



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:49 PM BST

PDB ID : 1HKB
Title : CRYSTAL STRUCTURE OF RECOMBINANT HUMAN BRAIN HEXOKINASE TYPE I COMPLEXED WITH GLUCOSE AND GLUCOSE-6-PHOSPHATE
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Deposited on : 1997-12-01
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 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

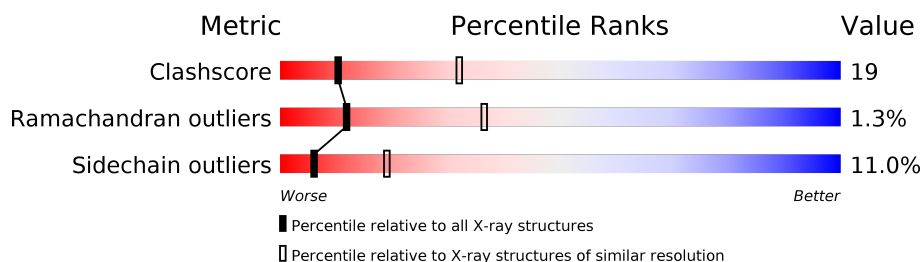
1 Overall quality at a glance

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)

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 ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	917	
1	B	917	

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	919	X	-	-	-
3	G6P	A	921	X	-	-	-
3	G6P	B	919	X	-	-	-
3	G6P	B	921	X	-	-	-

2 Entry composition [i](#)

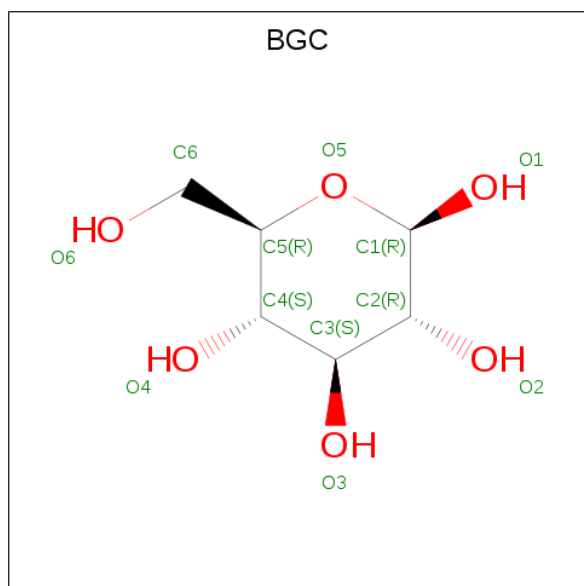
There are 5 unique types of molecules in this entry. The entry contains 14322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-GLUCOSE 6-PHOSPHOTRANSFERASE.

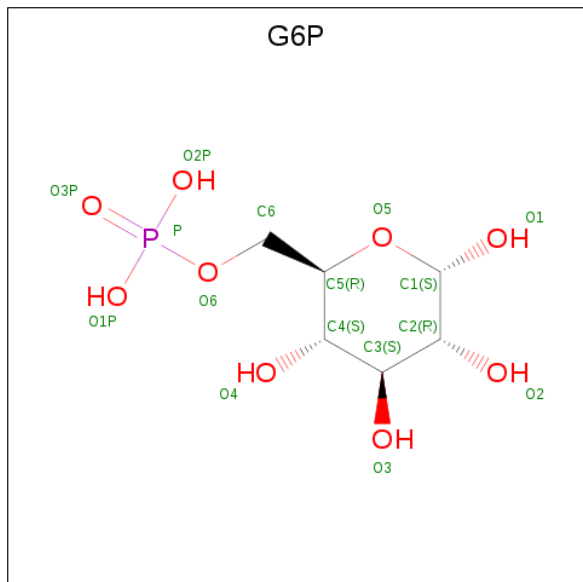
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	0	0	0
			7032	4407	1240	1332	53			
1	B	899	Total	C	N	O	S	0	0	0
			7032	4407	1240	1332	53			

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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	B	2	Total	Ca	0	0
			2	2		
4	A	2	Total	Ca	0	0
			2	2		

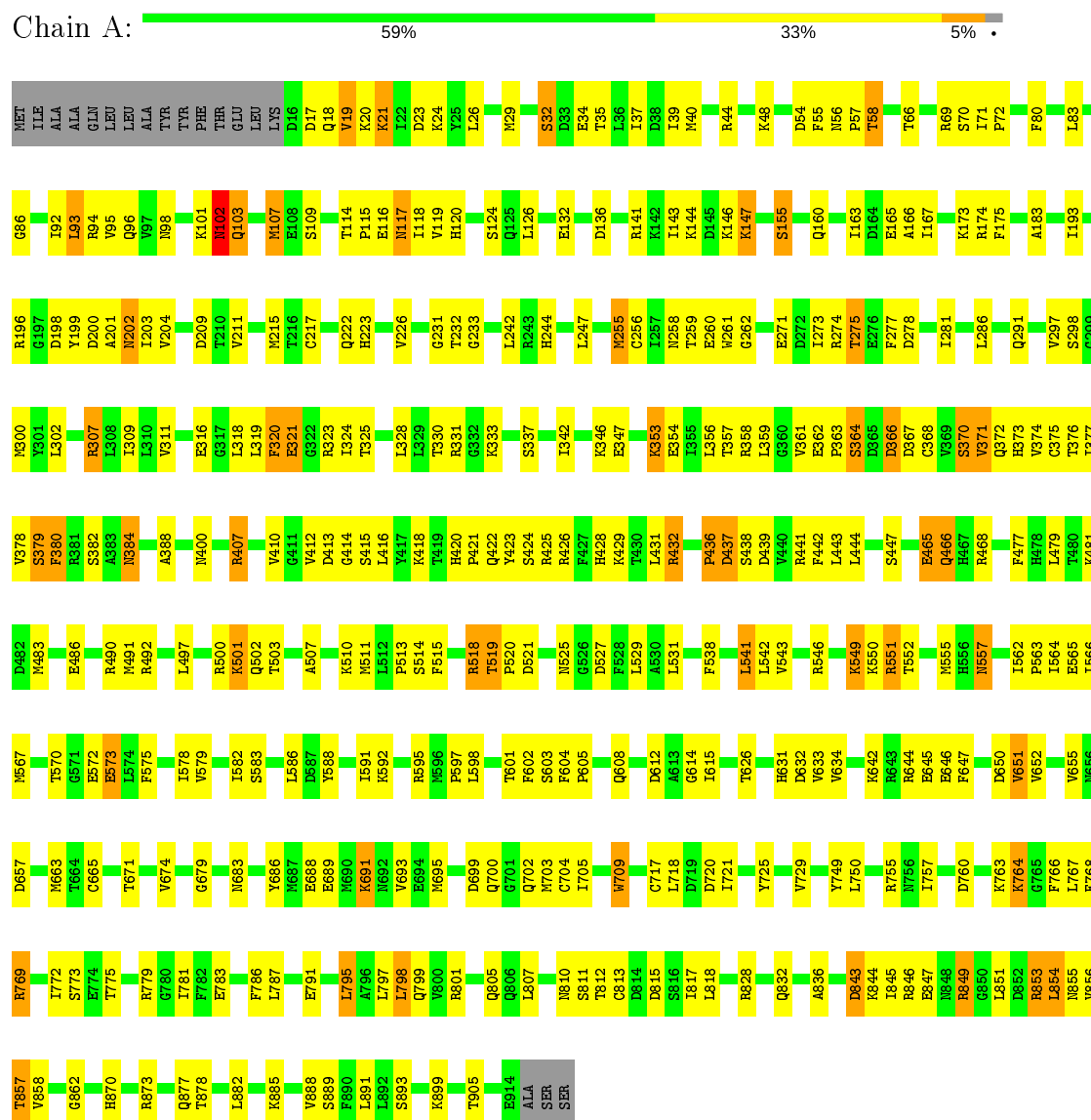
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	86	Total	O	0	0
			86	86		

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. 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. 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: D-GLUCOSE 6-PHOSPHOTRANSFERASE



• Molecule 1: D-GLUCOSE 6-PHOSPHOTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.00 Å 122.00 Å 123.00 Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 39.27 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.4 (8.00-2.80) 96.0 (39.27-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.81 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.200 , 0.270 0.268 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.007 for -h,-l,-k 0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14322	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/7138	0.60	0/9606
1	B	0.39	0/7138	0.61	2/9606 (0.0%)
All	All	0.39	0/14276	0.61	2/19212 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	GLN	N-CA-C	-6.91	92.33	111.00
1	B	516	VAL	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

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	7032	0	7090	282	0
1	B	7032	0	7090	259	0
2	A	24	0	24	3	0
2	B	24	0	24	2	0
3	A	32	0	22	6	0
3	B	32	0	22	5	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	56	0	0	2	0
5	B	86	0	0	2	0
All	All	14322	0	14272	531	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 19.

All (531) 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:691:LYS:HD2	1:A:691:LYS:H	1.01	1.13
1:A:307:ARG:HH21	1:A:331:ARG:HA	1.22	1.00
1:A:550:LYS:HE3	1:A:552:THR:HG21	1.47	0.97
1:B:307:ARG:HH21	1:B:331:ARG:HA	1.31	0.95
1:A:689:GLU:HB3	1:A:691:LYS:HD3	1.47	0.95
1:A:691:LYS:HD2	1:A:691:LYS:N	1.85	0.91
1:B:420:HIS:HD2	1:B:423:TYR:H	1.15	0.89
1:A:691:LYS:CD	1:A:691:LYS:H	1.87	0.88
1:A:420:HIS:HD2	1:A:423:TYR:H	1.17	0.88
1:B:115:PRO:HD2	1:B:118:ILE:HD13	1.54	0.87
1:A:115:PRO:HD2	1:A:118:ILE:HD13	1.55	0.87
1:A:541:LEU:HD23	1:A:557:ASN:HB3	1.56	0.87
1:A:132:GLU:HG3	1:A:196:ARG:HH12	1.39	0.86
1:A:465:GLU:HA	1:A:465:GLU:OE1	1.76	0.84
1:B:465:GLU:OE1	1:B:465:GLU:HA	1.77	0.84
1:B:132:GLU:HG3	1:B:196:ARG:HH12	1.41	0.83
1:B:541:LEU:HD23	1:B:557:ASN:HB3	1.61	0.83
1:A:307:ARG:NH2	1:A:331:ARG:HA	1.94	0.81
1:A:26:LEU:HD11	1:A:374:VAL:HG13	1.63	0.80
1:A:321:GLU:HB3	1:A:323:ARG:HE	1.48	0.79
1:A:34:GLU:HA	1:A:37:ILE:HD12	1.65	0.78
1:A:421:PRO:HB2	1:A:422:GLN:HE21	1.47	0.78
1:A:323:ARG:NH1	1:A:362:GLU:HB2	2.00	0.77
1:A:18:GLN:O	1:A:21:LYS:HB3	1.85	0.77
1:A:58:THR:HB	1:B:799:GLN:NE2	2.00	0.77
1:B:421:PRO:HB2	1:B:422:GLN:HE21	1.49	0.76
1:B:307:ARG:NH2	1:B:331:ARG:HA	2.01	0.75
1:A:17:ASP:O	1:A:21:LYS:N	2.20	0.75
1:A:420:HIS:CD2	1:A:423:TYR:H	2.04	0.75
1:B:34:GLU:HA	1:B:37:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:LEU:HD22	1:B:799:GLN:HG2	1.69	0.74
1:B:321:GLU:HB3	1:B:323:ARG:HE	1.53	0.74
1:B:323:ARG:NH1	1:B:362:GLU:HB2	2.02	0.74
1:B:428:HIS:O	1:B:432:ARG:HG2	1.87	0.74
1:A:769:ARG:NH2	1:A:812:THR:HG23	2.02	0.74
1:B:18:GLN:HE21	1:B:18:GLN:HA	1.52	0.73
1:A:549:LYS:HG3	1:A:550:LYS:H	1.54	0.73
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.02	0.72
1:A:550:LYS:CE	1:A:552:THR:HG21	2.18	0.72
1:B:843:ASP:O	1:B:847:GLU:HG3	1.89	0.72
1:A:320:PHE:HB3	1:A:361:VAL:CG1	2.19	0.72
1:A:843:ASP:O	1:A:847:GLU:HG3	1.88	0.72
1:B:769:ARG:NH2	1:B:815:ASP:OD2	2.22	0.72
1:B:18:GLN:O	1:B:21:LYS:HB2	1.89	0.72
1:A:39:ILE:HD11	1:A:273:ILE:HD13	1.71	0.71
1:A:769:ARG:NH2	1:A:815:ASP:OD2	2.24	0.71
1:A:428:HIS:O	1:A:432:ARG:HG2	1.90	0.71
1:B:769:ARG:NH2	1:B:812:THR:HG23	2.05	0.71
1:A:58:THR:HB	1:B:799:GLN:HE22	1.54	0.71
1:A:797:LEU:HD21	1:A:817:ILE:HD11	1.71	0.71
1:A:132:GLU:HG3	1:A:196:ARG:NH1	2.06	0.71
1:B:431:LEU:CD2	1:B:442:PHE:HZ	2.04	0.71
1:A:324:ILE:HG23	1:A:328:LEU:HD23	1.72	0.71
1:B:420:HIS:CD2	1:B:423:TYR:H	2.04	0.70
1:A:795:LEU:HD22	1:A:799:GLN:HG2	1.71	0.70
1:B:39:ILE:HD11	1:B:273:ILE:HD13	1.73	0.70
1:B:486:GLU:O	1:B:490:ARG:HG3	1.90	0.70
1:A:674:VAL:HB	1:A:858:VAL:HG22	1.72	0.70
1:B:98:ASN:HD22	1:B:98:ASN:H	1.38	0.70
1:B:421:PRO:HB2	1:B:422:GLN:NE2	2.07	0.70
1:B:357:THR:OG1	1:B:363:PRO:HG2	1.92	0.69
1:B:497:LEU:O	1:B:503:THR:HG23	1.92	0.69
1:B:320:PHE:HB3	1:B:361:VAL:CG1	2.23	0.69
1:A:357:THR:OG1	1:A:363:PRO:HG2	1.93	0.69
1:A:422:GLN:O	1:A:426:ARG:HG3	1.93	0.69
1:A:421:PRO:HB2	1:A:422:GLN:NE2	2.06	0.69
1:A:486:GLU:O	1:A:490:ARG:HG3	1.94	0.68
1:A:431:LEU:HD23	1:A:442:PHE:HZ	1.57	0.68
1:B:674:VAL:HB	1:B:858:VAL:HG22	1.75	0.68
1:B:132:GLU:HG3	1:B:196:ARG:NH1	2.09	0.68
1:A:356:LEU:HD21	1:A:371:VAL:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ARG:HH21	1:A:812:THR:HG23	1.58	0.67
1:B:356:LEU:HD21	1:B:371:VAL:HG21	1.77	0.67
1:B:115:PRO:C	1:B:117:ASN:H	1.98	0.67
1:A:497:LEU:O	1:A:503:THR:HG23	1.93	0.66
1:A:418:LYS:HG3	1:A:444:LEU:HD11	1.75	0.66
1:B:324:ILE:HG23	1:B:328:LEU:HD23	1.78	0.66
1:B:422:GLN:O	1:B:426:ARG:HG3	1.96	0.66
1:A:320:PHE:HB3	1:A:361:VAL:HG13	1.78	0.66
1:B:514:SER:OG	1:B:704:CYS:HB3	1.96	0.65
1:A:514:SER:OG	1:A:704:CYS:HB3	1.95	0.65
1:B:320:PHE:CD1	1:B:361:VAL:HG11	2.32	0.65
1:A:98:ASN:OD1	1:A:101:LYS:HB2	1.97	0.65
1:B:769:ARG:HH21	1:B:812:THR:HG23	1.61	0.65
1:A:466:GLN:HG2	1:A:766:PHE:CE1	2.32	0.64
1:B:418:LYS:HG3	1:B:444:LEU:HD11	1.79	0.64
1:A:115:PRO:C	1:A:117:ASN:H	1.98	0.64
1:A:56:ASN:N	1:A:57:PRO:HD2	2.12	0.64
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.32	0.64
1:B:193:ILE:HD13	1:B:201:ALA:CB	2.28	0.64
1:B:26:LEU:HD21	1:B:309:ILE:HG21	1.79	0.64
1:B:431:LEU:HD23	1:B:442:PHE:HZ	1.61	0.64
1:A:767:LEU:CD2	1:A:818:LEU:HD23	2.28	0.64
1:B:380:PHE:CE2	1:B:426:ARG:HD3	2.33	0.64
1:B:768:PHE:HA	1:B:769:ARG:CZ	2.28	0.64
1:B:320:PHE:HB3	1:B:361:VAL:HG13	1.79	0.63
1:A:26:LEU:CD1	1:A:374:VAL:HG13	2.28	0.63
1:A:147:LYS:H	1:A:147:LYS:CD	2.11	0.63
1:A:380:PHE:CE2	1:A:426:ARG:HD3	2.33	0.63
1:A:795:LEU:CD2	1:A:799:GLN:HG2	2.29	0.63
1:A:799:GLN:NE2	1:B:58:THR:HB	2.13	0.63
1:A:767:LEU:HD21	1:A:818:LEU:HD23	1.80	0.63
1:A:160:GLN:HG2	1:A:165:GLU:O	1.99	0.62
1:B:147:LYS:CD	1:B:147:LYS:H	2.12	0.62
1:B:75:SER:HA	1:B:99:HIS:NE2	2.15	0.62
1:B:797:LEU:HD21	1:B:817:ILE:HD11	1.81	0.62
1:B:795:LEU:CD2	1:B:799:GLN:HG2	2.29	0.62
1:A:354:GLU:O	1:A:358:ARG:HG3	2.00	0.61
1:B:32:SER:O	1:B:35:THR:HB	1.99	0.61
1:B:307:ARG:HG2	1:B:307:ARG:NH1	2.14	0.61
1:A:768:PHE:HA	1:A:769:ARG:CZ	2.30	0.61
1:B:431:LEU:HD23	1:B:442:PHE:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HH21	1:B:395:ASN:HB3	1.63	0.61
1:A:320:PHE:CD1	1:A:361:VAL:HG11	2.35	0.61
1:A:500:ARG:HB2	1:A:503:THR:CG2	2.31	0.61
1:A:95:VAL:HG22	1:A:107:MET:HB3	1.83	0.60
1:A:40:MET:HG3	1:A:388:ALA:O	2.01	0.60
1:A:193:ILE:HD13	1:A:201:ALA:CB	2.31	0.60
1:B:114:THR:HG22	1:B:119:VAL:HG23	1.83	0.60
1:B:441:ARG:NH2	1:B:443:LEU:HD13	2.15	0.60
1:B:466:GLN:HG2	1:B:766:PHE:CE1	2.37	0.60
1:A:209:ASP:HB2	3:A:919:G6P:H1	1.84	0.59
1:B:321:GLU:HB2	1:B:323:ARG:HH21	1.67	0.59
1:B:354:GLU:O	1:B:358:ARG:HG3	2.01	0.59
1:B:502:GLN:OE1	1:B:502:GLN:N	2.33	0.59
1:B:56:ASN:N	1:B:57:PRO:HD2	2.16	0.59
1:B:437:ASP:OD1	1:B:437:ASP:N	2.36	0.59
1:A:725:TYR:O	1:A:729:VAL:HG23	2.02	0.59
1:B:18:GLN:NE2	1:B:18:GLN:HA	2.16	0.59
1:B:361:VAL:O	1:B:363:PRO:HD3	2.03	0.59
1:A:665:CYS:HB3	1:A:891:LEU:HD23	1.85	0.59
1:B:597:PRO:HA	1:B:650:ASP:HB3	1.84	0.59
1:A:114:THR:HG22	1:A:119:VAL:HG23	1.84	0.58
1:B:95:VAL:HG22	1:B:107:MET:HB3	1.85	0.58
1:A:502:GLN:OE1	1:A:502:GLN:N	2.33	0.58
1:A:54:ASP:HB3	1:B:798:LEU:HD22	1.84	0.58
1:A:361:VAL:O	1:A:363:PRO:HD3	2.03	0.58
1:B:118:ILE:HG23	1:B:126:LEU:HA	1.85	0.58
1:B:870:HIS:CD2	1:B:873:ARG:HH21	2.21	0.58
1:B:420:HIS:CD2	1:B:423:TYR:HB2	2.39	0.58
1:B:501:LYS:HA	1:B:695:MET:SD	2.43	0.58
1:A:321:GLU:HB2	1:A:323:ARG:HH21	1.67	0.58
1:B:688:GLU:O	1:B:702:GLN:HB3	2.03	0.58
1:A:320:PHE:HB3	1:A:361:VAL:HG11	1.85	0.58
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.17	0.58
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.69	0.58
1:A:32:SER:O	1:A:35:THR:HB	2.04	0.57
1:A:23:ASP:OD1	1:A:373:HIS:NE2	2.30	0.57
1:A:783:GLU:HB2	1:A:786:PHE:CD2	2.39	0.57
1:B:98:ASN:HD22	1:B:98:ASN:N	1.98	0.57
1:A:307:ARG:CG	1:A:307:ARG:HH11	2.16	0.57
1:B:307:ARG:CG	1:B:307:ARG:HH11	2.17	0.57
1:A:854:LEU:HD12	1:A:855:ASN:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:ARG:HB2	1:B:503:THR:CG2	2.34	0.57
1:B:767:LEU:CD2	1:B:818:LEU:HD23	2.34	0.57
1:A:325:THR:HG23	1:A:361:VAL:HG23	1.85	0.57
1:B:507:ALA:O	1:B:510:LYS:HD3	2.04	0.56
1:A:797:LEU:HD21	1:A:817:ILE:CD1	2.34	0.56
1:A:380:PHE:CD2	1:A:426:ARG:HD3	2.41	0.56
1:B:854:LEU:HD12	1:B:855:ASN:N	2.20	0.56
1:A:330:THR:HB	1:A:333:LYS:HG3	1.87	0.56
1:B:330:THR:HB	1:B:333:LYS:HG3	1.86	0.56
1:A:328:LEU:O	1:A:328:LEU:HG	2.03	0.56
1:A:118:ILE:HG23	1:A:126:LEU:HA	1.87	0.56
1:B:196:ARG:C	1:B:198:ASP:H	2.08	0.56
1:B:513:PRO:HA	1:B:705:ILE:HD13	1.87	0.56
1:A:420:HIS:CD2	1:A:423:TYR:HB2	2.41	0.56
1:A:465:GLU:OE1	1:A:468:ARG:NE	2.38	0.56
1:A:570:THR:OG1	1:A:573:GLU:HG3	2.06	0.56
1:A:689:GLU:HB3	1:A:691:LYS:CD	2.30	0.56
1:A:646:GLU:HB3	1:A:647:PHE:CD1	2.41	0.55
1:A:331:ARG:HD2	1:B:588:TYR:CZ	2.41	0.55
1:B:862:GLY:HA2	3:B:921:G6P:H61	1.88	0.55
1:A:513:PRO:HA	1:A:705:ILE:HD13	1.88	0.55
1:A:202:ASN:O	1:A:204:VAL:HG23	2.06	0.55
1:A:173:LYS:HE2	2:A:918:BGC:O5	2.06	0.55
1:A:147:LYS:H	1:A:147:LYS:HD3	1.72	0.55
1:A:437:ASP:N	1:A:437:ASP:OD1	2.40	0.55
1:B:718:LEU:C	1:B:720:ASP:H	2.08	0.55
1:B:725:TYR:O	1:B:729:VAL:HG23	2.07	0.55
1:B:646:GLU:HB3	1:B:647:PHE:CD1	2.42	0.54
1:A:26:LEU:HD21	1:A:309:ILE:HG21	1.90	0.54
1:A:500:ARG:HB2	1:A:503:THR:HG22	1.89	0.54
1:B:693:VAL:HG12	1:B:693:VAL:O	2.07	0.54
1:B:325:THR:HG23	1:B:361:VAL:HG23	1.88	0.54
1:A:441:ARG:NH2	1:A:443:LEU:HD13	2.23	0.54
1:B:18:GLN:HA	1:B:21:LYS:HG3	1.89	0.54
1:A:597:PRO:HA	1:A:650:ASP:HB3	1.90	0.54
1:A:26:LEU:HD12	1:A:377:ILE:HD12	1.90	0.54
1:B:598:LEU:HD23	1:B:598:LEU:C	2.28	0.54
1:B:328:LEU:HG	1:B:328:LEU:O	2.08	0.54
1:A:196:ARG:C	1:A:198:ASP:H	2.12	0.54
1:A:277:PHE:CE1	1:A:309:ILE:HA	2.43	0.54
1:A:226:VAL:HB	1:A:410:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLY:HA3	3:B:919:G6P:O2P	2.07	0.53
1:B:767:LEU:HD21	1:B:818:LEU:HD23	1.90	0.53
1:B:604:PHE:HB3	1:B:605:PRO:HD2	1.90	0.53
1:A:86:GLY:HA3	1:A:155:SER:OG	2.09	0.53
1:A:700:GLN:OE1	1:A:700:GLN:N	2.36	0.53
1:B:380:PHE:CD2	1:B:426:ARG:HD3	2.44	0.53
1:B:500:ARG:HB2	1:B:503:THR:HG22	1.90	0.53
1:A:274:ARG:HH11	1:A:274:ARG:HG2	1.74	0.53
1:B:441:ARG:HH21	1:B:443:LEU:HD13	1.73	0.53
1:A:688:GLU:O	1:A:702:GLN:HB3	2.09	0.52
1:B:86:GLY:HA3	1:B:155:SER:OG	2.08	0.52
1:B:209:ASP:HB2	3:B:919:G6P:H1	1.91	0.52
1:A:588:TYR:CZ	1:B:331:ARG:HD2	2.45	0.52
1:A:101:LYS:O	1:A:102:ASN:CB	2.56	0.52
1:B:320:PHE:HB3	1:B:361:VAL:HG11	1.90	0.52
1:B:718:LEU:C	1:B:720:ASP:N	2.63	0.52
1:B:783:GLU:HB2	1:B:786:PHE:CD2	2.44	0.52
1:B:832:GLN:NE2	5:B:1125:HOH:O	2.43	0.52
1:B:160:GLN:HG2	1:B:165:GLU:O	2.10	0.52
1:A:321:GLU:CB	1:A:323:ARG:HE	2.21	0.52
1:A:376:THR:O	1:A:380:PHE:HB2	2.10	0.52
1:A:501:LYS:HA	1:A:695:MET:SD	2.50	0.52
1:A:755:ARG:HG2	1:A:755:ARG:HH11	1.75	0.52
1:B:26:LEU:HD11	1:B:374:VAL:HG13	1.92	0.52
1:B:88:SER:HB3	3:B:919:G6P:O1P	2.10	0.52
1:B:689:GLU:HB2	1:B:692:ASN:HD22	1.75	0.52
1:A:380:PHE:HE1	1:A:384:ASN:HD21	1.56	0.52
1:A:691:LYS:HB3	1:A:699:ASP:HB2	1.91	0.52
1:B:644:ARG:HG3	1:B:644:ARG:HH11	1.75	0.52
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.73	0.51
1:A:507:ALA:O	1:A:510:LYS:HD3	2.10	0.51
1:A:19:VAL:HG12	1:A:20:LYS:N	2.26	0.51
1:B:259:THR:O	1:B:260:GLU:HB2	2.09	0.51
1:B:307:ARG:O	1:B:311:VAL:HG23	2.09	0.51
1:B:543:VAL:HG22	1:B:555:MET:HB3	1.91	0.51
1:B:797:LEU:HD21	1:B:817:ILE:CD1	2.40	0.51
1:A:768:PHE:HA	1:A:769:ARG:NH1	2.26	0.51
1:B:83:LEU:HD23	1:B:92:ILE:HG23	1.93	0.51
1:A:353:LYS:HA	1:A:368:CYS:SG	2.51	0.51
1:A:20:LYS:O	1:A:24:LYS:HG3	2.11	0.51
1:B:103:GLN:O	1:B:105:VAL:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:GLU:OE1	1:B:468:ARG:NE	2.42	0.51
1:B:93:LEU:HD12	1:B:93:LEU:N	2.26	0.51
1:A:878:THR:O	1:A:882:LEU:HG	2.11	0.50
1:B:274:ARG:HG2	1:B:274:ARG:HH11	1.75	0.50
1:A:477:PHE:CZ	1:A:757:ILE:HD11	2.46	0.50
1:A:520:PRO:HD3	1:A:663:MET:CE	2.41	0.50
1:B:409:THR:HG23	1:B:441:ARG:HG2	1.93	0.50
1:B:614:GLY:O	1:B:632:ASP:HA	2.11	0.50
1:A:490:ARG:NH1	1:A:717:CYS:O	2.43	0.50
1:A:115:PRO:C	1:A:117:ASN:N	2.64	0.50
1:A:320:PHE:CG	1:A:361:VAL:HG11	2.47	0.50
1:A:307:ARG:CG	1:A:307:ARG:NH1	2.75	0.50
1:B:209:ASP:CB	3:B:919:G6P:H1	2.42	0.50
1:A:441:ARG:HH21	1:A:443:LEU:HD13	1.76	0.50
1:A:575:PHE:O	1:A:579:VAL:HG23	2.12	0.50
1:A:652:VAL:HB	1:A:905:THR:HG23	1.93	0.50
1:A:17:ASP:HA	1:A:20:LYS:HB2	1.92	0.50
1:A:518:ARG:NH1	1:A:521:ASP:N	2.59	0.50
1:B:575:PHE:O	1:B:579:VAL:HG23	2.11	0.50
1:A:259:THR:O	1:A:260:GLU:HB2	2.12	0.49
1:A:546:ARG:O	1:A:551:ARG:HA	2.12	0.49
1:A:598:LEU:HD23	1:A:598:LEU:C	2.32	0.49
1:A:604:PHE:HB3	1:A:605:PRO:HD2	1.93	0.49
1:B:193:ILE:HD13	1:B:201:ALA:HB3	1.93	0.49
1:B:878:THR:O	1:B:882:LEU:HG	2.12	0.49
1:A:718:LEU:C	1:A:720:ASP:H	2.14	0.49
1:B:320:PHE:CG	1:B:361:VAL:HG11	2.46	0.49
1:B:775:THR:HG21	1:B:807:LEU:O	2.12	0.49
1:A:870:HIS:CD2	1:A:873:ARG:HH21	2.30	0.49
1:A:93:LEU:N	1:A:93:LEU:HD12	2.27	0.49
1:A:232:THR:O	1:A:300:MET:HB2	2.13	0.49
1:B:325:THR:HG21	1:B:361:VAL:N	2.28	0.49
1:B:375:CYS:O	1:B:379:SER:HB3	2.13	0.49
1:B:196:ARG:C	1:B:198:ASP:N	2.65	0.49
1:B:376:THR:O	1:B:380:PHE:HB2	2.13	0.49
1:B:578:ILE:O	1:B:582:ILE:HG13	2.13	0.49
1:A:119:VAL:HG13	1:A:175:PHE:HA	1.94	0.49
1:A:66:THR:HG21	1:A:211:VAL:HG21	1.95	0.49
1:B:40:MET:HG3	1:B:388:ALA:O	2.13	0.49
1:B:836:ALA:HA	1:B:882:LEU:HD12	1.95	0.49
1:B:147:LYS:H	1:B:147:LYS:CE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ASN:HB2	2:A:920:BGC:H5	1.94	0.49
1:B:425:ARG:HG2	1:B:425:ARG:HH11	1.77	0.49
1:A:479:LEU:HA	1:A:483:MET:SD	2.53	0.48
1:B:232:THR:O	1:B:300:MET:HB2	2.13	0.48
1:B:634:VAL:HG13	1:B:651:VAL:HG11	1.94	0.48
1:A:325:THR:HG21	1:A:361:VAL:N	2.28	0.48
1:B:115:PRO:C	1:B:117:ASN:N	2.65	0.48
1:B:689:GLU:HB2	1:B:692:ASN:ND2	2.29	0.48
1:A:193:ILE:HD13	1:A:201:ALA:HB3	1.95	0.48
1:A:258:ASN:OD1	1:A:258:ASN:C	2.52	0.48
1:A:797:LEU:HD11	1:A:817:ILE:HG13	1.95	0.48
1:B:71:ILE:HA	1:B:215:MET:HE1	1.96	0.48
1:B:147:LYS:HD3	1:B:147:LYS:H	1.76	0.48
1:B:755:ARG:HH11	1:B:755:ARG:HG2	1.78	0.48
1:A:66:THR:OG1	1:A:256:CYS:HB3	2.14	0.48
1:A:275:THR:HG23	1:A:278:ASP:OD2	2.14	0.48
1:B:307:ARG:CG	1:B:307:ARG:NH1	2.75	0.48
1:B:202:ASN:O	1:B:204:VAL:HG23	2.14	0.48
1:A:578:ILE:O	1:A:582:ILE:HG13	2.14	0.47
1:A:307:ARG:O	1:A:311:VAL:HG23	2.14	0.47
1:A:425:ARG:HG2	1:A:425:ARG:HH11	1.79	0.47
1:A:549:LYS:CG	1:A:550:LYS:H	2.24	0.47
1:A:779:ARG:NH1	5:A:1145:HOH:O	2.47	0.47
1:B:277:PHE:CE1	1:B:309:ILE:HA	2.49	0.47
1:B:570:THR:OG1	1:B:573:GLU:HG3	2.14	0.47
1:A:115:PRO:O	1:A:117:ASN:N	2.46	0.47
1:A:83:LEU:HD23	1:A:92:ILE:HG23	1.96	0.47
1:B:860:VAL:HG12	1:B:861:ASP:N	2.29	0.47
1:B:105:VAL:HG11	1:B:451:LYS:HG3	1.96	0.47
1:B:62:LYS:NZ	5:B:1012:HOH:O	2.47	0.47
1:B:640:ALA:CA	1:B:643:ARG:HH21	2.27	0.47
1:B:98:ASN:N	1:B:98:ASN:ND2	2.61	0.47
1:A:364:SER:C	1:A:366:ASP:H	2.17	0.47
1:A:412:VAL:HG12	1:A:413:ASP:N	2.30	0.47
1:A:755:ARG:NH1	1:A:755:ARG:HG2	2.28	0.47
1:A:854:LEU:HD11	1:A:856:VAL:HB	1.97	0.47
1:B:119:VAL:HG13	1:B:175:PHE:HA	1.97	0.47
1:A:718:LEU:C	1:A:720:ASP:N	2.68	0.47
1:A:760:ASP:O	1:A:764:LYS:HG2	2.14	0.47
1:B:115:PRO:O	1:B:117:ASN:N	2.48	0.47
1:A:557:ASN:HD22	1:A:557:ASN:C	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:PHE:HE2	1:A:608:GLN:C	2.18	0.47
1:A:120:HIS:NE2	1:A:174:ARG:O	2.46	0.47
1:A:167:ILE:HA	1:A:183:ALA:O	2.15	0.47
1:B:97:VAL:HA	1:B:104:ASN:O	2.15	0.47
1:B:320:PHE:HE1	1:B:356:LEU:HD22	1.80	0.47
1:A:18:GLN:OE1	1:A:18:GLN:HA	2.15	0.47
1:B:121:GLY:O	1:B:177:ALA:HA	2.15	0.47
1:B:380:PHE:HE1	1:B:384:ASN:HD21	1.63	0.47
1:B:479:LEU:HA	1:B:483:MET:SD	2.55	0.47
1:B:514:SER:O	1:B:515:PHE:HB2	2.15	0.47
1:B:492:ARG:NE	1:B:844:LYS:HD2	2.29	0.47
1:A:763:LYS:HG2	1:A:772:ILE:HD11	1.95	0.46
1:B:703:MET:HG3	1:B:704:CYS:N	2.31	0.46
1:B:665:CYS:HB3	1:B:891:LEU:HD23	1.97	0.46
1:B:103:GLN:O	1:B:104:ASN:C	2.54	0.46
1:B:221:ASP:OD1	1:B:223:HIS:HB2	2.15	0.46
1:A:644:ARG:HH11	1:A:644:ARG:HG3	1.80	0.46
1:A:775:THR:HG21	1:A:807:LEU:O	2.15	0.46
1:B:167:ILE:HA	1:B:183:ALA:O	2.15	0.46
1:B:477:PHE:CZ	1:B:757:ILE:HD11	2.50	0.46
1:A:55:PHE:C	1:A:57:PRO:HD2	2.35	0.46
1:A:813:CYS:O	1:A:817:ILE:HD12	2.15	0.46
1:A:657:ASP:HB2	3:A:921:G6P:H1	1.98	0.46
1:B:196:ARG:O	1:B:198:ASP:N	2.49	0.46
1:B:531:LEU:HD21	1:B:582:ILE:HD11	1.98	0.46
1:A:147:LYS:CE	1:A:147:LYS:H	2.28	0.46
1:A:514:SER:O	1:A:515:PHE:HB2	2.16	0.46
1:A:20:LYS:O	1:A:24:LYS:HE3	2.16	0.46
1:B:364:SER:C	1:B:366:ASP:H	2.19	0.46
1:A:614:GLY:O	1:A:632:ASP:HA	2.16	0.46
1:B:570:THR:HA	1:B:626:THR:OG1	2.15	0.46
1:A:320:PHE:HE1	1:A:356:LEU:HD22	1.81	0.46
1:B:193:ILE:HD13	1:B:201:ALA:HB2	1.98	0.46
1:B:55:PHE:C	1:B:57:PRO:HD2	2.36	0.46
1:B:854:LEU:HD11	1:B:856:VAL:HB	1.97	0.46
1:B:26:LEU:CD1	1:B:374:VAL:HG13	2.46	0.45
1:A:543:VAL:HG22	1:A:555:MET:HB3	1.98	0.45
1:B:161:SER:OG	1:B:165:GLU:OE1	2.22	0.45
1:A:196:ARG:C	1:A:198:ASP:N	2.68	0.45
1:A:370:SER:O	1:A:374:VAL:HG23	2.16	0.45
1:A:564:ILE:HA	1:A:567:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASN:N	1:A:57:PRO:CD	2.79	0.45
1:B:173:LYS:HE2	2:B:918:BGC:O5	2.16	0.45
1:B:491:MET:O	1:B:495:MET:HG3	2.16	0.45
1:B:612:ASP:O	1:B:634:VAL:HG21	2.16	0.45
1:A:323:ARG:HH12	1:A:362:GLU:HB2	1.78	0.45
1:A:371:VAL:HG12	1:A:372:GLN:N	2.31	0.45
1:A:563:PRO:HG2	1:A:566:ILE:HG13	1.98	0.45
1:B:853:ARG:HA	1:B:885:LYS:O	2.17	0.45
1:A:93:LEU:HD23	1:A:109:SER:HB3	1.98	0.45
1:A:510:LYS:O	1:A:511:MET:C	2.54	0.45
1:A:570:THR:HA	1:A:626:THR:OG1	2.16	0.45
1:B:755:ARG:NH1	1:B:755:ARG:HG2	2.32	0.45
1:B:768:PHE:HA	1:B:769:ARG:NH1	2.32	0.45
1:A:247:LEU:HG	5:A:1034:HOH:O	2.17	0.45
1:A:846:ARG:HB2	1:A:854:LEU:HD23	1.98	0.45
1:B:120:HIS:NE2	1:B:174:ARG:O	2.49	0.45
1:B:252:GLU:OE1	1:B:812:THR:HB	2.17	0.45
1:B:26:LEU:HD21	1:B:309:ILE:CG2	2.46	0.45
1:B:490:ARG:NH1	1:B:717:CYS:O	2.49	0.45
1:A:71:ILE:HA	1:A:215:MET:HE1	1.98	0.45
1:A:233:GLY:HA2	1:A:298:SER:CB	2.47	0.45
1:A:492:ARG:NE	1:A:844:LYS:HD2	2.32	0.45
1:B:242:LEU:HD23	1:B:252:GLU:O	2.17	0.45
1:B:538:PHE:CD2	1:B:562:ILE:HD11	2.51	0.45
1:A:612:ASP:O	1:A:634:VAL:HG21	2.17	0.44
1:A:703:MET:HG3	1:A:704:CYS:N	2.32	0.44
1:A:828:ARG:O	1:A:832:GLN:HG3	2.17	0.44
1:B:763:LYS:HG2	1:B:772:ILE:HD11	1.99	0.44
1:B:758:LEU:HD22	1:B:767:LEU:HD11	1.99	0.44
1:B:262:GLY:O	1:B:291:GLN:HA	2.17	0.44
1:B:275:THR:HG23	1:B:278:ASP:OD2	2.17	0.44
1:A:244:HIS:HE1	1:A:400:ASN:ND2	2.15	0.44
1:B:17:ASP:O	1:B:18:GLN:C	2.55	0.44
1:B:72:PRO:HD3	1:B:215:MET:CE	2.47	0.44
1:B:856:VAL:O	1:B:888:VAL:HA	2.17	0.44
1:B:564:ILE:HA	1:B:567:MET:HB2	1.99	0.44
1:B:797:LEU:HD11	1:B:817:ILE:HG13	2.00	0.44
1:B:371:VAL:HG12	1:B:372:GLN:N	2.32	0.44
1:A:364:SER:O	1:A:367:ASP:N	2.48	0.44
1:A:436:PRO:C	1:A:438:SER:H	2.21	0.44
1:A:518:ARG:HH12	1:A:521:ASP:N	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASP:OD1	1:A:546:ARG:NH1	2.44	0.44
1:A:244:HIS:CE1	1:A:400:ASN:HD21	2.35	0.44
1:A:302:LEU:HD22	1:A:378:VAL:HG12	2.00	0.44
1:A:364:SER:C	1:A:366:ASP:N	2.71	0.44
1:A:787:LEU:O	1:A:791:GLU:HG3	2.18	0.44
1:B:228:LEU:HD23	1:B:412:VAL:HG13	2.00	0.44
1:B:105:VAL:HG11	1:B:451:LYS:CG	2.48	0.43
1:A:552:THR:HB	1:B:117:ASN:OD1	2.17	0.43
1:A:500:ARG:NH2	1:A:503:THR:HG21	2.32	0.43
1:B:543:VAL:HG22	1:B:555:MET:CB	2.48	0.43
1:A:518:ARG:HH12	1:A:521:ASP:H	1.66	0.43
1:A:853:ARG:HA	1:A:885:LYS:O	2.17	0.43
1:B:211:VAL:HG22	1:B:256:CYS:SG	2.58	0.43
1:B:718:LEU:HD22	1:B:721:ILE:HD11	2.00	0.43
1:A:311:VAL:HG22	1:A:328:LEU:HG	2.00	0.43
1:A:862:GLY:HA2	3:A:921:G6P:H61	2.00	0.43
1:B:702:GLN:HE22	1:B:849:ARG:HH21	1.67	0.43
1:A:836:ALA:HA	1:A:882:LEU:HD12	1.99	0.43
1:B:518:ARG:NH1	1:B:521:ASP:N	2.66	0.43
1:A:798:LEU:HD21	1:B:55:PHE:CE1	2.52	0.43
1:B:718:LEU:O	1:B:720:ASP:N	2.52	0.43
1:A:211:VAL:HG22	1:A:256:CYS:SG	2.59	0.43
1:A:29:MET:CE	1:A:275:THR:HG21	2.49	0.43
1:A:342:ILE:O	1:A:372:GLN:HG3	2.18	0.43
1:A:518:ARG:HG3	1:A:519:THR:O	2.19	0.43
1:B:551:ARG:NH1	1:B:551:ARG:HG3	2.33	0.43
1:B:601:THR:HA	1:B:655:VAL:O	2.19	0.43
1:B:66:THR:OG1	1:B:256:CYS:HB3	2.19	0.43
1:B:669:GLU:HA	1:B:670:PRO:HD2	1.84	0.43
1:A:316:GLU:HB2	1:A:318:LEU:HD12	1.99	0.43
1:A:432:ARG:HG2	1:A:432:ARG:H	1.52	0.43
1:A:407:ARG:HG2	1:A:439:ASP:HB2	2.00	0.43
1:A:573:GLU:H	1:A:573:GLU:HG3	1.57	0.43
1:B:44:ARG:NH2	1:B:395:ASN:HB3	2.32	0.43
1:A:320:PHE:CE1	1:A:356:LEU:HD22	2.54	0.43
1:B:146:LYS:HA	1:B:147:LYS:NZ	2.34	0.43
1:B:321:GLU:CB	1:B:323:ARG:HE	2.26	0.43
1:A:646:GLU:HB3	1:A:647:PHE:HD1	1.83	0.43
1:A:94:ARG:NH1	1:A:143:ILE:HG21	2.33	0.43
1:A:375:CYS:O	1:A:379:SER:HB3	2.18	0.43
1:B:551:ARG:HH11	1:B:551:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASN:N	1:B:57:PRO:CD	2.81	0.43
1:B:845:ILE:O	1:B:849:ARG:HD2	2.19	0.43
1:A:209:ASP:CB	3:A:919:G6P:H1	2.49	0.42
1:B:23:ASP:OD1	1:B:23:ASP:N	2.52	0.42
1:B:370:SER:O	1:B:374:VAL:HG23	2.18	0.42
1:A:255:MET:HG3	1:A:256:CYS:N	2.34	0.42
1:A:601:THR:HA	1:A:655:VAL:O	2.19	0.42
1:A:602:PHE:CE2	1:A:633:VAL:HG11	2.54	0.42
1:B:436:PRO:C	1:B:438:SER:H	2.23	0.42
1:B:529:LEU:HD11	1:B:586:LEU:HD21	2.01	0.42
1:B:805:GLN:HA	1:B:809:LEU:O	2.19	0.42
1:B:860:VAL:HG12	1:B:861:ASP:H	1.85	0.42
1:A:709:TRP:CD1	1:A:709:TRP:C	2.92	0.42
1:B:93:LEU:HD23	1:B:109:SER:HB3	2.01	0.42
1:A:538:PHE:CD2	1:A:562:ILE:HD11	2.54	0.42
1:A:671:THR:OG1	1:A:857:THR:HG23	2.20	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.82	0.42
1:A:231:GLY:HA3	3:A:919:G6P:O1P	2.20	0.42
1:B:563:PRO:HG2	1:B:566:ILE:HG13	2.01	0.42
1:A:217:CYS:HB3	1:A:443:LEU:HD23	2.00	0.42
1:B:118:ILE:CG2	1:B:126:LEU:HA	2.48	0.42
1:A:297:VAL:HG13	1:A:382:SER:OG	2.20	0.42
1:A:54:ASP:HB3	1:B:798:LEU:CD2	2.50	0.42
1:A:849:ARG:HB3	1:A:851:LEU:HG	2.01	0.42
1:B:136:ASP:C	1:B:136:ASP:OD1	2.58	0.42
1:B:244:HIS:HE1	1:B:400:ASN:ND2	2.17	0.42
1:B:364:SER:C	1:B:366:ASP:N	2.73	0.42
1:A:693:VAL:O	1:A:693:VAL:HG12	2.20	0.42
1:B:233:GLY:HA2	1:B:298:SER:CB	2.50	0.42
1:B:342:ILE:O	1:B:372:GLN:HG3	2.19	0.42
1:B:828:ARG:O	1:B:832:GLN:HG3	2.20	0.42
1:B:258:ASN:OD1	1:B:258:ASN:C	2.59	0.41
1:B:226:VAL:HB	1:B:410:VAL:HG22	2.01	0.41
1:A:586:LEU:HA	1:A:586:LEU:HD23	1.87	0.41
1:B:518:ARG:CG	1:B:518:ARG:HH11	2.33	0.41
1:A:400:ASN:HD22	1:A:400:ASN:HA	1.66	0.41
1:B:320:PHE:CE1	1:B:356:LEU:HD22	2.55	0.41
1:B:713:GLY:HA2	1:B:717:CYS:SG	2.60	0.41
1:A:173:LYS:HE2	2:A:918:BGC:C1	2.50	0.41
1:A:531:LEU:HD21	1:A:582:ILE:HD11	2.02	0.41
1:A:650:ASP:O	1:A:652:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:VAL:O	1:A:888:VAL:HA	2.21	0.41
1:A:428:HIS:O	1:A:431:LEU:HB3	2.21	0.41
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.56	0.41
1:B:432:ARG:H	1:B:432:ARG:HG2	1.51	0.41
1:B:760:ASP:O	1:B:764:LYS:HG2	2.20	0.41
1:A:319:LEU:HD21	1:A:370:SER:HB2	2.01	0.41
1:A:48:LYS:HE3	1:A:48:LYS:HB2	1.90	0.41
1:A:529:LEU:HD11	1:A:586:LEU:HD21	2.03	0.41
1:A:634:VAL:HG13	1:A:651:VAL:HG11	2.02	0.41
1:B:316:GLU:HB2	1:B:318:LEU:HD12	2.01	0.41
1:A:146:LYS:HA	1:A:147:LYS:NZ	2.36	0.41
1:A:72:PRO:HD3	1:A:215:MET:CE	2.50	0.41
1:B:100:GLU:CG	1:B:101:LYS:H	2.34	0.41
1:B:48:LYS:HE3	1:B:48:LYS:HB2	1.88	0.41
1:A:160:GLN:HG2	1:A:166:ALA:HA	2.02	0.41
1:A:320:PHE:CB	1:A:361:VAL:HG11	2.51	0.41
1:B:215:MET:HG3	1:B:456:VAL:CG2	2.51	0.41
1:B:641:ILE:HD11	1:B:649:LEU:HD12	2.03	0.41
1:B:650:ASP:O	1:B:652:VAL:HG23	2.20	0.41
1:B:683:ASN:HA	1:B:709:TRP:CD1	2.56	0.41
1:A:101:LYS:HD2	1:A:103:GLN:HE22	1.86	0.41
1:A:749:TYR:O	1:A:750:LEU:C	2.59	0.41
1:A:798:LEU:HD21	1:B:55:PHE:CZ	2.56	0.41
1:A:679:GLY:HA3	3:A:921:G6P:O1P	2.21	0.41
1:A:302:LEU:HD12	1:A:416:LEU:HD11	2.03	0.41
1:A:413:ASP:OD1	1:A:414:GLY:N	2.54	0.41
1:B:154:PHE:CE2	1:B:185:VAL:HG11	2.55	0.41
1:A:232:THR:O	1:A:298:SER:OG	2.34	0.40
1:A:615:ILE:HA	1:A:631:HIS:O	2.22	0.40
1:B:274:ARG:NH1	1:B:274:ARG:HG2	2.35	0.40
1:B:615:ILE:HA	1:B:631:HIS:O	2.21	0.40
1:A:262:GLY:O	1:A:291:GLN:HA	2.21	0.40
1:A:671:THR:OG1	1:A:857:THR:CG2	2.69	0.40
1:B:510:LYS:O	1:B:511:MET:C	2.59	0.40
1:B:707:MET:O	1:B:708:GLU:HB2	2.20	0.40
1:A:144:LYS:HD3	1:A:199:TYR:HB3	2.03	0.40
1:A:598:LEU:HD23	1:A:598:LEU:O	2.21	0.40
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.87	0.40
1:A:491:MET:HE3	1:A:709:TRP:CE3	2.57	0.40
1:A:518:ARG:CG	1:A:518:ARG:HH11	2.34	0.40
1:A:686:TYR:HB2	1:A:845:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ILE:HD13	1:A:705:ILE:HA	1.91	0.40
1:B:520:PRO:HD3	1:B:663:MET:CE	2.52	0.40
1:A:29:MET:HE3	1:A:275:THR:HG21	2.03	0.40
1:A:642:LYS:O	1:A:645:GLU:HG2	2.21	0.40
1:A:801:ARG:NH1	1:A:813:CYS:SG	2.94	0.40
1:B:215:MET:HG3	1:B:456:VAL:HG23	2.02	0.40
1:B:551:ARG:H	1:B:551:ARG:HG2	1.61	0.40
1:B:683:ASN:HB2	2:B:920:BGC:H5	2.03	0.40
1:B:818:LEU:O	1:B:822:VAL:HG23	2.21	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	897/917 (98%)	810 (90%)	76 (8%)	11 (1%)	13	39
1	B	897/917 (98%)	811 (90%)	73 (8%)	13 (1%)	11	34
All	All	1794/1834 (98%)	1621 (90%)	149 (8%)	24 (1%)	12	36

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	346	LYS
1	B	100	GLU
1	B	104	ASN
1	B	346	LYS
1	B	549	LYS
1	A	116	GLU
1	A	591	ILE
1	B	116	GLU

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Mol	Chain	Res	Type
1	B	591	ILE
1	A	222	GLN
1	B	222	GLN
1	A	437	ASP
1	B	320	PHE
1	B	372	GLN
1	B	694	GLU
1	A	415	SER
1	B	436	PRO
1	A	436	PRO
1	A	203	ILE
1	A	371	VAL
1	B	651	VAL
1	A	651	VAL
1	B	404	PRO

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	774/788 (98%)	687 (89%)	87 (11%)	6	18
1	B	774/788 (98%)	691 (89%)	83 (11%)	6	20
All	All	1548/1576 (98%)	1378 (89%)	170 (11%)	6	19

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	21	LYS
1	A	32	SER
1	A	44	ARG
1	A	58	THR
1	A	69	ARG
1	A	70	SER
1	A	80	PHE

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Mol	Chain	Res	Type
1	A	93	LEU
1	A	96	GLN
1	A	102	ASN
1	A	103	GLN
1	A	107	MET
1	A	117	ASN
1	A	124	SER
1	A	136	ASP
1	A	141	ARG
1	A	147	LYS
1	A	155	SER
1	A	163	ILE
1	A	200	ASP
1	A	202	ASN
1	A	223	HIS
1	A	242	LEU
1	A	255	MET
1	A	261	TRP
1	A	271	GLU
1	A	275	THR
1	A	281	ILE
1	A	286	LEU
1	A	307	ARG
1	A	320	PHE
1	A	321	GLU
1	A	337	SER
1	A	347	GLU
1	A	353	LYS
1	A	364	SER
1	A	366	ASP
1	A	370	SER
1	A	379	SER
1	A	380	PHE
1	A	384	ASN
1	A	407	ARG
1	A	424	SER
1	A	429	LYS
1	A	432	ARG
1	A	447	SER
1	A	465	GLU
1	A	466	GLN
1	A	481	LYS

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Mol	Chain	Res	Type
1	A	501	LYS
1	A	518	ARG
1	A	519	THR
1	A	525	ASN
1	A	541	LEU
1	A	542	LEU
1	A	549	LYS
1	A	551	ARG
1	A	557	ASN
1	A	565	GLU
1	A	572	GLU
1	A	573	GLU
1	A	583	SER
1	A	592	LYS
1	A	595	ARG
1	A	603	SER
1	A	691	LYS
1	A	709	TRP
1	A	721	ILE
1	A	764	LYS
1	A	769	ARG
1	A	773	SER
1	A	781	ILE
1	A	795	LEU
1	A	798	LEU
1	A	805	GLN
1	A	810	ASN
1	A	811	SER
1	A	843	ASP
1	A	849	ARG
1	A	853	ARG
1	A	854	LEU
1	A	857	THR
1	A	877	GLN
1	A	889	SER
1	A	893	SER
1	A	899	LYS
1	B	21	LYS
1	B	23	ASP
1	B	32	SER
1	B	58	THR
1	B	69	ARG

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Mol	Chain	Res	Type
1	B	70	SER
1	B	80	PHE
1	B	93	LEU
1	B	96	GLN
1	B	98	ASN
1	B	100	GLU
1	B	101	LYS
1	B	107	MET
1	B	117	ASN
1	B	124	SER
1	B	136	ASP
1	B	141	ARG
1	B	147	LYS
1	B	155	SER
1	B	163	ILE
1	B	174	ARG
1	B	200	ASP
1	B	242	LEU
1	B	255	MET
1	B	261	TRP
1	B	271	GLU
1	B	275	THR
1	B	281	ILE
1	B	286	LEU
1	B	307	ARG
1	B	320	PHE
1	B	321	GLU
1	B	337	SER
1	B	347	GLU
1	B	353	LYS
1	B	364	SER
1	B	366	ASP
1	B	370	SER
1	B	379	SER
1	B	380	PHE
1	B	384	ASN
1	B	405	ARG
1	B	407	ARG
1	B	424	SER
1	B	432	ARG
1	B	447	SER
1	B	465	GLU

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Mol	Chain	Res	Type
1	B	466	GLN
1	B	481	LYS
1	B	501	LYS
1	B	518	ARG
1	B	519	THR
1	B	525	ASN
1	B	541	LEU
1	B	542	LEU
1	B	551	ARG
1	B	557	ASN
1	B	565	GLU
1	B	572	GLU
1	B	573	GLU
1	B	583	SER
1	B	592	LYS
1	B	595	ARG
1	B	603	SER
1	B	709	TRP
1	B	721	ILE
1	B	764	LYS
1	B	769	ARG
1	B	773	SER
1	B	781	ILE
1	B	795	LEU
1	B	798	LEU
1	B	805	GLN
1	B	810	ASN
1	B	811	SER
1	B	843	ASP
1	B	849	ARG
1	B	853	ARG
1	B	854	LEU
1	B	857	THR
1	B	877	GLN
1	B	889	SER
1	B	899	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	117	ASN
1	A	159	GLN
1	A	202	ASN
1	A	222	GLN
1	A	384	ASN
1	A	400	ASN
1	A	466	GLN
1	A	525	ASN
1	A	556	HIS
1	A	557	ASN
1	A	692	ASN
1	A	805	GLN
1	A	806	GLN
1	A	848	ASN
1	A	870	HIS
1	B	96	GLN
1	B	98	ASN
1	B	103	GLN
1	B	104	ASN
1	B	159	GLN
1	B	202	ASN
1	B	222	GLN
1	B	384	ASN
1	B	400	ASN
1	B	466	GLN
1	B	525	ASN
1	B	556	HIS
1	B	557	ASN
1	B	692	ASN
1	B	702	GLN
1	B	771	GLN
1	B	805	GLN
1	B	806	GLN
1	B	848	ASN
1	B	870	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are 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	918	-	12,12,12	0.40	0	17,17,17	0.73	0
3	G6P	A	919	-	16,16,16	0.72	0	24,24,24	0.91	1 (4%)
3	G6P	B	919	-	16,16,16	0.81	1 (6%)	24,24,24	1.04	2 (8%)
3	G6P	B	921	-	16,16,16	0.80	0	24,24,24	0.98	2 (8%)
2	BGC	B	920	-	12,12,12	0.36	0	17,17,17	0.58	0
2	BGC	A	918	-	12,12,12	0.44	0	17,17,17	0.85	1 (5%)
3	G6P	A	921	-	16,16,16	0.77	0	24,24,24	1.24	4 (16%)
2	BGC	A	920	-	12,12,12	0.43	0	17,17,17	0.79	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
3	G6P	A	921	-	1/1/6/6	0/6/26/26	0/1/1/1
3	G6P	A	919	-	1/1/6/6	3/6/26/26	0/1/1/1
3	G6P	B	919	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	B	921	-	1/1/6/6	1/6/26/26	0/1/1/1
2	BGC	B	920	-	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	918	-	-	0/2/22/22	0/1/1/1
2	BGC	B	918	-	-	2/2/22/22	0/1/1/1
2	BGC	A	920	-	-	1/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	919	G6P	P-O1P	-2.08	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	921	G6P	O1P-P-O6	2.58	113.60	106.73
3	A	921	G6P	C6-C5-C4	2.49	117.30	112.09
3	A	919	G6P	O2P-P-O6	2.43	113.19	106.73
3	A	921	G6P	O2P-P-O6	2.42	113.17	106.73
3	B	921	G6P	O1P-P-O6	2.33	112.94	106.73
3	B	919	G6P	O6-P-O3P	2.33	113.00	106.47
3	B	919	G6P	O2P-P-O6	2.26	112.75	106.73
2	A	918	BGC	O5-C1-C2	2.15	114.11	110.28
3	A	921	G6P	C3-C4-C5	-2.14	106.41	110.24
3	B	921	G6P	O2P-P-O6	2.09	112.29	106.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	919	G6P	C1
3	B	919	G6P	C1
3	B	921	G6P	C1
3	A	921	G6P	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	919	G6P	C6-O6-P-O1P
3	A	919	G6P	C6-O6-P-O2P
3	A	919	G6P	C6-O6-P-O3P
2	B	920	BGC	C4-C5-C6-O6
2	B	918	BGC	C4-C5-C6-O6
3	B	919	G6P	C6-O6-P-O3P
2	B	920	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	921	G6P	C4-C5-C6-O6
2	B	918	BGC	O5-C5-C6-O6
3	B	919	G6P	C6-O6-P-O1P
2	A	920	BGC	C4-C5-C6-O6

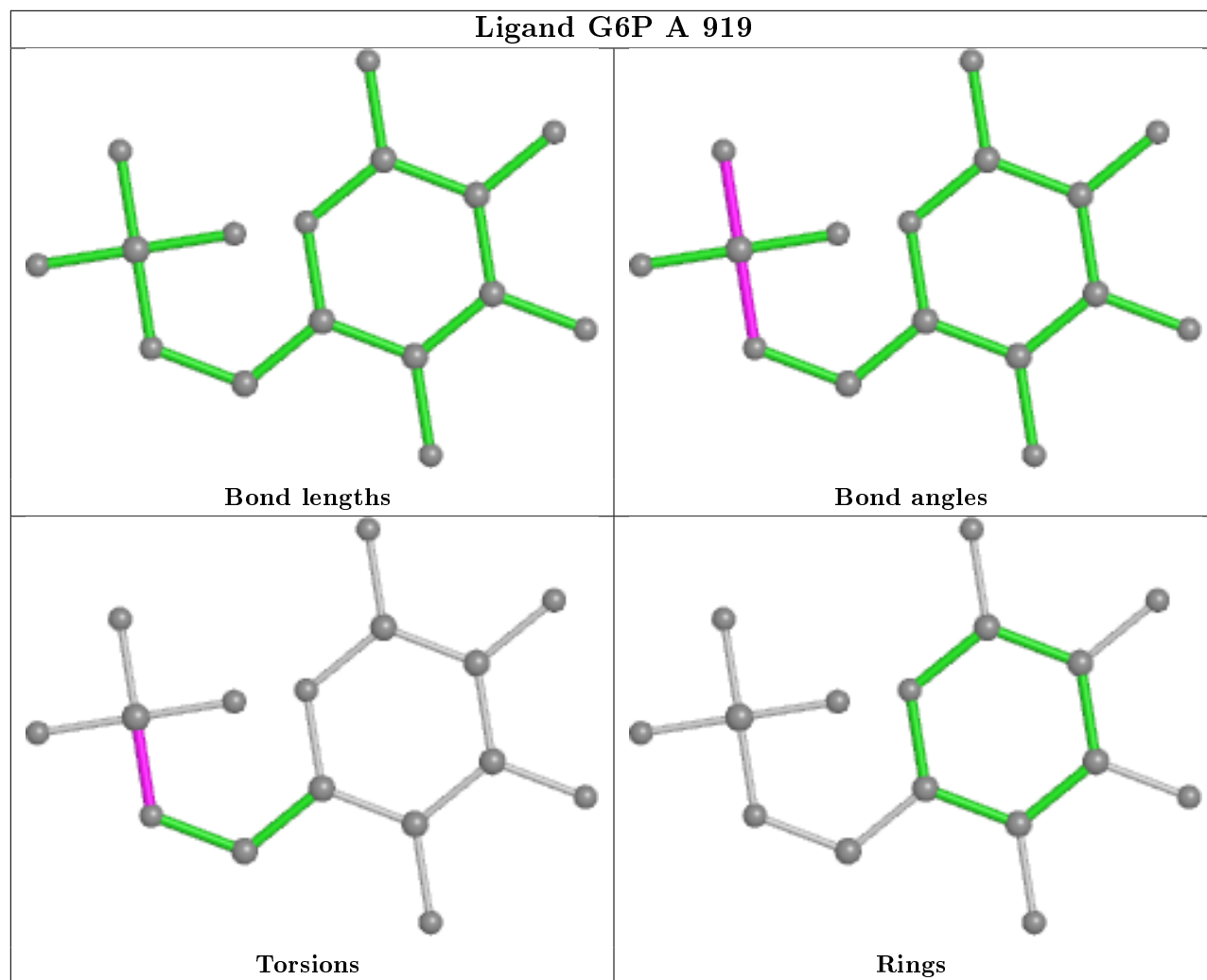
There are no ring outliers.

8 monomers are involved in 16 short contacts:

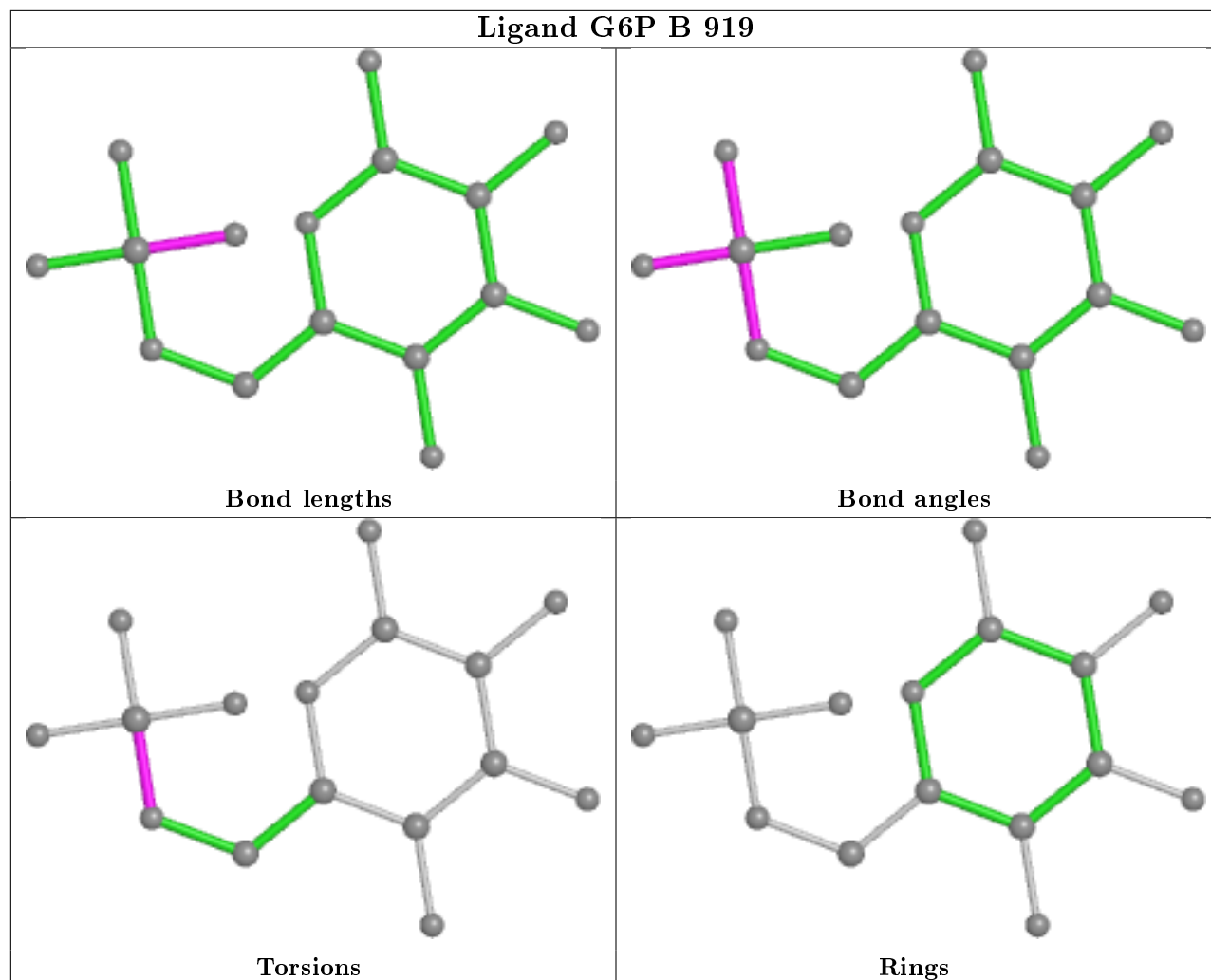
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	918	BGC	1	0
3	A	919	G6P	3	0
3	B	919	G6P	4	0
3	B	921	G6P	1	0
2	B	920	BGC	1	0
2	A	918	BGC	2	0
3	A	921	G6P	3	0
2	A	920	BGC	1	0

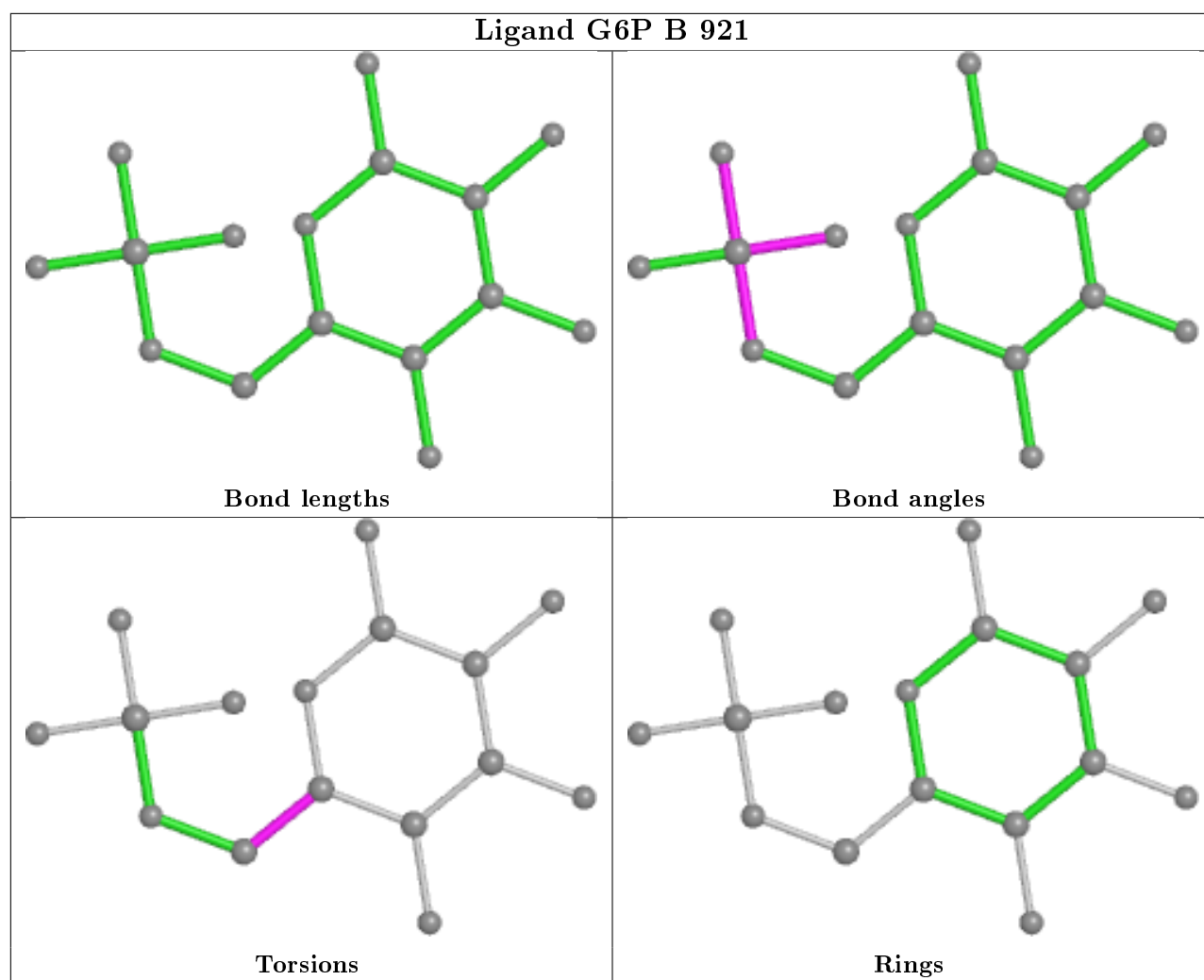
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

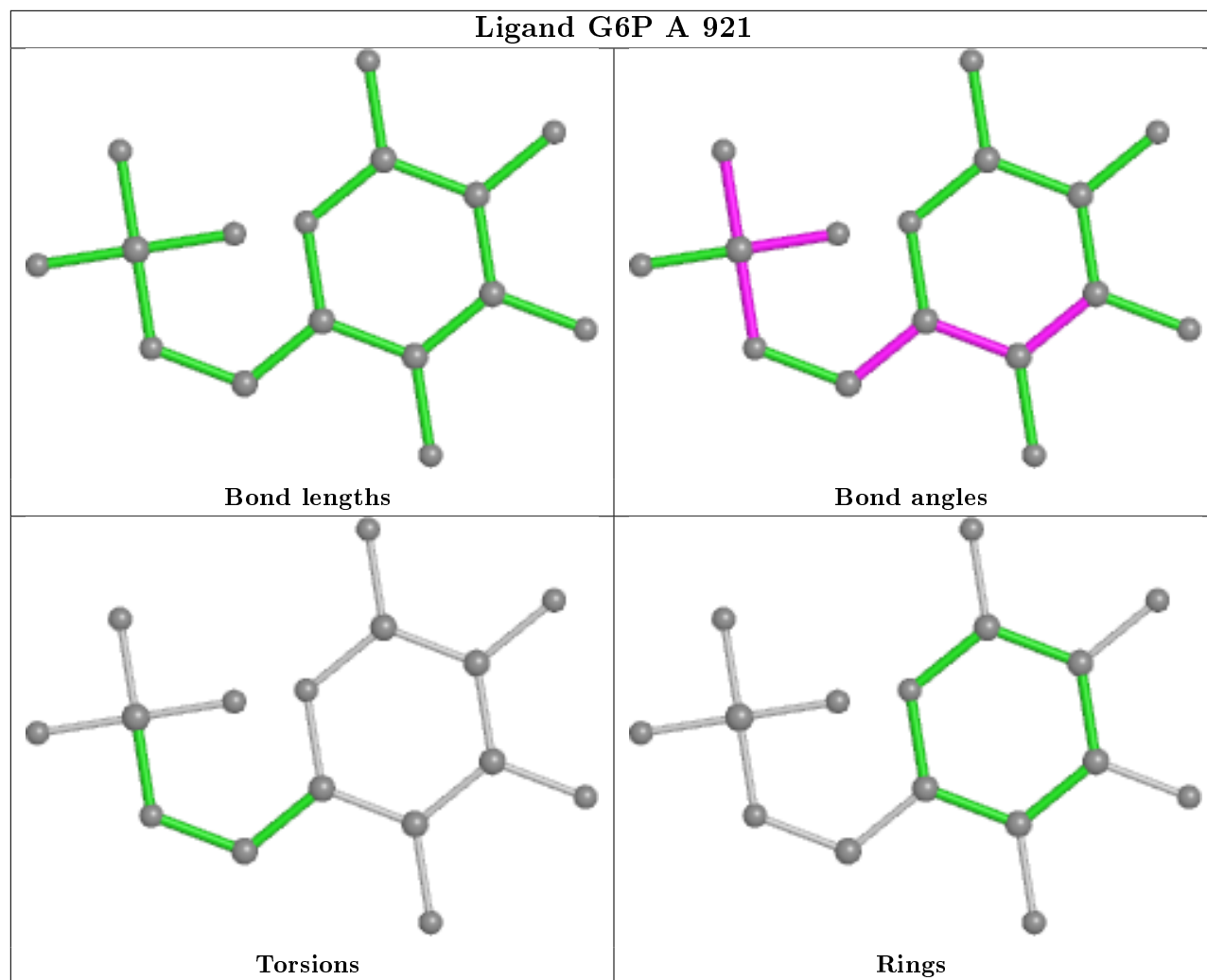
Ligand G6P A 919



Ligand G6P B 919







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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

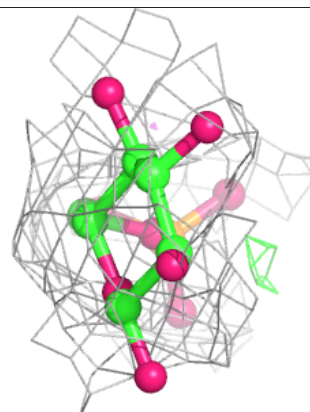
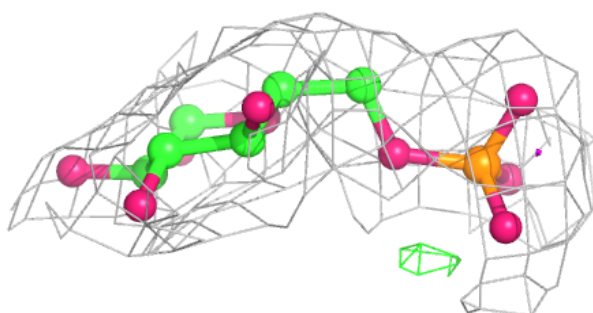
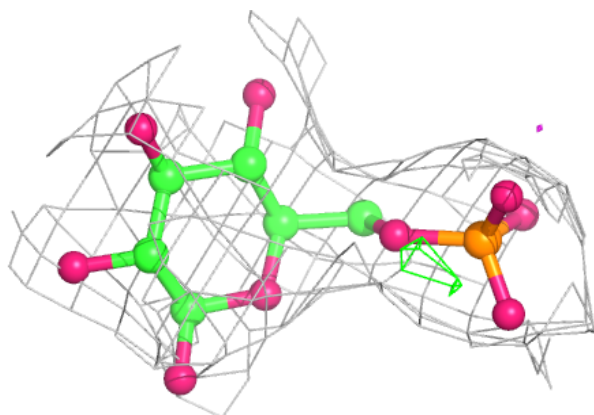
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

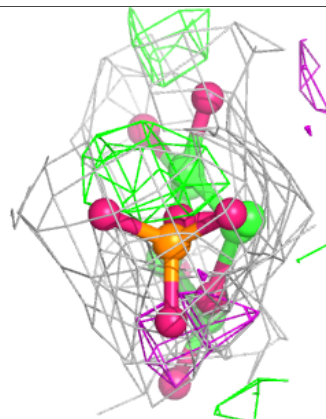
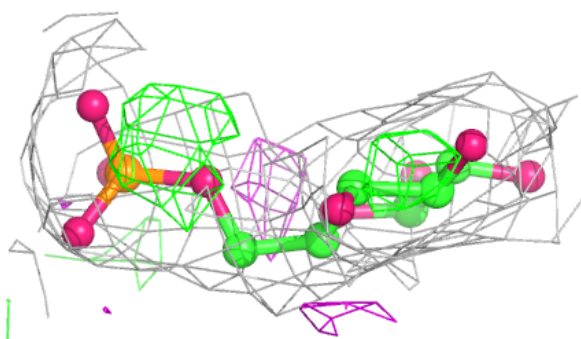
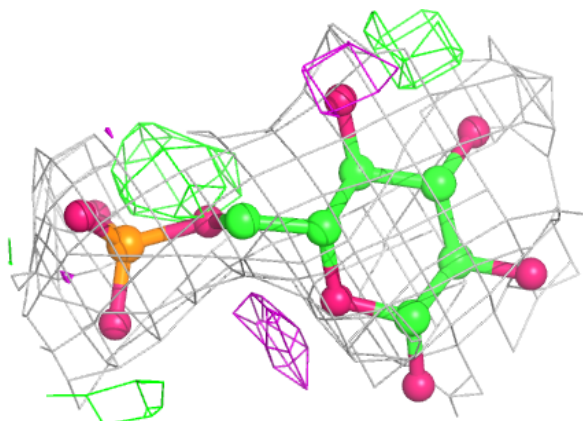
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G6P A 919:

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

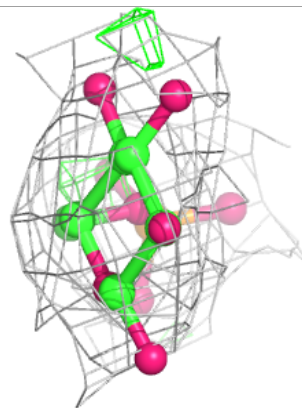
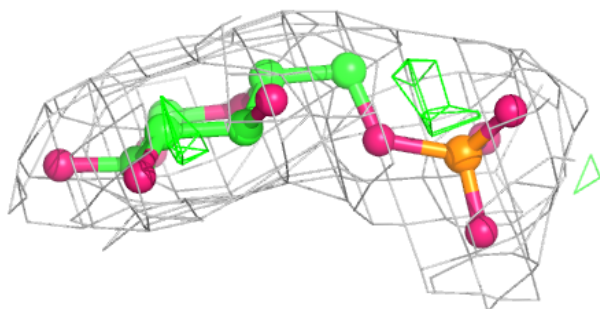
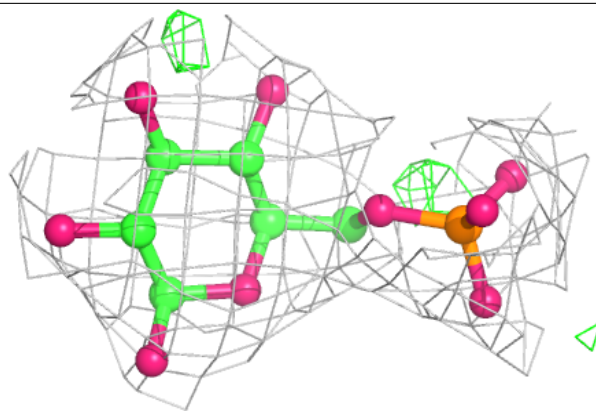
**Electron density around G6P B 919:**

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



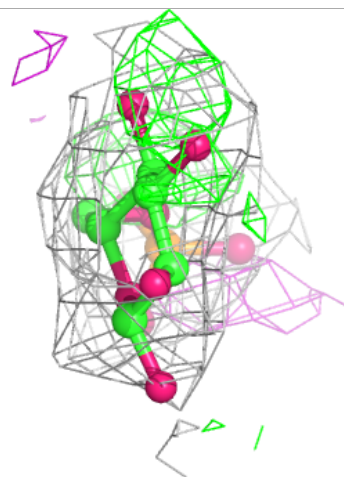
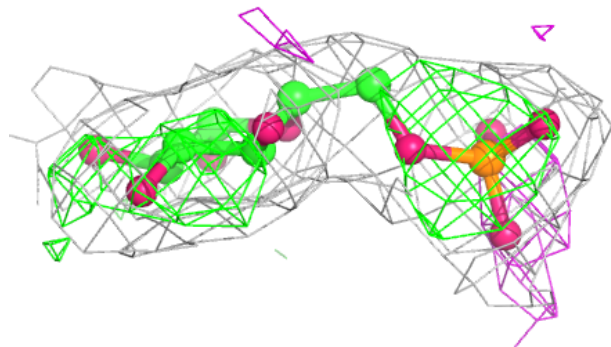
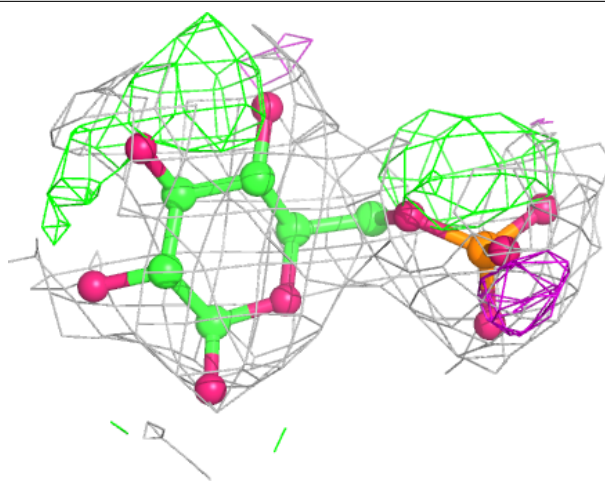
Electron density around G6P B 921:

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



Electron density around G6P A 921:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.