



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:50 AM BST

PDB ID : 1BG3  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

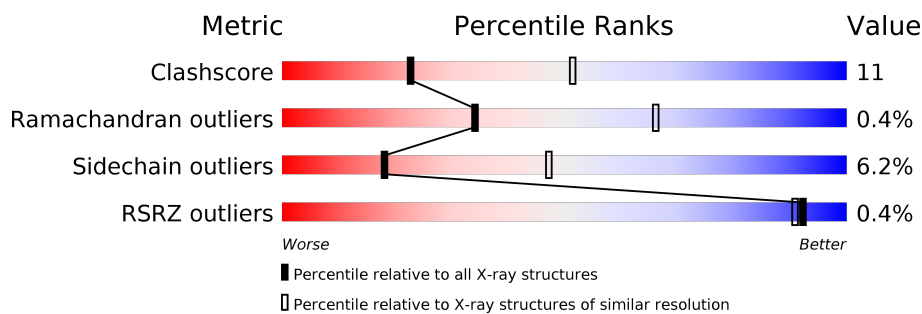
# 1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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](#)

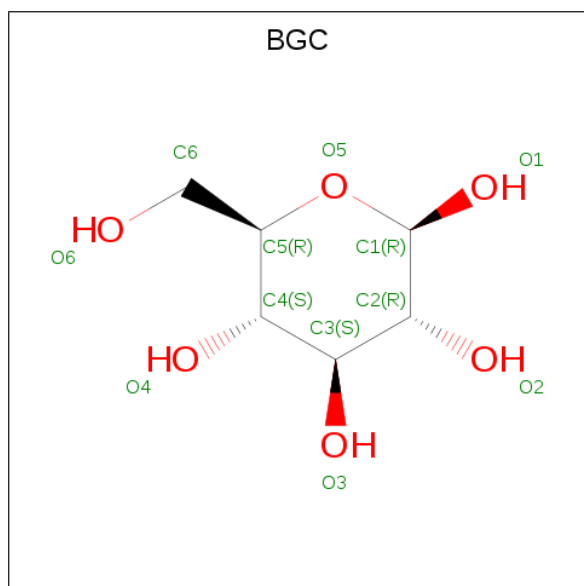
There are 5 unique types of molecules in this entry. The entry contains 13962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

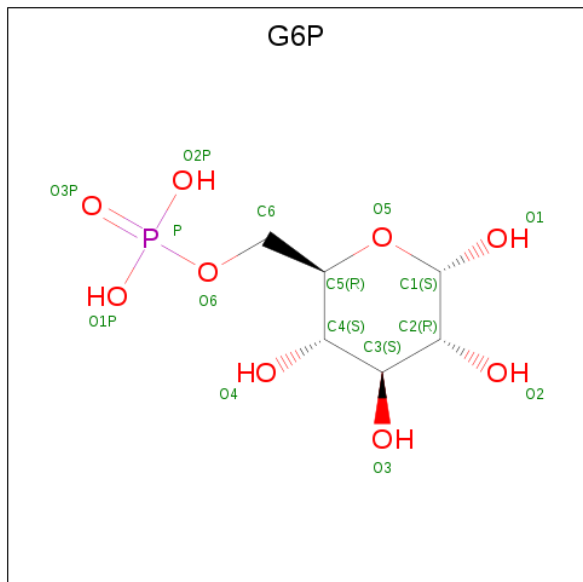
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	0	0
			6832	4304	1177	1296	55			
1	B	902	Total	C	N	O	S	0	0	0
			6783	4276	1157	1295	55			

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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 (three-letter code: 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 (three-letter code: CA) (formula: Ca).

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

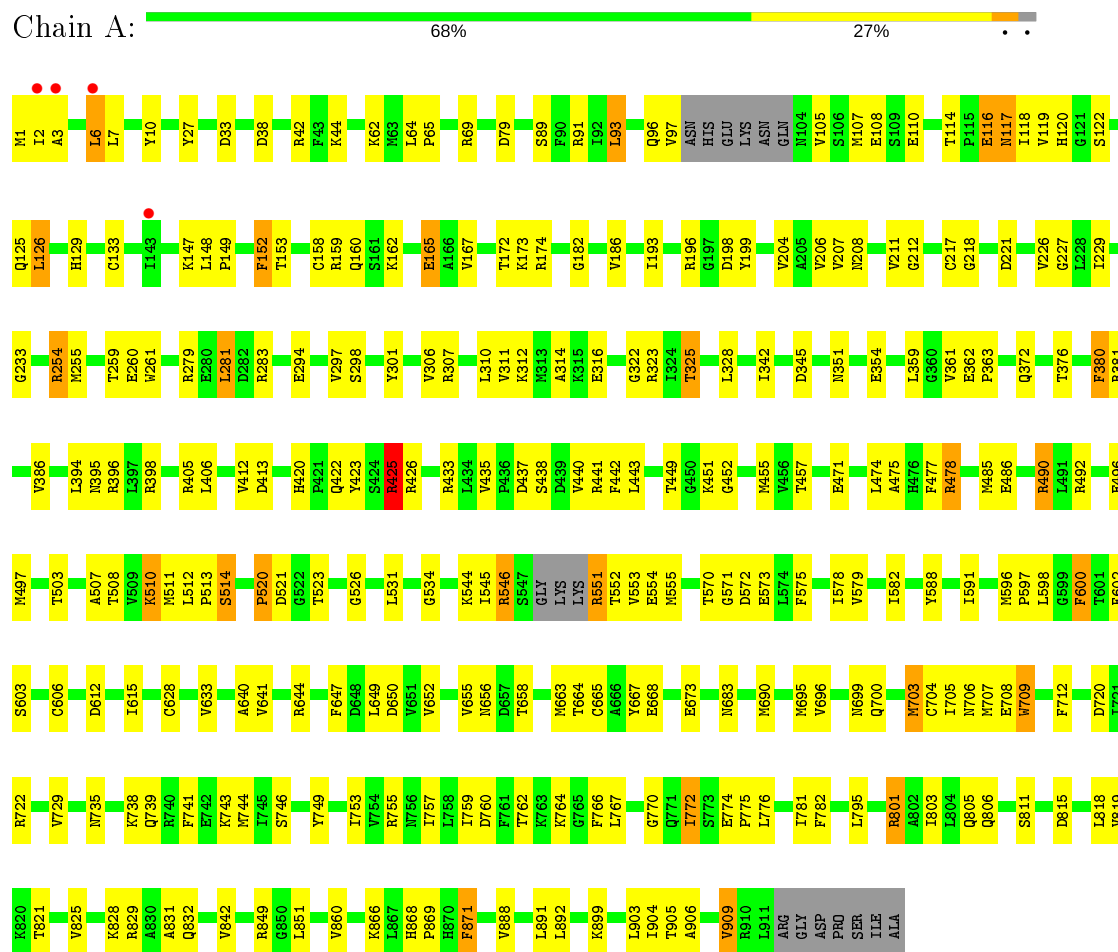
- Molecule 5 is water.

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

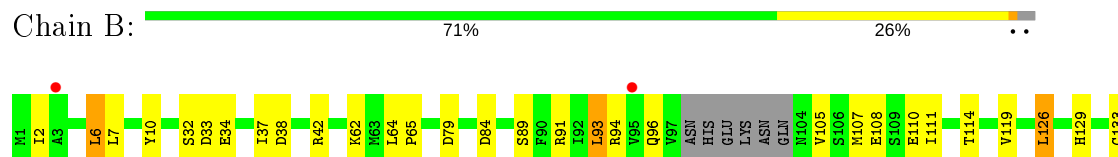
### 3 Residue-property plots

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



L892	L903	T904	T905	A906	V909	R910	L911	ARG	GLY	ASP	PRO	SER	ILE	ALA	I757	L758	I759	D760	F761	I762	L767	G770	S773	L776	K777	I781	R801	C813	D814	D815	L818	V819	V825	K828	R829	Q832	V842	E843	K844	T845	R846	E847	N848	H853	V860	K866	H870	F871	S872	R873	I874	L882	K885	G886	T887	V888	V651	V652	V655	T658	N663	T664	C665	E668	E669	F670	T671	N683	E688	E689	N690	V693	E694	N695	Q700	M703	C704	I705	N706	N707	E708	N709	G710	A711	F712	D720	I721	R722	V729	N735	S736	G737	K738	Q739	R740	F741	E742	K743	N744	I753	V754	N756	V553	E554	M555	H556	N557	K558	G569	T570	C571	E572	E573	L574	F575	I578	V579	I582	L586	I591	K592	G593	M596	P597	L598	G599	F600	F601	F602	S603	F604	P605	C606	D612	C613	G614	I615	L616	I617	S618	A625	T626	D627	C628	V633	A640	F647	D648	L649	D650	L443	T449	G450	K451	G452	M455	V456	T457	R468	E471	A475	H476	F477	R478	K481	M485	E486	R492	E496	M497	K501	A507	T508	V509	K510	M511	S514	P520	D521	G522	T523	E524	H525	L529	A530	L531	G534	L541	L542	V543	K544	I545	R546	G322	R323	I324	T325	L328	R331	I342	D345	G348	I349	Q350	N351	A352	K353	E354	R358	L359	G360	V361	E362	P363	F380	R381	V386	L397	K401	G402	T403	P404	V412	D413	L416	H420	P421	Q422	Y423	S424	R425	F427	R426	H428	R433	L434	R441	F442	K140	LYS	LYS	ILE	K144	F152	T153	Q160	E165	T172	K173	V186	V204	A205	V206	V207	G212	C217	Q223	V226	G227	L228	I229	I230	G233	R284	M285	W261	R279	E280	L281	V297	S298	Y301	K312	K313	A314	K315	E316	F320	E321
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.10Å 77.10Å 137.10Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 38.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	71.0 (20.00-2.80) 70.6 (38.48-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.196 , 0.251 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 74.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, BGC, 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	0.62	1/6935 (0.0%)	0.89	15/9367 (0.2%)
1	B	0.62	0/6885	0.90	15/9310 (0.2%)
All	All	0.62	1/13820 (0.0%)	0.90	30/18677 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	CYS	CB-SG	-5.23	1.73	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH2	-14.98	112.81	120.30
1	B	279	ARG	NE-CZ-NH2	-14.97	112.81	120.30
1	A	279	ARG	NE-CZ-NH2	-14.74	112.93	120.30
1	B	425	ARG	NE-CZ-NH2	-14.09	113.26	120.30
1	B	279	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	B	381	ARG	NE-CZ-NH2	-14.07	113.27	120.30
1	A	381	ARG	NE-CZ-NH1	13.93	127.26	120.30
1	A	381	ARG	NE-CZ-NH2	-13.71	113.44	120.30
1	B	381	ARG	NE-CZ-NH1	13.63	127.12	120.30
1	A	254	ARG	NE-CZ-NH1	13.56	127.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	A	254	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	B	254	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	B	425	ARG	NE-CZ-NH1	11.87	126.23	120.30
1	B	254	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	A	425	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	A	490	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	A	254	ARG	CD-NE-CZ	7.34	133.88	123.60
1	B	279	ARG	CD-NE-CZ	6.90	133.26	123.60
1	A	381	ARG	CD-NE-CZ	6.55	132.77	123.60
1	A	279	ARG	CD-NE-CZ	6.48	132.67	123.60
1	B	514	SER	N-CA-C	-6.26	94.11	111.00
1	A	514	SER	N-CA-C	-6.24	94.14	111.00
1	A	425	ARG	CD-NE-CZ	6.11	132.15	123.60
1	B	254	ARG	CG-CD-NE	5.98	124.35	111.80
1	B	425	ARG	CD-NE-CZ	5.98	131.97	123.60
1	B	381	ARG	CD-NE-CZ	5.72	131.61	123.60
1	B	254	ARG	CB-CG-CD	-5.58	97.09	111.60
1	A	281	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	254	ARG	CD-NE-CZ	5.08	130.72	123.60

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 [i](#)

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	177	0
1	B	6783	0	6623	136	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	311	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 11.

All (311) 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:361:VAL:O	1:B:363:PRO:HD3	1.67	0.93
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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:SER:HB2	1:B:91:ARG:NH1	2.10	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: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: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
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: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: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: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: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:A:107:MET:SD	1:A:451:LYS:HB2	2.45	0.56
1:B:65:PRO:HB3	1:B:255:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:755:ARG:HD3	1:B:781:ILE:HG22	1.87	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: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:B:755:ARG:O	1:B:759:ILE:HG13	2.07	0.54
1:B:477:PHE:HB2	1:B:825:VAL:CG1	2.36	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:226:VAL:HG12	1:B:227:GLY:N	2.25	0.51
1:B:152:PHE:HB3	1:B:206:VAL:HG22	1.92	0.51
1:B:38:ASP:O	1:B:42:ARG:HG3	2.10	0.51
1:A:193:ILE:HG23	1:A:199:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ARG:HG2	1:A:442:PHE:N	2.25	0.51
1:A:690:MET:HE3	1:A:703:MET:HB2	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:A:62:LYS:HB3	1:A:64:LEU:HG	1.93	0.51
1:B:606:CYS:HA	1:B:615:ILE:O	2.10	0.51
1:A:93:LEU:HD12	1:A:93:LEU:N	2.26	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:A:673:GLU:CD	1:A:849:ARG:HH22	2.14	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: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:A:65:PRO:HB3	1:A:255:MET:HE3	1.93	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:541:LEU:HG	1:B:557:ASN:HB3	1.95	0.49
1:B:534:GLY:HA3	1:B:603:SER:HB2	1.94	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:1:MET:C	1:A:3:ALA:N	2.64	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:579:VAL:HG13	1:A:647:PHE:CZ	2.48	0.49
1:A:520:PRO:HG2	1:A:903:LEU:HD13	1.95	0.49
1:B:614:GLY:O	1:B:633:VAL:HG22	2.13	0.49
1:A:1:MET:C	1:A:3:ALA:H	2.15	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:B:690:MET:CE	1:B:703:MET:HB2	2.44	0.48
1:A:380:PHE:CE1	1:A:426:ARG:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG11	1:A:451:LYS:HG3	1.96	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:B:722:ARG:HG2	1:B:744:MET:CE	2.44	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: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:33:ASP:OD2	1:B:433:ARG:NH1	2.48	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: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:690:MET:HE3	1:B:703:MET:HB2	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:452:GLY:O	1:A:455:MET:HB2	2.15	0.47
1:A:722:ARG:HG2	1:A:744:MET:CE	2.45	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: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:147:LYS:C	1:A:148:LEU:HD23	2.36	0.46
1:A:755:ARG:HD2	1:A:776:LEU:O	2.16	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:571:GLY:CA	1:A:628:CYS:SG	3.01	0.45
1:A:828:LYS:HD3	5:A:2125:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:602:PHE:HD2	1:A:606:CYS:HG	1.66	0.44
1:B:477:PHE:N	1:B:477:PHE:CD1	2.85	0.44
1:B:866:LYS:CE	1:B:892:LEU:HD11	2.48	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:422:GLN:OE1	1:A:425:ARG:NH2	2.51	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: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:283:ARG:HH21	1:B:558:LYS:HE3	1.82	0.43
1:A:709:TRP:C	1:A:709:TRP:CD1	2.92	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:A:690:MET:CE	1:A:703:MET:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:THR:HG23	1:A:426:ARG:NH1	2.34	0.43
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.78	0.43
1:B:757:ILE:O	1:B:760:ASP:HB3	2.18	0.43
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: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:B:401:LYS:C	1:B:403:THR:H	2.21	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:A:97:VAL:HG11	1:A:455:MET:HE1	2.00	0.42
1:B:37:ILE:HD13	1:B:434:LEU:HD22	2.01	0.42
1:B:689:GLU:O	1:B:693:VAL:HG23	2.19	0.42
1:A:117:ASN:O	1:A:125:GLN:NE2	2.52	0.42
1:A:259:THR:O	1:A:260:GLU:HB2	2.20	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:MET:HA	1:B:597:PRO:HD3	1.75	0.41
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:A:65:PRO:HB3	1:A:255:MET:CE	2.51	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:853:HIS:HE1	1:B:887:THR:OG1	2.02	0.41
1:B:79:ASP:HA	1:B:96:GLN:HA	2.01	0.41
1:A:868:HIS:ND1	1:A:869:PRO:HD2	2.36	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:512:LEU:HA	1:A:513:PRO:HD3	1.80	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:477:PHE:N	1:A:477:PHE:CD1	2.88	0.41
1:A:781:ILE:HG23	1:A:782:PHE:CD2	2.56	0.41
1:A:376:THR:O	1:A:380:PHE:HB2	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: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: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:868:HIS:HA	1:A:869:PRO:HD3	1.92	0.40
1:A:831:ALA:HB2	1:A:871:PHE:HA	2.03	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
1:B:882:LEU:HA	1:B:882:LEU:HD23	1.89	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	896/918 (98%)	829 (92%)	65 (7%)	2 (0%)	47	78
1	B	896/918 (98%)	835 (93%)	55 (6%)	6 (1%)	22	53
All	All	1792/1836 (98%)	1664 (93%)	120 (7%)	8 (0%)	34	66

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

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%)	676 (94%)	46 (6%)	17	45
1	B	714/791 (90%)	671 (94%)	43 (6%)	19	48
All	All	1436/1582 (91%)	1347 (94%)	89 (6%)	18	47

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	27	TYR
1	A	93	LEU
1	A	116	GLU
1	A	117	ASN
1	A	122	SER
1	A	126	LEU
1	A	152	PHE
1	A	165	GLU
1	A	174	ARG
1	A	254	ARG
1	A	261	TRP
1	A	281	LEU
1	A	325	THR
1	A	380	PHE
1	A	396	ARG
1	A	405	ARG
1	A	412	VAL
1	A	425	ARG
1	A	478	ARG
1	A	485	MET
1	A	486	GLU
1	A	492	ARG
1	A	496	GLU
1	A	503	THR
1	A	508	THR
1	A	510	LYS
1	A	520	PRO
1	A	546	ARG
1	A	551	ARG
1	A	552	THR
1	A	555	MET
1	A	598	LEU
1	A	600	PHE
1	A	612	ASP
1	A	649	LEU
1	A	703	MET
1	A	707	MET
1	A	709	TRP
1	A	720	ASP
1	A	772	ILE
1	A	795	LEU
1	A	801	ARG

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Mol	Chain	Res	Type
1	A	829	ARG
1	A	860	VAL
1	A	909	VAL
1	B	6	LEU
1	B	93	LEU
1	B	94	ARG
1	B	126	LEU
1	B	152	PHE
1	B	254	ARG
1	B	261	TRP
1	B	281	LEU
1	B	320	PHE
1	B	325	THR
1	B	349	ILE
1	B	380	PHE
1	B	412	VAL
1	B	425	ARG
1	B	428	HIS
1	B	468	ARG
1	B	478	ARG
1	B	485	MET
1	B	486	GLU
1	B	492	ARG
1	B	496	GLU
1	B	508	THR
1	B	510	LYS
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	707	MET
1	B	709	TRP
1	B	720	ASP
1	B	736	SER
1	B	801	ARG
1	B	813	CYS

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Mol	Chain	Res	Type
1	B	829	ARG
1	B	844	LYS
1	B	860	VAL
1	B	911	LEU

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

Mol	Chain	Res	Type
1	A	125	GLN
1	A	384	ASN
1	A	692	ASN
1	B	125	GLN
1	B	384	ASN
1	B	692	ASN
1	B	853	HIS

### 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 monosaccharides 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
3	G6P	B	1002	-	16,16,16	0.73	0	24,24,24	0.92	1 (4%)
3	G6P	A	1002	-	16,16,16	0.74	0	24,24,24	0.74	0
2	BGC	B	1003	-	12,12,12	0.38	0	17,17,17	0.64	0
2	BGC	A	1001	-	12,12,12	0.61	0	17,17,17	1.02	1 (5%)
3	G6P	A	1004	-	16,16,16	0.69	0	24,24,24	0.79	1 (4%)
3	G6P	B	1004	-	16,16,16	0.73	0	24,24,24	0.83	1 (4%)
2	BGC	A	1003	-	12,12,12	0.32	0	17,17,17	0.54	0
2	BGC	B	1001	-	12,12,12	0.53	0	17,17,17	0.97	1 (5%)

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	G6P	B	1002	-	1/1/6/6	3/6/26/26	0/1/1/1
3	G6P	A	1002	-	1/1/6/6	3/6/26/26	0/1/1/1
2	BGC	B	1003	-	-	2/2/22/22	0/1/1/1
2	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
3	G6P	A	1004	-	1/1/6/6	4/6/26/26	0/1/1/1
3	G6P	B	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
2	BGC	B	1001	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	BGC	C1-C2-C3	-3.00	104.09	110.31
2	B	1001	BGC	C1-C2-C3	-2.63	104.85	110.31
3	B	1002	G6P	P-O6-C6	2.13	124.15	118.30
3	B	1004	G6P	P-O6-C6	2.09	124.05	118.30
3	A	1004	G6P	P-O6-C6	2.01	123.82	118.30

All (4) chirality outliers are listed below:

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

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

There are no ring outliers.

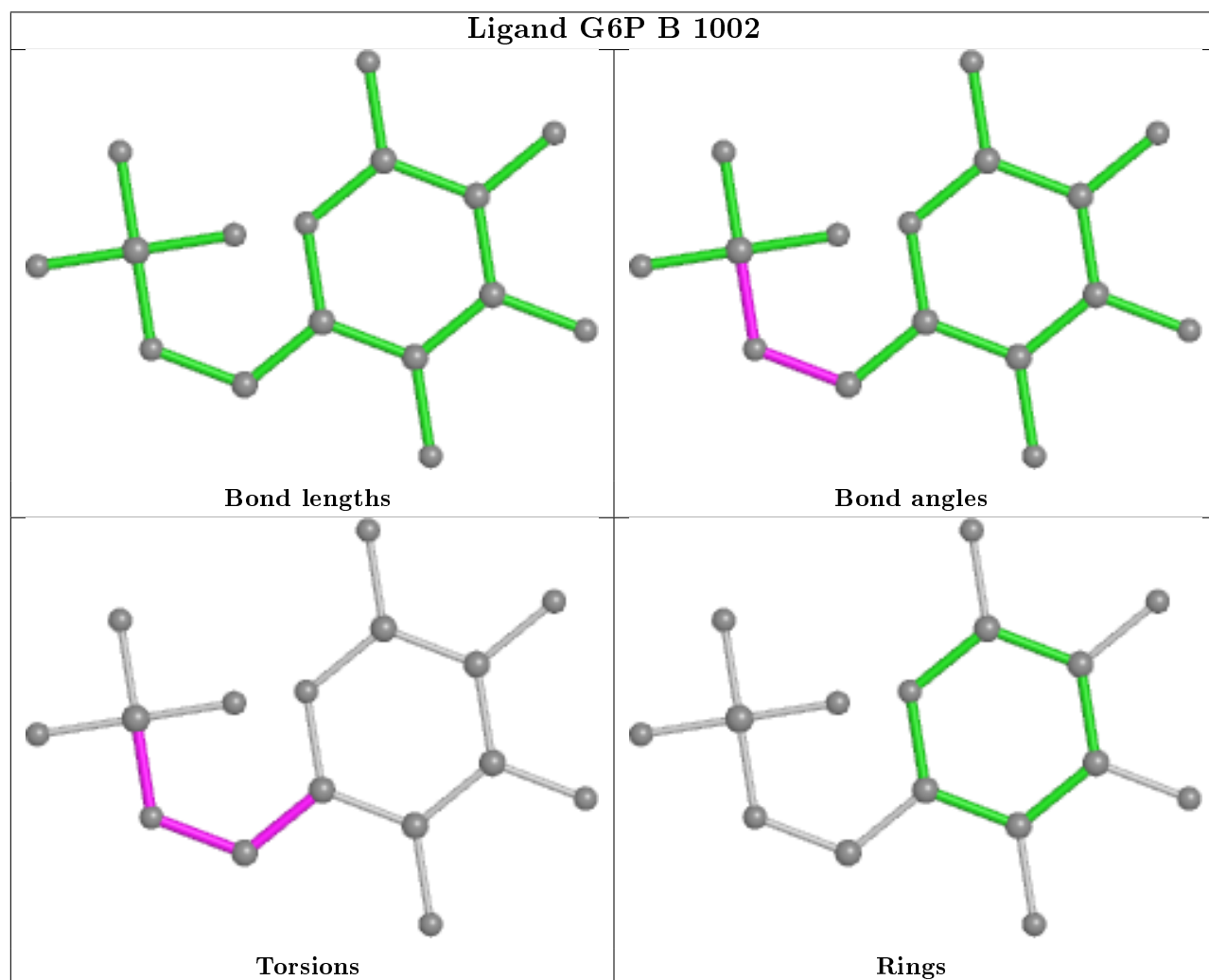
2 monomers are involved in 3 short contacts:

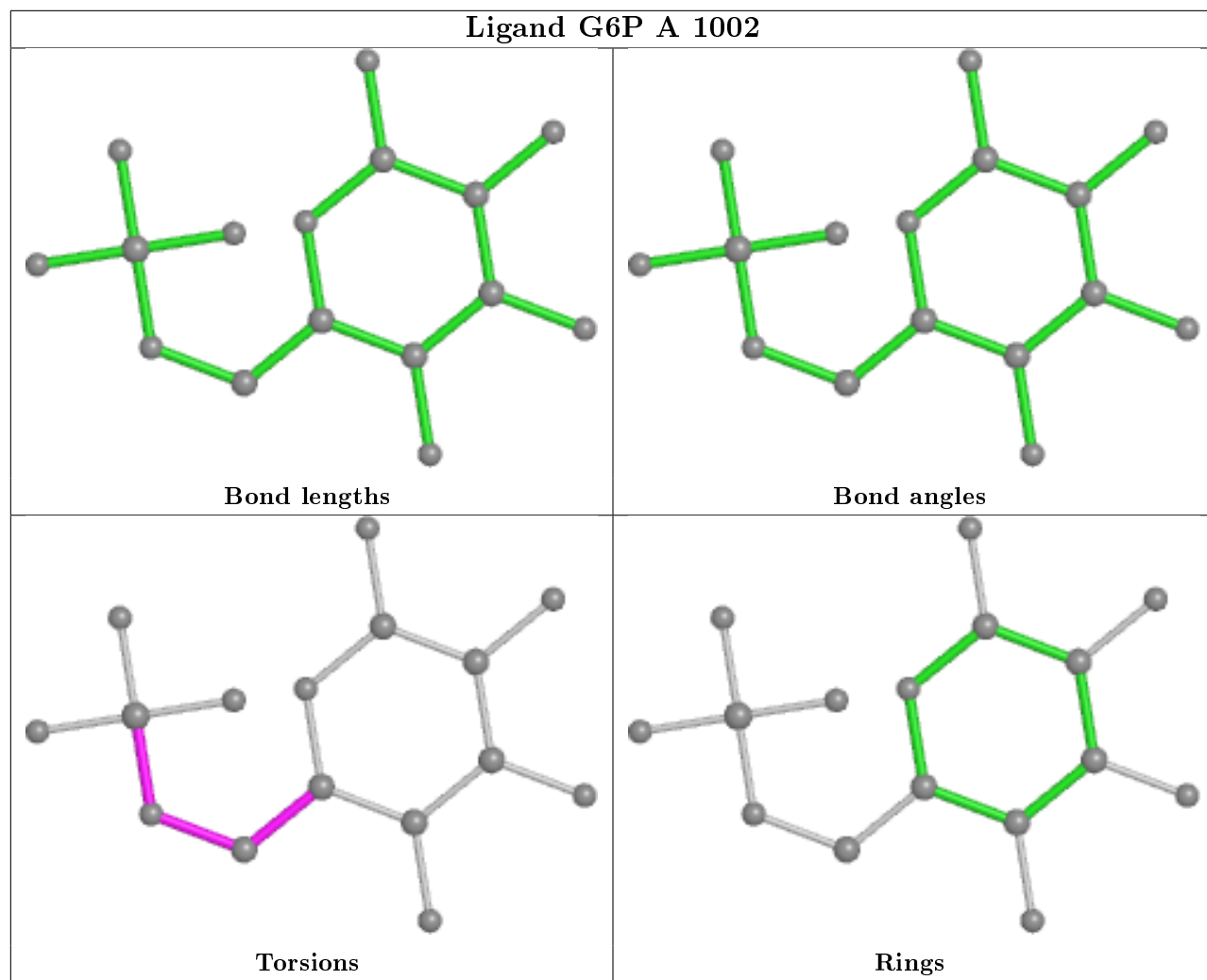
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	BGC	2	0
2	B	1001	BGC	1	0

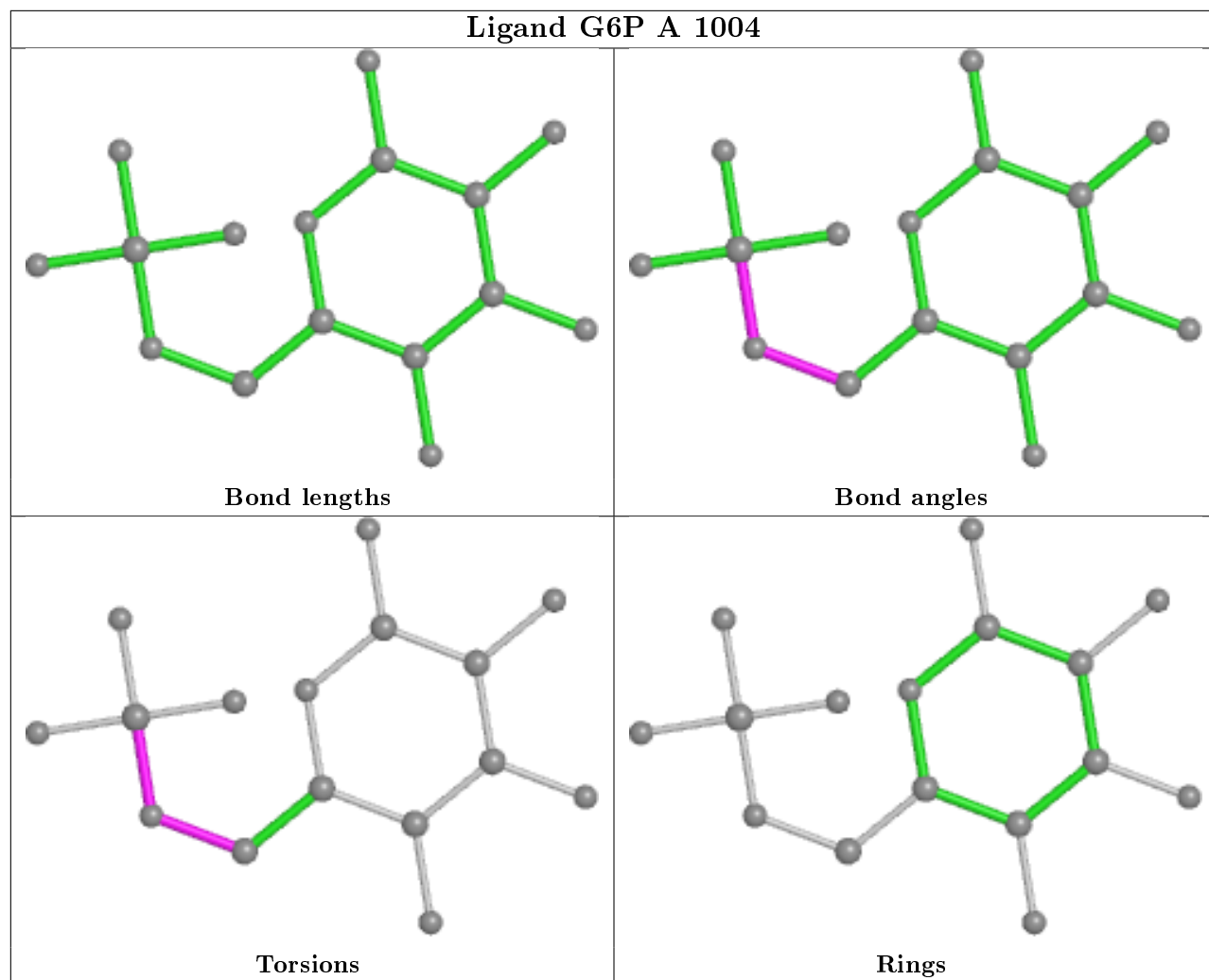
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

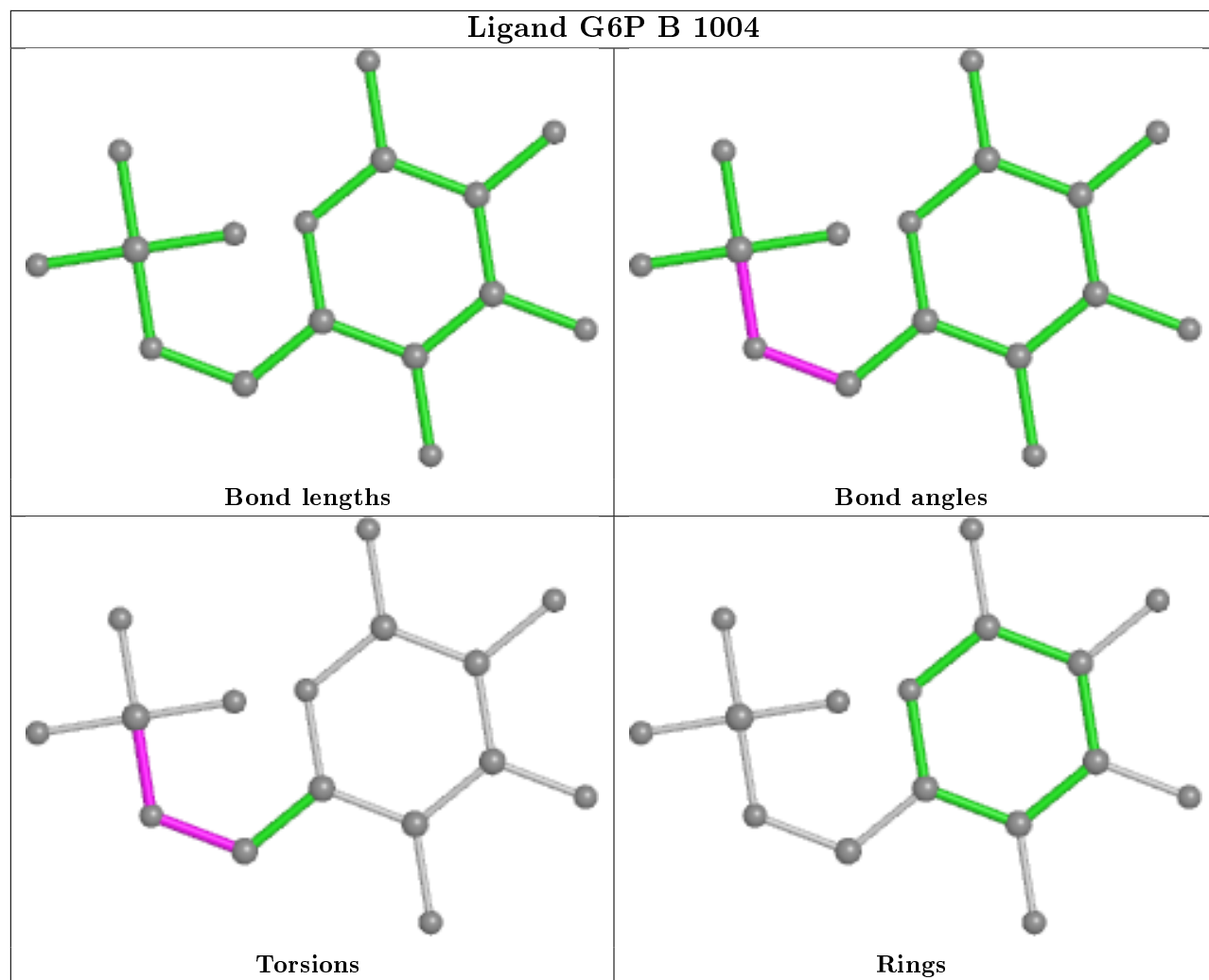


The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	902/918 (98%)	-0.44	4 (0%) 92 91	14, 33, 47, 59	0
1	B	902/918 (98%)	-0.46	3 (0%) 94 93	15, 33, 47, 59	0
All	All	1804/1836 (98%)	-0.45	7 (0%) 92 91	14, 33, 47, 59	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	3.3
1	B	95	VAL	3.2
1	A	3	ALA	3.0
1	A	2	ILE	2.9
1	A	6	LEU	2.7
1	B	593	GLY	2.2
1	A	143	ILE	2.2

### 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](#)

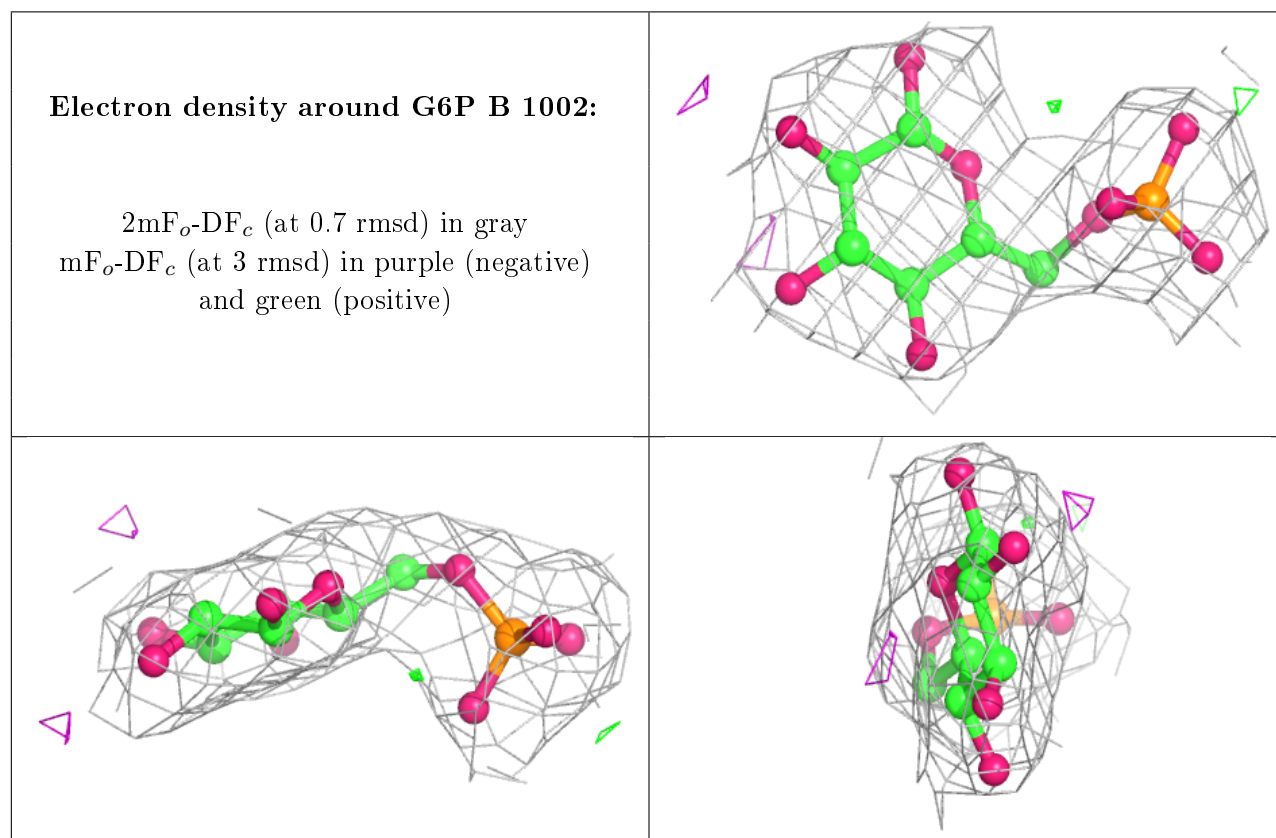
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

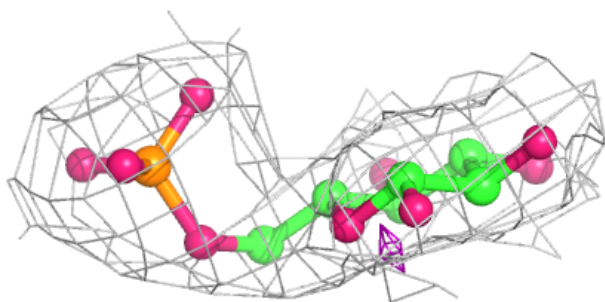
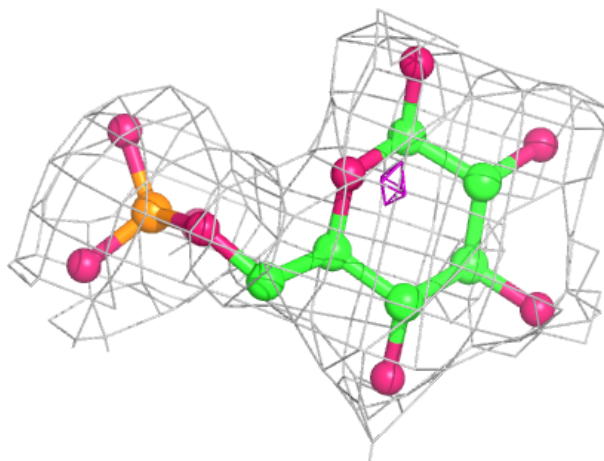
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	1005	1/1	0.96	0.18	10,10,10,10	0
2	BGC	A	1003	12/12	0.96	0.25	21,26,31,33	0
2	BGC	B	1001	12/12	0.96	0.18	23,29,31,31	0
2	BGC	A	1001	12/12	0.97	0.18	25,27,29,29	0
3	G6P	B	1002	16/16	0.97	0.11	30,34,42,44	0
3	G6P	A	1004	16/16	0.97	0.19	36,38,41,45	0
3	G6P	A	1002	16/16	0.97	0.14	28,31,36,37	0
2	BGC	B	1003	12/12	0.97	0.23	21,26,29,31	0
3	G6P	B	1004	16/16	0.98	0.18	35,37,42,43	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.



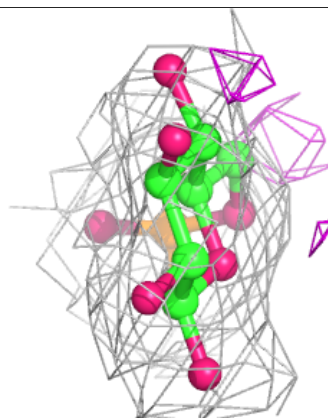
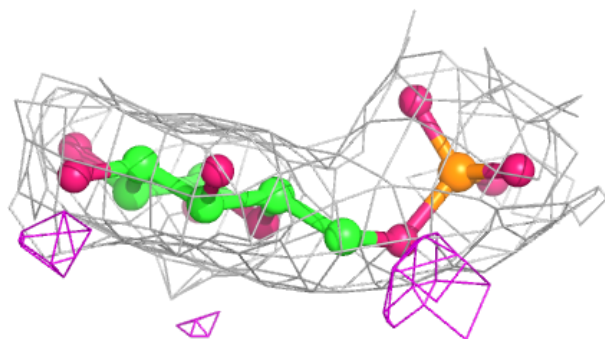
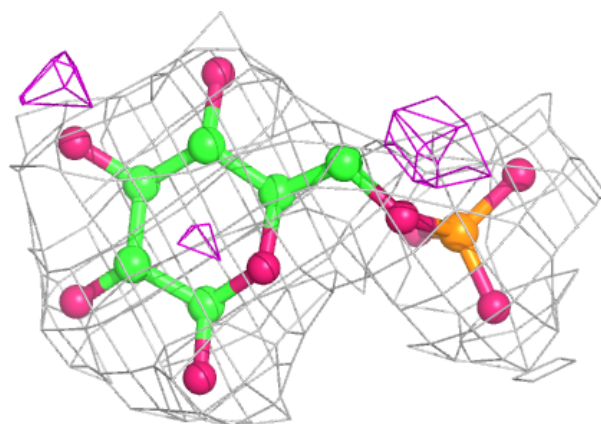
**Electron density around G6P A 1004:**

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

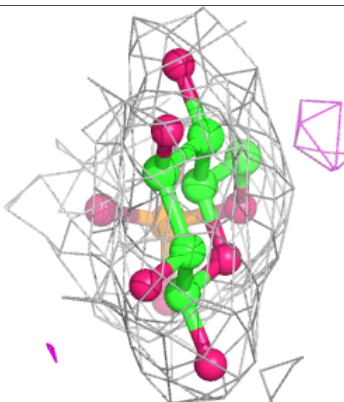
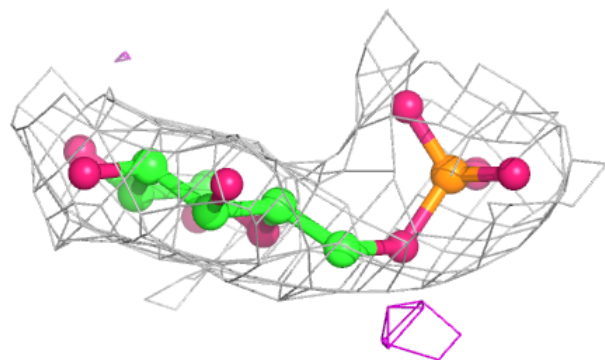
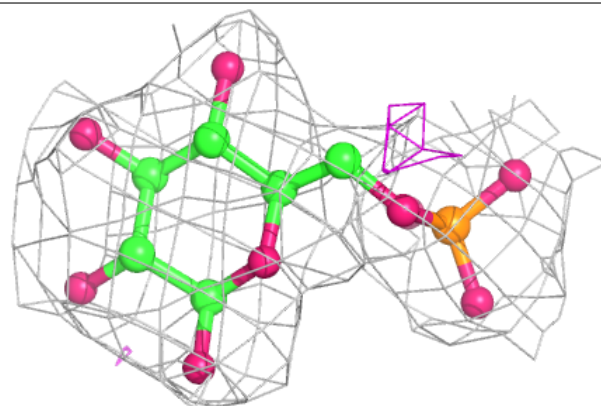


**Electron density around G6P A 1002:**

$2mF_o-DF_c$  (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

There are no such residues in this entry.