GLU:O	2.09	0.53
1:A:152:PHE:HB3	1:A:206:VAL:HG22	1.91	0.53
1:A:811:SER:OG	1:A:815:ASP:HB2	2.08	0.53
1:A:591:ILE:CG2	1:A:596:MET:SD	2.97	0.52
1:B:422:GLN:O	1:B:426:ARG:HG3	2.09	0.52
1:B:354:GLU:O	1:B:358:ARG:HG3	2.09	0.52
1:A:147:LYS:O	1:A:148:LEU:HD23	2.10	0.52
1:A:665:CYS:O	1:A:668:GLU:HG2	2.10	0.52
1:B:323:ARG:NH1	1:B:362:GLU:H	2.08	0.52
1:A:376:THR:HG23	1:A:426:ARG:HH12	1.75	0.51
1:B:815:ASP:O	1:B:819:VAL:HG23	2.09	0.51
1:A:551:ARG:NH2	1:A:667:TYR:O	2.42	0.51
1:B:579:VAL:HG13	1:B:647:PHE:CZ	2.45	0.51
1:A:531:LEU:HD12	1:A:600:PHE:CD1	2.45	0.51
1:B:38:ASP:O	1:B:42:ARG:HG3	2.10	0.51
1:B:152:PHE:HB3	1:B:206:VAL:HG22	1.92	0.51
1:A:193:ILE:HG23	1:A:199:TYR:CE1	2.45	0.51
1:A:441:ARG:HG2	1:A:442:PHE:N	2.25	0.51
1:A:62:LYS:HB3	1:A:64:LEU:HG	1.93	0.51
1:A:116:GLU:HG2	1:A:120:HIS:ND1	2.25	0.51
1:A:323:ARG:NH1	1:A:362:GLU:H	2.08	0.51
1:B:606:CYS:HA	1:B:615:ILE:O	2.10	0.51
1:A:93:LEU:N	1:A:93:LEU:HD12	2.26	0.51
1:A:147:LYS:C	1:A:148:LEU:HD23	2.36	0.51
1:B:325:THR:HG23	1:B:328:LEU:HB2	1.93	0.51
1:A:217:CYS:HB3	1:A:443:LEU:HD23	1.92	0.51
1:B:7:LEU:O	1:B:10:TYR:HB3	2.11	0.51
1:B:93:LEU:HD12	1:B:93:LEU:N	2.26	0.50
1:A:186:VAL:HG22	1:A:206:VAL:HG21	1.93	0.50
1:B:226:VAL:HG12	1:B:227:GLY:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:VAL:HG11	1:B:899:LYS:HG3	1.93	0.50
1:A:606:CYS:HA	1:A:615:ILE:O	2.12	0.50
1:B:93:LEU:HA	1:B:108:GLU:O	2.12	0.50
1:B:172:THR:HG21	2:B:1001:BGC:O1	2.12	0.50
1:A:33:ASP:OD2	1:A:433:ARG:NH1	2.45	0.50
1:B:105:VAL:HG11	1:B:451:LYS:HG3	1.94	0.50
1:B:129:HIS:CE1	1:B:133:CYS:SG	3.05	0.49
1:B:521:ASP:O	1:B:523:THR:HG23	2.13	0.49
1:B:534:GLY:HA3	1:B:603:SER:HB2	1.94	0.49
1:B:541:LEU:HG	1:B:557:ASN:HB3	1.95	0.49
1:A:441:ARG:HG2	1:A:442:PHE:H	1.76	0.49
1:B:712:PHE:O	1:B:741:PHE:HB2	2.12	0.49
1:B:186:VAL:HG22	1:B:206:VAL:HG21	1.94	0.49
1:A:521:ASP:O	1:A:523:THR:HG23	2.13	0.49
1:B:664:THR:HG23	1:B:899:LYS:HD2	1.93	0.49
1:A:422:GLN:O	1:A:426:ARG:HG3	2.13	0.49
1:A:597:PRO:HA	1:A:650:ASP:HB3	1.95	0.49
1:A:520:PRO:HG2	1:A:903:LEU:HD13	1.95	0.49
1:A:579:VAL:HG13	1:A:647:PHE:CZ	2.48	0.49
1:B:614:GLY:O	1:B:633:VAL:HG22	2.13	0.49
1:B:545:ILE:HG22	1:B:546:ARG:N	2.28	0.48
1:A:534:GLY:HA3	1:A:603:SER:HB2	1.95	0.48
1:B:312:LYS:O	1:B:316:GLU:HG3	2.13	0.48
1:A:380:PHE:CE1	1:A:426:ARG:HB3	2.48	0.48
1:A:105:VAL:HG11	1:A:451:LYS:HG3	1.96	0.48
1:A:300:MET:HE2	1:A:301:TYR:CE1	2.49	0.48
1:A:325:THR:HG23	1:A:328:LEU:HB2	1.96	0.48
1:A:511:MET:HB3	1:A:705:ILE:HG21	1.96	0.48
1:A:160:GLN:HG2	1:A:165:GLU:O	2.13	0.48
1:B:602:PHE:CE2	1:B:633:VAL:HG11	2.48	0.48
1:A:815:ASP:O	1:A:819:VAL:HG23	2.14	0.48
1:A:118:ILE:HG21	1:A:129:HIS:HD2	1.79	0.47
1:A:307:ARG:O	1:A:311:VAL:HG23	2.13	0.47
1:B:870:HIS:ND1	1:B:873:ARG:NH2	2.62	0.47
1:A:739:GLN:HG3	5:A:2017:HOH:O	2.14	0.47
1:A:153:THR:HA	1:A:207:VAL:O	2.15	0.47
1:A:172:THR:HG21	2:A:1001:BGC:O1	2.13	0.47
1:A:656:ASN:HB2	5:A:2111:HOH:O	2.13	0.47
1:B:380:PHE:CD1	1:B:426:ARG:HD3	2.49	0.47
1:B:401:LYS:C	1:B:403:THR:H	2.21	0.47
1:B:33:ASP:OD2	1:B:433:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PRO:HB3	1:B:255:MET:CE	2.44	0.47
1:B:297:VAL:HG11	1:B:386:VAL:CG2	2.45	0.47
1:B:683:ASN:OD1	1:B:708:GLU:HA	2.15	0.47
1:A:7:LEU:O	1:A:10:TYR:HB3	2.14	0.47
1:A:118:ILE:HG21	1:A:129:HIS:CD2	2.50	0.47
1:A:134:LEU:HD11	1:A:138:MET:HE3	1.96	0.47
1:A:394:LEU:HD13	1:A:440:VAL:HG21	1.97	0.47
1:B:652:VAL:HB	1:B:905:THR:HG23	1.95	0.47
1:B:511:MET:HB3	1:B:705:ILE:HG21	1.97	0.47
1:B:828:LYS:HG3	1:B:874:ILE:HD13	1.96	0.47
1:A:664:THR:HG23	1:A:899:LYS:HD2	1.97	0.47
1:A:97:VAL:HG11	1:A:455:MET:HE1	1.97	0.47
1:A:452:GLY:O	1:A:455:MET:HB2	2.15	0.47
1:B:314:ALA:O	1:B:322:GLY:HA2	2.15	0.46
1:A:229:ILE:HD13	1:A:413:ASP:HB3	1.97	0.46
1:A:709:TRP:C	1:A:709:TRP:CD1	2.92	0.46
1:A:314:ALA:O	1:A:322:GLY:HA2	2.16	0.46
1:A:803:ILE:O	1:A:806:GLN:HB3	2.16	0.46
1:A:690:MET:HE2	1:A:693:VAL:HG21	1.98	0.46
1:A:755:ARG:HD2	1:A:776:LEU:O	2.16	0.46
1:B:418:LYS:O	1:B:419:MET:HE2	2.15	0.46
1:B:229:ILE:HD13	1:B:413:ASP:HB3	1.98	0.46
1:B:452:GLY:O	1:B:455:MET:HB2	2.15	0.46
1:A:79:ASP:HA	1:A:96:GLN:HA	1.98	0.46
1:A:38:ASP:O	1:A:42:ARG:HG3	2.16	0.46
1:A:245:ILE:HD13	1:A:255:MET:HE2	1.97	0.46
1:B:302:MET:HE1	1:B:416:LEU:HD11	1.97	0.46
1:A:571:GLY:CA	1:A:628:CYS:SG	3.01	0.45
1:A:497:MET:HE3	1:A:503:THR:HG22	1.97	0.45
1:A:828:LYS:HD3	5:A:2125:HOH:O	2.16	0.45
1:B:160:GLN:HG2	1:B:165:GLU:O	2.16	0.45
1:B:451:LYS:O	1:B:455:MET:HG2	2.16	0.45
1:B:755:ARG:HD2	1:B:776:LEU:O	2.16	0.45
1:B:773:SER:O	1:B:777:LYS:HG3	2.16	0.45
1:A:683:ASN:OD1	1:A:708:GLU:HA	2.16	0.45
1:B:153:THR:HA	1:B:207:VAL:O	2.16	0.45
1:A:471:GLU:O	1:A:475:ALA:HB2	2.16	0.45
1:A:735:ASN:HB2	1:A:738:LYS:HB2	1.97	0.45
1:A:699:ASN:OD1	1:A:700:GLN:HG2	2.17	0.45
1:B:545:ILE:CD1	1:B:903:LEU:HD23	2.46	0.45
1:A:474:LEU:O	1:A:478:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LEU:HD11	1:B:586:LEU:HD21	1.99	0.45
1:A:129:HIS:CE1	1:A:133:CYS:SG	3.10	0.45
1:B:690:MET:CE	1:B:703:MET:HB2	2.44	0.45
1:A:642:LYS:O	1:A:643:ARG:C	2.60	0.44
1:A:757:ILE:O	1:A:760:ASP:HB3	2.17	0.44
1:B:526:GLY:O	1:B:545:ILE:N	2.50	0.44
1:B:542:LEU:HD13	1:B:591:ILE:HD13	1.99	0.44
1:B:709:TRP:CD1	1:B:709:TRP:C	2.93	0.44
1:A:93:LEU:HA	1:A:108:GLU:O	2.16	0.44
1:A:764:LYS:HE2	1:A:766:PHE:CZ	2.52	0.44
1:A:323:ARG:HH11	1:A:362:GLU:H	1.66	0.44
1:B:477:PHE:CD1	1:B:477:PHE:N	2.85	0.44
1:B:866:LYS:CE	1:B:892:LEU:HD11	2.48	0.44
1:A:434:LEU:C	1:A:436:PRO:HD3	2.43	0.44
1:A:652:VAL:CG1	1:A:905:THR:HG23	2.48	0.44
1:B:688:GLU:OE1	1:B:848:ASN:ND2	2.51	0.44
1:A:406:LEU:HB3	1:A:438:SER:HB3	2.00	0.44
1:B:665:CYS:O	1:B:668:GLU:HG3	2.18	0.44
1:A:302:MET:HE1	1:A:416:LEU:HD11	2.00	0.44
1:A:422:GLN:OE1	1:A:425:ARG:NH2	2.51	0.44
1:B:47:MET:HE2	1:B:63:MET:HE1	1.99	0.44
1:A:772:ILE:HG23	1:A:776:LEU:HD23	1.99	0.44
1:B:323:ARG:HH11	1:B:362:GLU:H	1.65	0.44
1:B:501:LYS:HE3	1:B:694:GLU:O	2.18	0.44
1:A:283:ARG:HH21	1:B:558:LYS:HE3	1.82	0.43
1:A:706:ASN:ND2	1:A:708:GLU:OE1	2.51	0.43
1:A:801:ARG:O	1:A:805:GLN:HG3	2.18	0.43
1:B:420:HIS:HB3	1:B:423:TYR:HB2	2.00	0.43
1:A:553:VAL:HG11	1:A:899:LYS:HG3	2.00	0.43
1:A:579:VAL:HG21	1:A:640:ALA:CB	2.48	0.43
1:B:605:PRO:HD2	1:B:618:SER:O	2.19	0.43
1:A:696:VAL:HG21	1:A:703:MET:CE	2.48	0.43
1:A:497:MET:HB3	1:A:507:ALA:HB2	2.01	0.43
1:B:401:LYS:C	1:B:403:THR:N	2.76	0.43
1:A:63:MET:HE3	1:A:257:ILE:HG21	2.01	0.43
1:A:226:VAL:HG12	1:A:227:GLY:N	2.33	0.43
1:B:230:ILE:HG22	1:B:416:LEU:HB3	2.00	0.43
1:B:706:ASN:ND2	1:B:708:GLU:OE1	2.51	0.43
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.78	0.43
1:A:376:THR:HG23	1:A:426:ARG:NH1	2.34	0.43
1:B:757:ILE:O	1:B:760:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG11	1:A:386:VAL:CG2	2.49	0.43
1:A:571:GLY:O	1:A:575:PHE:HD1	2.02	0.43
1:A:821:THR:O	1:A:825:VAL:HG23	2.19	0.43
1:B:300:MET:HE2	1:B:301:TYR:CE1	2.54	0.43
1:A:398:ARG:NH1	1:A:437:ASP:OD2	2.51	0.43
1:A:526:GLY:O	1:A:545:ILE:N	2.52	0.43
1:B:233:GLY:HA2	1:B:298:SER:OG	2.19	0.43
1:B:525:HIS:NE2	1:B:546:ARG:HD2	2.34	0.43
1:A:44:LYS:HE3	1:A:395:ASN:HD22	1.83	0.42
1:B:84:ASP:HA	1:B:153:THR:HB	2.01	0.42
1:B:350:GLN:HG3	1:B:354:GLU:OE2	2.19	0.42
1:A:300:MET:HE2	1:A:301:TYR:CZ	2.54	0.42
1:B:846:ARG:CD	1:B:885:LYS:HB3	2.49	0.42
1:A:729:VAL:HG21	1:A:753:ILE:HG12	2.01	0.42
1:A:735:ASN:O	1:A:743:LYS:NZ	2.52	0.42
1:A:828:LYS:O	1:A:832:GLN:HG3	2.20	0.42
1:B:37:ILE:HD13	1:B:434:LEU:HD22	2.01	0.42
1:B:642:LYS:O	1:B:643:ARG:C	2.62	0.42
1:B:689:GLU:O	1:B:693:VAL:HG23	2.19	0.42
1:B:798:LEU:C	1:B:798:LEU:HD23	2.44	0.42
1:A:117:ASN:O	1:A:125:GLN:NE2	2.52	0.42
1:A:504:ASN:OD1	1:A:695:MET:HE2	2.19	0.42
1:A:764:LYS:HD3	1:A:766:PHE:CE2	2.54	0.42
1:B:571:GLY:O	1:B:575:PHE:HD1	2.03	0.42
1:B:579:VAL:HG21	1:B:640:ALA:CB	2.50	0.42
1:A:47:MET:HE1	1:A:393:ILE:HG12	2.01	0.42
1:B:471:GLU:O	1:B:475:ALA:HB2	2.19	0.42
1:B:32:SER:OG	1:B:34:GLU:HG2	2.20	0.42
1:A:514:SER:OG	1:A:704:CYS:HB3	2.20	0.42
1:A:842:VAL:HG11	1:A:888:VAL:HG22	2.02	0.42
1:A:259:THR:O	1:A:260:GLU:HB2	2.20	0.41
1:A:294:GLU:OE2	2:A:1001:BGC:O1	2.38	0.41
1:A:746:SER:OG	1:A:749:TYR:HD2	2.03	0.41
1:B:729:VAL:HG21	1:B:753:ILE:HG12	2.01	0.41
1:A:148:LEU:HA	1:A:149:PRO:HD3	1.74	0.41
1:B:842:VAL:HG11	1:B:888:VAL:HG22	2.02	0.41
1:A:233:GLY:HA2	1:A:298:SER:OG	2.20	0.41
1:A:588:TYR:CE1	1:B:331:ARG:HB2	2.55	0.41
1:B:91:ARG:CG	1:B:111:ILE:HG12	2.50	0.41
1:B:519:ILE:O	1:B:520:PRO:C	2.62	0.41
1:B:596:MET:HA	1:B:597:PRO:HD3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PHE:HZ	5:A:2205:HOH:O	2.01	0.41
1:A:602:PHE:CD2	1:A:606:CYS:SG	3.13	0.41
1:A:655:VAL:HG11	1:A:904:ILE:HG21	2.01	0.41
1:B:342:ILE:HG12	1:B:352:ALA:HA	2.03	0.41
1:B:690:MET:HG3	1:B:700:GLN:O	2.21	0.41
1:A:3:ALA:O	1:A:6:LEU:N	2.54	0.41
1:A:420:HIS:HB3	1:A:423:TYR:HB2	2.02	0.41
1:B:79:ASP:HA	1:B:96:GLN:HA	2.01	0.41
1:B:853:HIS:HE1	1:B:887:THR:OG1	2.02	0.41
1:A:868:HIS:ND1	1:A:869:PRO:HD2	2.36	0.41
1:B:71:ILE:HG22	1:B:214:MET:HE3	2.02	0.41
1:B:710:GLY:O	1:B:739:GLN:HA	2.21	0.41
1:A:118:ILE:HD12	1:A:125:GLN:HE21	1.86	0.41
1:A:167:VAL:HG13	1:A:182:GLY:O	2.21	0.41
1:A:306:VAL:O	1:A:310:LEU:HG	2.21	0.41
1:A:477:PHE:CD1	1:A:477:PHE:N	2.88	0.41
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.80	0.41
1:A:696:VAL:HG21	1:A:703:MET:HE2	2.03	0.41
1:A:781:ILE:HG23	1:A:782:PHE:CD2	2.56	0.41
1:B:669:GLU:HA	1:B:670:PRO:HD2	1.73	0.41
1:B:737:GLY:HA2	1:B:740:ARG:HH21	1.86	0.41
1:A:376:THR:O	1:A:380:PHE:HB2	2.21	0.41
1:A:418:LYS:O	1:A:419:MET:HE2	2.21	0.41
1:A:774:GLU:N	1:A:775:PRO:HD2	2.36	0.41
1:B:497:MET:HB3	1:B:507:ALA:HB2	2.03	0.41
1:B:655:VAL:HG11	1:B:904:ILE:HG21	2.02	0.41
1:A:71:ILE:HG22	1:A:214:MET:HE3	2.03	0.40
1:B:555:MET:HB2	1:B:555:MET:HE3	1.74	0.40
1:A:641:VAL:O	1:A:644:ARG:HB3	2.22	0.40
1:B:735:ASN:O	1:B:743:LYS:NZ	2.54	0.40
1:A:218:GLY:HA2	1:A:221:ASP:O	2.22	0.40
1:A:690:MET:CE	1:A:703:MET:HB2	2.48	0.40
1:B:40:LEU:HD23	1:B:40:LEU:C	2.47	0.40
1:B:63:MET:HE3	1:B:257:ILE:HG21	2.02	0.40
1:A:208:ASN:HB3	1:A:211:VAL:HG23	2.02	0.40
1:A:342:ILE:O	1:A:372:GLN:HG3	2.20	0.40
1:A:511:MET:HE3	1:A:705:ILE:HG21	2.03	0.40
1:A:831:ALA:HB2	1:A:871:PHE:HA	2.03	0.40
1:A:868:HIS:HA	1:A:869:PRO:HD3	1.92	0.40
1:B:126:LEU:O	1:B:129:HIS:HB3	2.22	0.40
1:A:602:PHE:HD2	1:A:606:CYS:SG	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:LEU:HD23	1:B:882:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	896/918 (98%)	829 (92%)	65 (7%)	2 (0%)	43	72
1	B	896/918 (98%)	835 (93%)	55 (6%)	6 (1%)	18	47
All	All	1792/1836 (98%)	1664 (93%)	120 (7%)	8 (0%)	30	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	ASP
1	A	345	ASP
1	A	871	PHE
1	B	871	PHE
1	B	404	PRO
1	B	651	VAL
1	B	348	GLY
1	B	593	GLY

5.3.2 Protein sidechains [i](#)

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	722/791 (91%)	677 (94%)	45 (6%)	16	45
1	B	714/791 (90%)	675 (94%)	39 (6%)	19	51
All	All	1436/1582 (91%)	1352 (94%)	84 (6%)	18	49

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	93	LEU
1	A	97	VAL
1	A	116	GLU
1	A	117	ASN
1	A	122	SER
1	A	126	LEU
1	A	143	ILE
1	A	163	ILE
1	A	165	GLU
1	A	174	ARG
1	A	254	ARG
1	A	281	LEU
1	A	325	THR
1	A	349	ILE
1	A	369	VAL
1	A	405	ARG
1	A	412	VAL
1	A	425	ARG
1	A	462	ARG
1	A	472	GLU
1	A	478	ARG
1	A	486	GLU
1	A	492	ARG
1	A	496	GLU
1	A	503	THR
1	A	508	THR
1	A	520	PRO
1	A	546	ARG
1	A	552	THR
1	A	555	MET
1	A	563	PRO
1	A	598	LEU
1	A	612	ASP
1	A	649	LEU

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Mol	Chain	Res	Type
1	A	703	MET
1	A	709	TRP
1	A	720	ASP
1	A	772	ILE
1	A	795	LEU
1	A	801	ARG
1	A	829	ARG
1	A	845	ILE
1	A	860	VAL
1	A	909	VAL
1	B	6	LEU
1	B	93	LEU
1	B	126	LEU
1	B	163	ILE
1	B	254	ARG
1	B	281	LEU
1	B	325	THR
1	B	344	LYS
1	B	349	ILE
1	B	369	VAL
1	B	412	VAL
1	B	425	ARG
1	B	468	ARG
1	B	472	GLU
1	B	478	ARG
1	B	486	GLU
1	B	492	ARG
1	B	496	GLU
1	B	508	THR
1	B	520	PRO
1	B	546	ARG
1	B	555	MET
1	B	592	LYS
1	B	598	LEU
1	B	612	ASP
1	B	626	THR
1	B	649	LEU
1	B	671	THR
1	B	703	MET
1	B	709	TRP
1	B	720	ASP
1	B	736	SER

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Mol	Chain	Res	Type
1	B	801	ARG
1	B	813	CYS
1	B	816	SER
1	B	829	ARG
1	B	844	LYS
1	B	860	VAL
1	B	911	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	384	ASN
1	A	469	GLN
1	A	577	HIS
1	A	683	ASN
1	A	789	GLN
1	A	805	GLN
1	A	855	ASN
1	B	125	GLN
1	B	190	ASN
1	B	384	ASN
1	B	656	ASN
1	B	683	ASN
1	B	692	ASN
1	B	702	GLN
1	B	832	GLN
1	B	848	ASN
1	B	853	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	BGC	B	1003	-	12,12,12	0.38	0	17,17,17	0.64	0
2	BGC	B	1001	-	12,12,12	0.52	0	17,17,17	0.97	1 (5%)
2	BGC	A	1001	-	12,12,12	0.60	0	17,17,17	1.02	1 (5%)
3	G6P	B	1002	-	16,16,16	0.73	0	23,24,24	0.84	0
3	G6P	B	1004	-	16,16,16	0.75	0	23,24,24	0.75	0
3	G6P	A	1004	-	16,16,16	0.70	0	23,24,24	0.70	0
2	BGC	A	1003	-	12,12,12	0.32	0	17,17,17	0.55	0
3	G6P	A	1002	-	16,16,16	0.75	0	23,24,24	0.71	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	BGC	B	1003	-	-	2/2/22/22	0/1/1/1
2	BGC	B	1001	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
3	G6P	B	1002	-	1/1/6/6	3/6/26/26	0/1/1/1
3	G6P	B	1004	-	1/1/6/6	4/6/26/26	0/1/1/1
3	G6P	A	1004	-	1/1/6/6	4/6/26/26	0/1/1/1
2	BGC	A	1003	-	-	2/2/22/22	0/1/1/1
3	G6P	A	1002	-	1/1/6/6	3/6/26/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	BGC	C1-C2-C3	-3.07	104.09	110.36
2	B	1001	BGC	C1-C2-C3	-2.70	104.85	110.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1002	G6P	C1
3	A	1004	G6P	C1
3	B	1002	G6P	C1
3	B	1004	G6P	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	G6P	C5-C6-O6-P
3	A	1004	G6P	C6-O6-P-O1P
3	B	1004	G6P	C5-C6-O6-P
3	B	1004	G6P	C6-O6-P-O1P
3	B	1002	G6P	C5-C6-O6-P
3	A	1002	G6P	C5-C6-O6-P
2	B	1003	BGC	C4-C5-C6-O6
3	A	1004	G6P	C6-O6-P-O3P
3	B	1004	G6P	C6-O6-P-O3P
2	A	1003	BGC	C4-C5-C6-O6
2	A	1003	BGC	O5-C5-C6-O6
3	A	1002	G6P	O5-C5-C6-O6
3	B	1002	G6P	O5-C5-C6-O6
2	B	1003	BGC	O5-C5-C6-O6
3	A	1004	G6P	C6-O6-P-O2P
3	B	1004	G6P	C6-O6-P-O2P
3	A	1002	G6P	C6-O6-P-O1P
3	B	1002	G6P	C6-O6-P-O1P

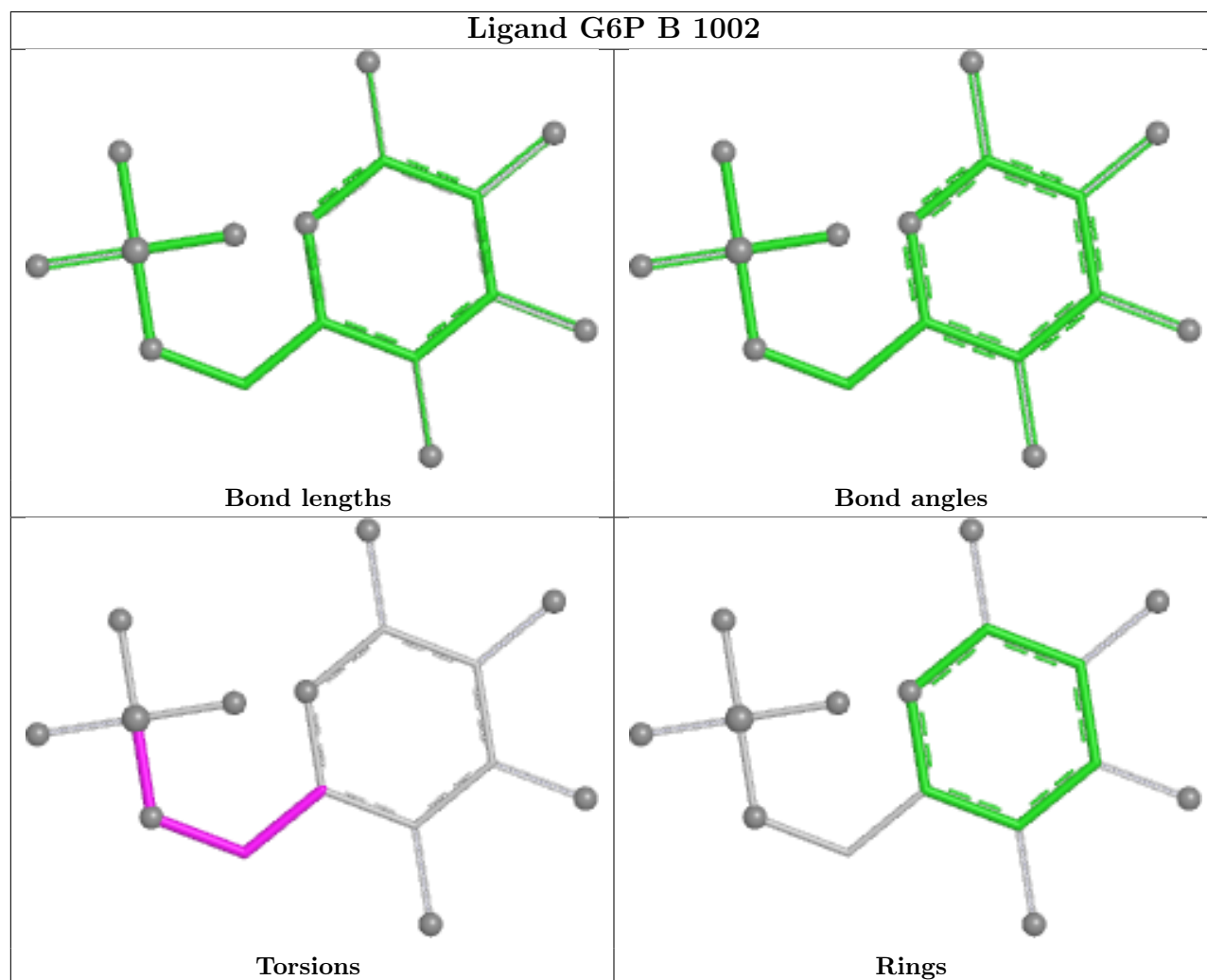
There are no ring outliers.

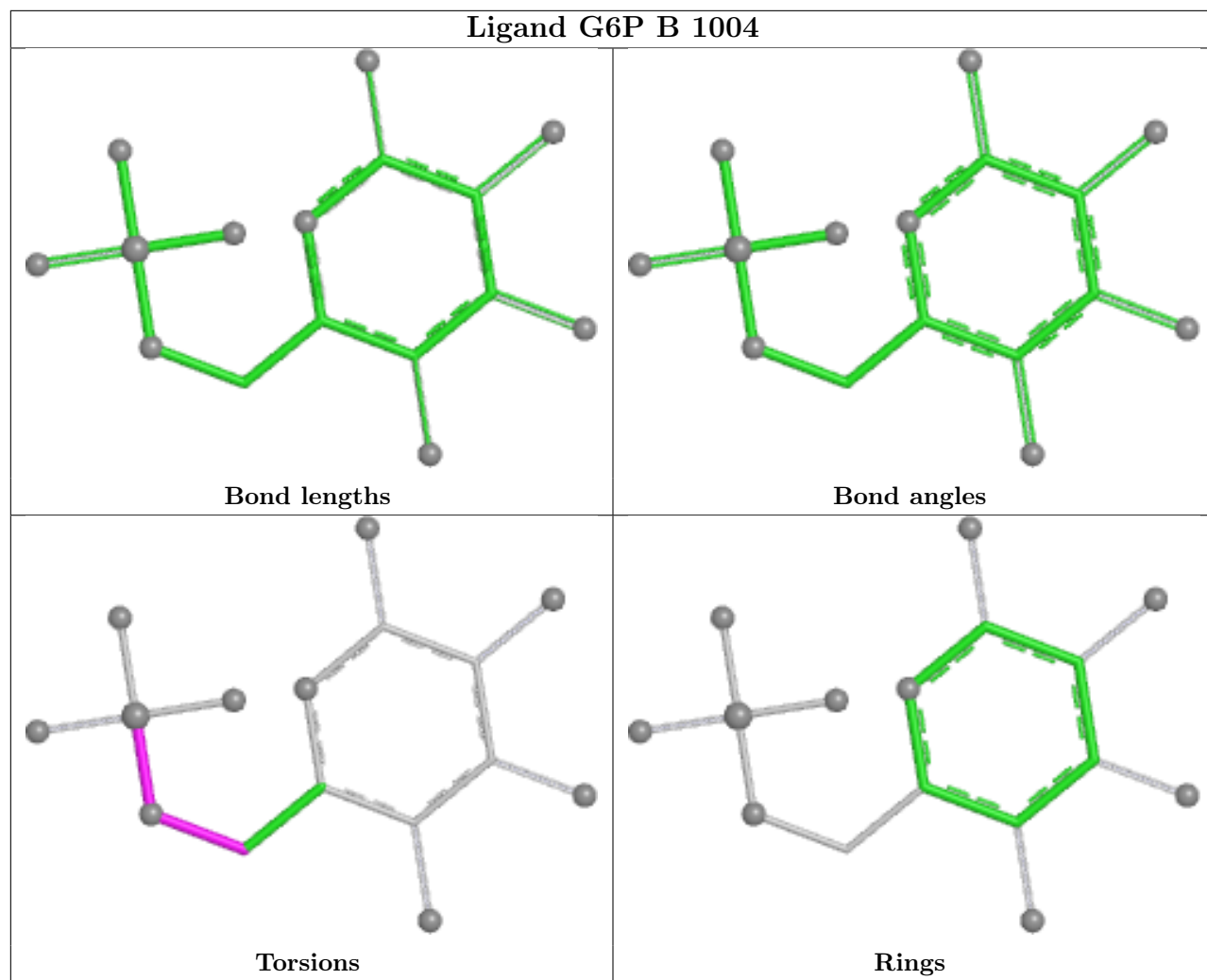
2 monomers are involved in 3 short contacts:

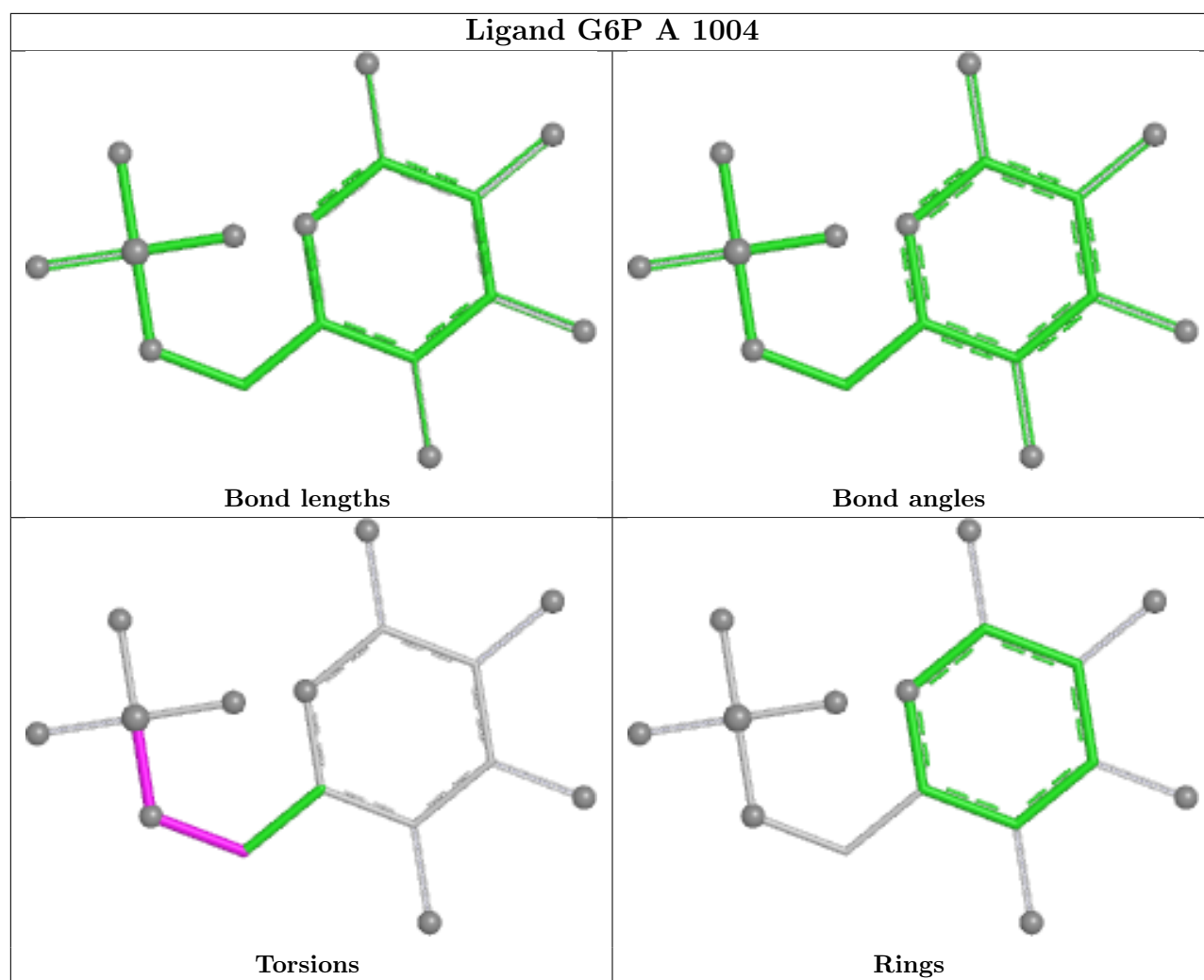
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	BGC	1	0
2	A	1001	BGC	2	0

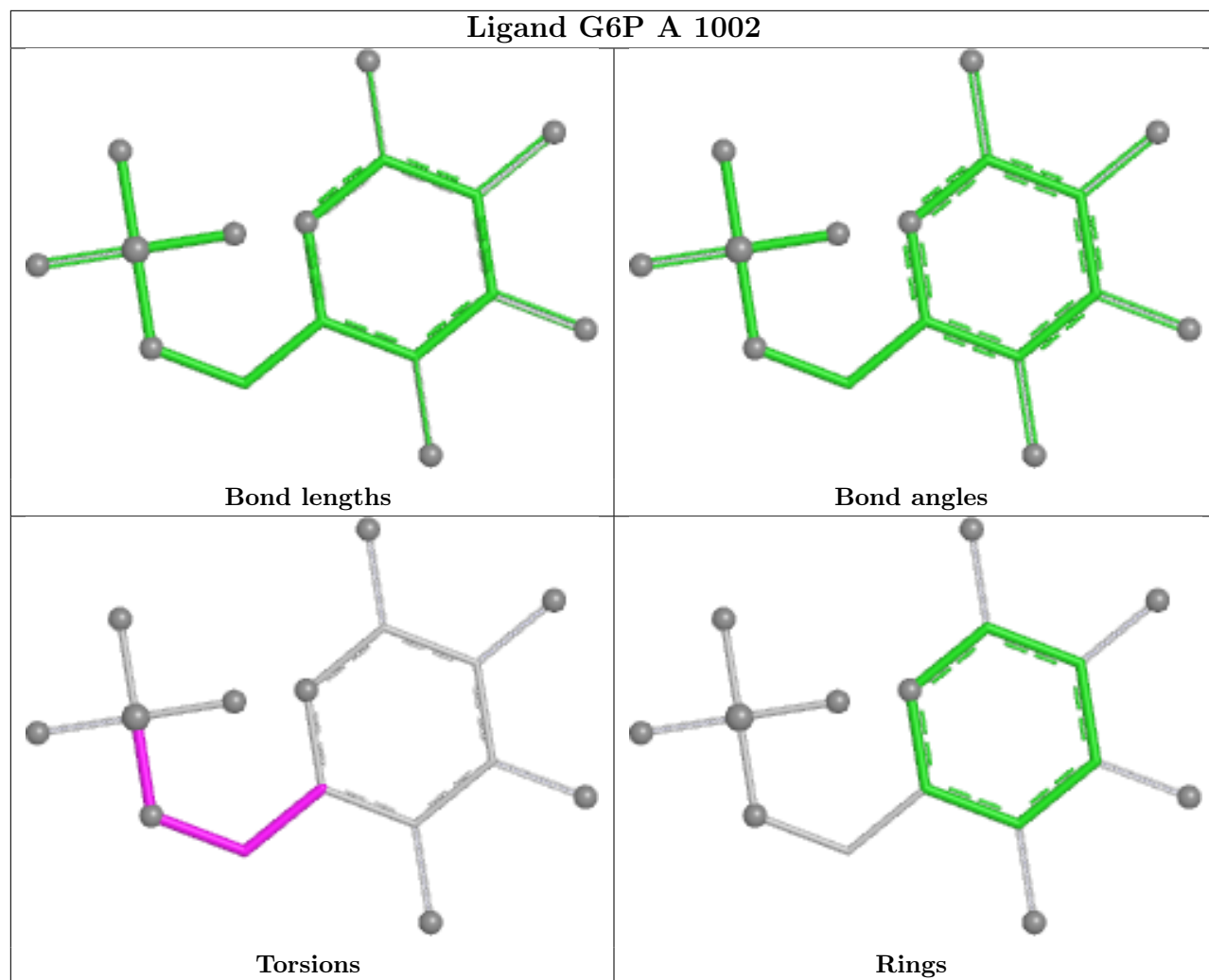
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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	902/918 (98%)	-0.33	2 (0%) 91 88	14, 33, 47, 59	0
1	B	902/918 (98%)	-0.31	1 (0%) 92 90	15, 33, 47, 59	0
All	All	1804/1836 (98%)	-0.32	3 (0%) 91 88	14, 33, 47, 59	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	SER	3.4
1	B	550	LYS	3.1
1	A	2	ILE	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
2	BGC	B	1001	12/12	0.93	0.08	23,29,31,31	0
2	BGC	A	1003	12/12	0.94	0.08	21,26,31,33	0

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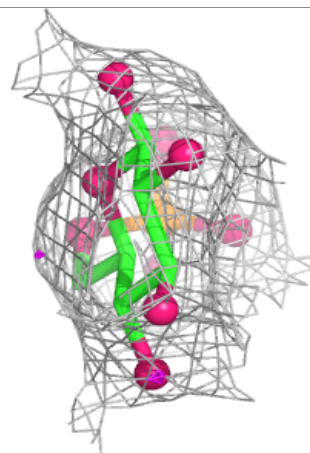
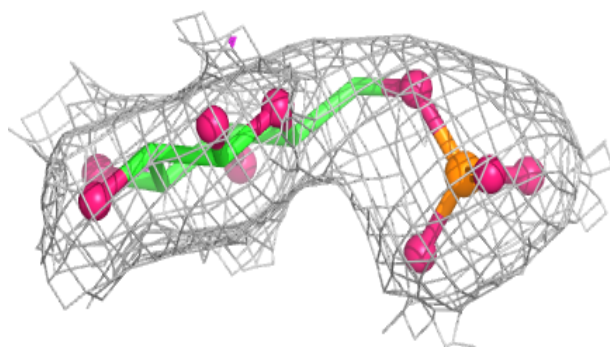
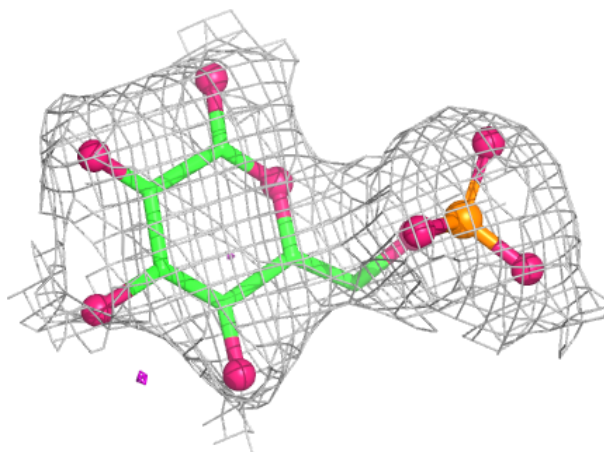
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	B	1003	12/12	0.94	0.10	21,26,29,31	0
3	G6P	A	1004	16/16	0.95	0.09	36,38,41,45	0
4	CA	A	1005	1/1	0.95	0.24	10,10,10,10	0
3	G6P	B	1002	16/16	0.96	0.07	30,34,42,44	0
3	G6P	B	1004	16/16	0.96	0.07	35,37,42,43	0
2	BGC	A	1001	12/12	0.96	0.08	25,27,29,29	0
3	G6P	A	1002	16/16	0.97	0.08	28,31,36,37	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.

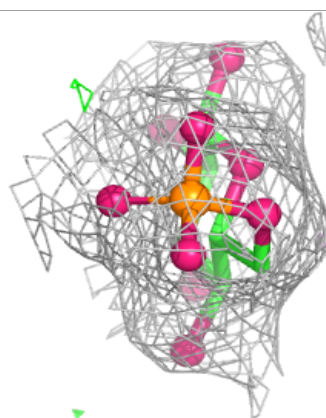
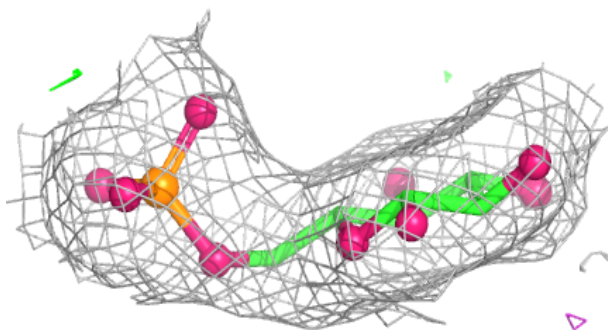
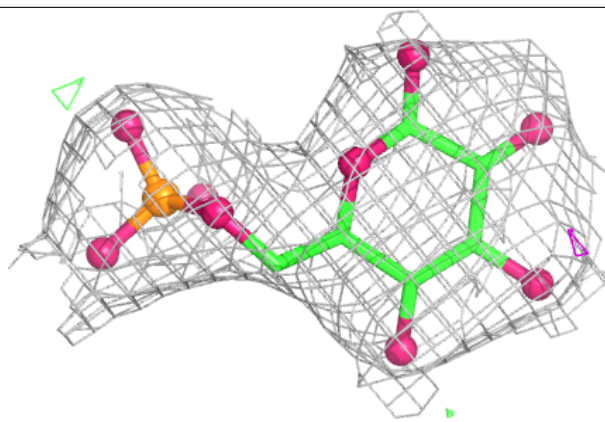
Electron density around G6P A 1004:

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



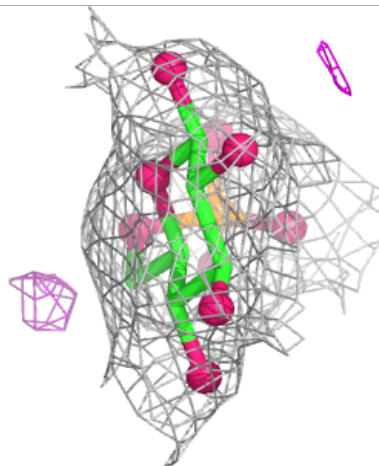
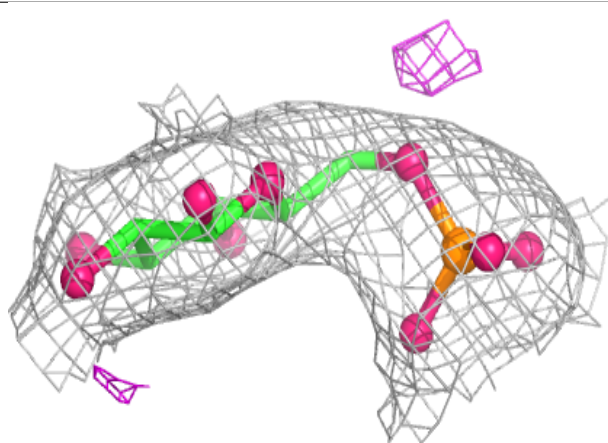
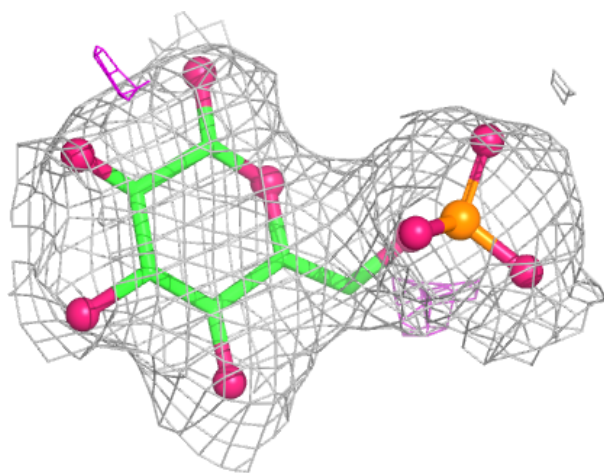
Electron density around G6P B 1002:

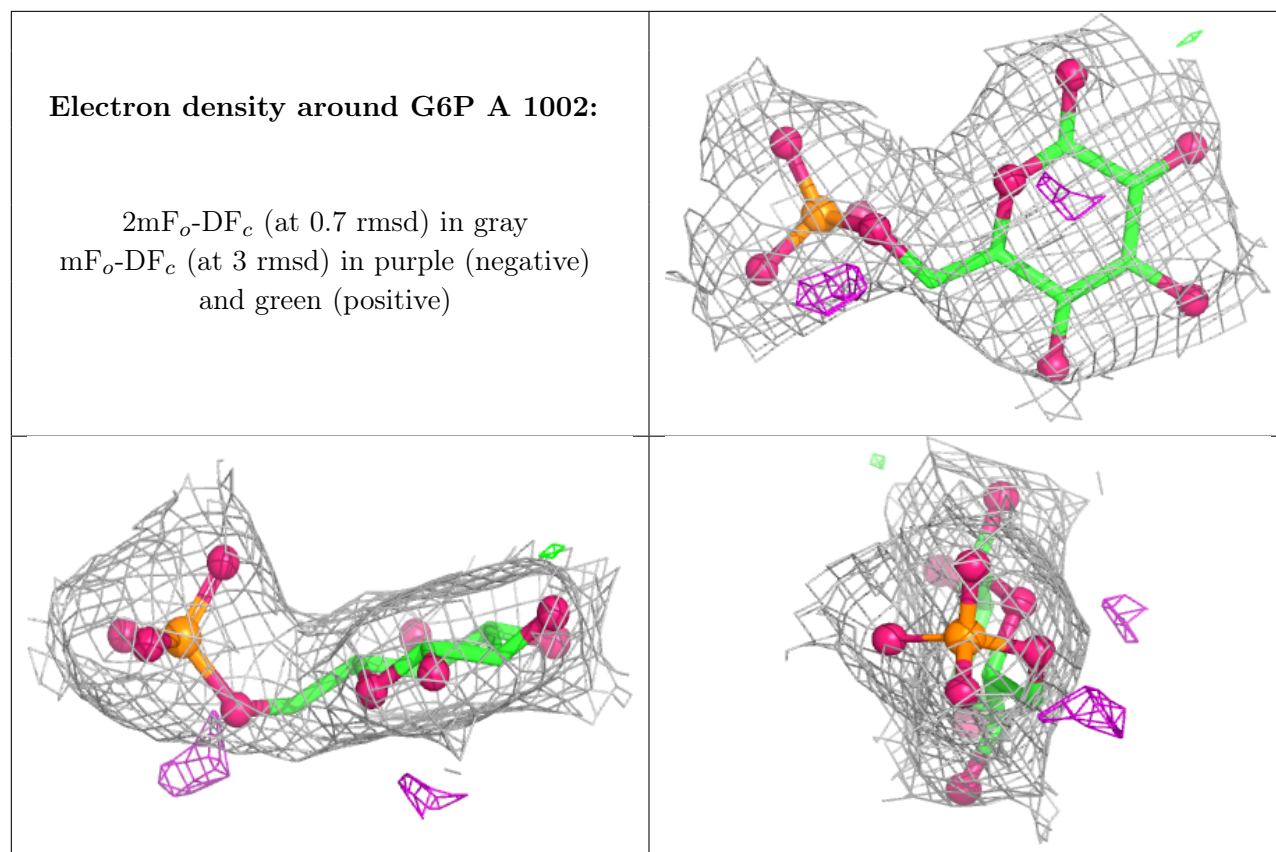
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G6P B 1004:

$2mF_o-DF_c$ (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.