



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:07 PM BST

PDB ID : 2PUW  
Title : The crystal structure of isomerase domain of glucosamine-6-phosphate synthase from *Candida albicans*  
Authors : Raczynska, J.; Olchow, J.; Milewski, S.; Rypniewski, W.  
Deposited on : 2007-05-09  
Resolution : 3.15 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

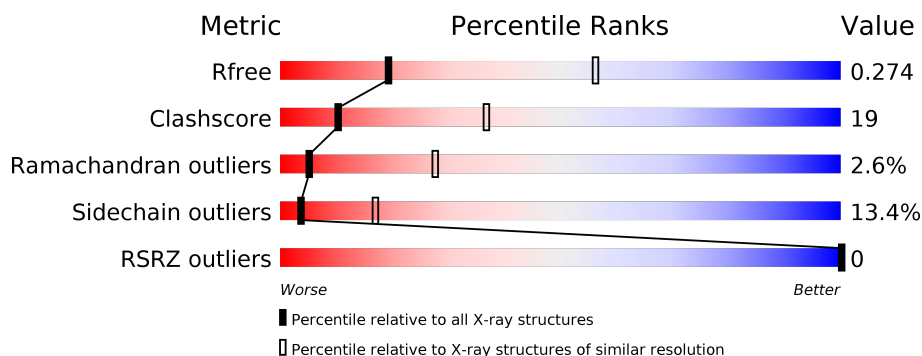
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	367	
1	B	367	

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
2	BG6	A	713	X	-	-	-
2	BG6	B	713	X	-	-	-

## 2 Entry composition [i](#)

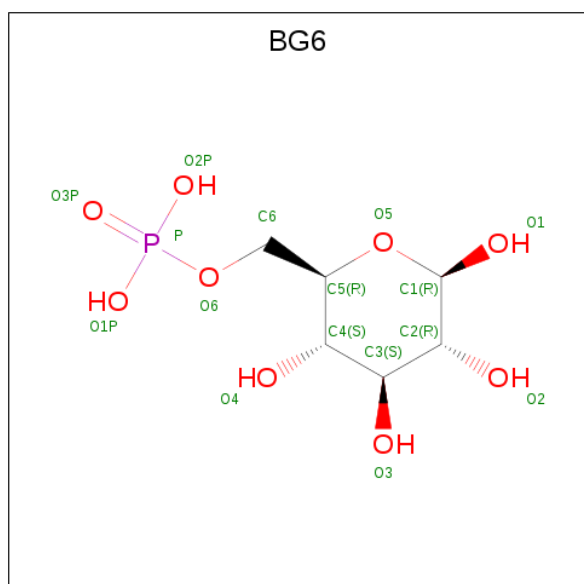
There are 3 unique types of molecules in this entry. The entry contains 5235 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2635	1662	454	502	17			
1	B	331	Total	C	N	O	S	0	0	0
			2566	1621	443	485	17			

- Molecule 2 is 6-O-phosphono-beta-D-glucopyranose (three-letter code: BG6) (formula:  $C_6H_{13}O_9P$ ).



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

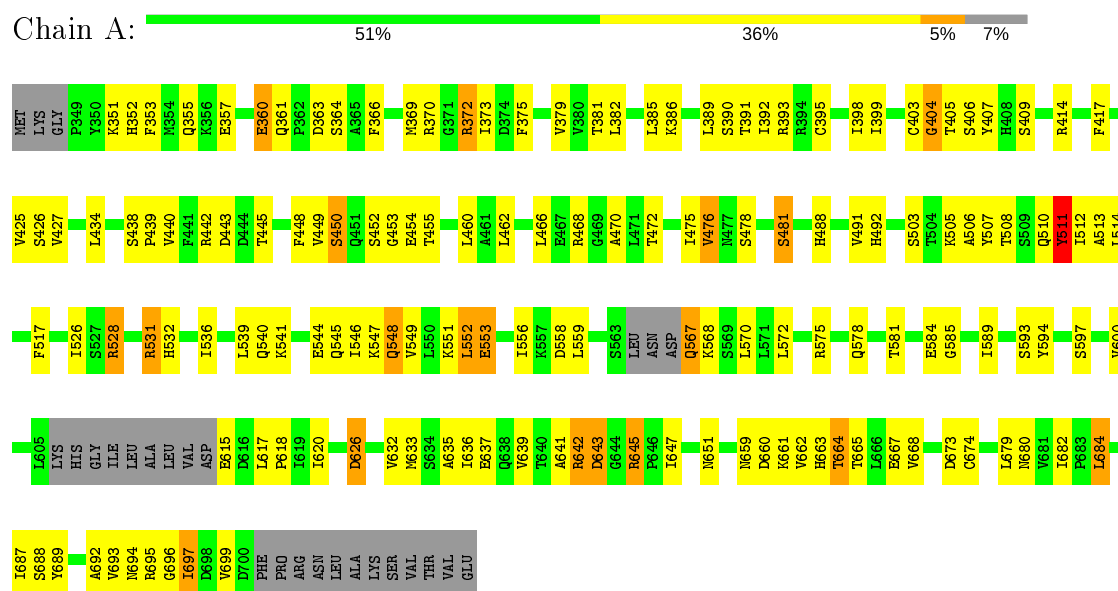
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

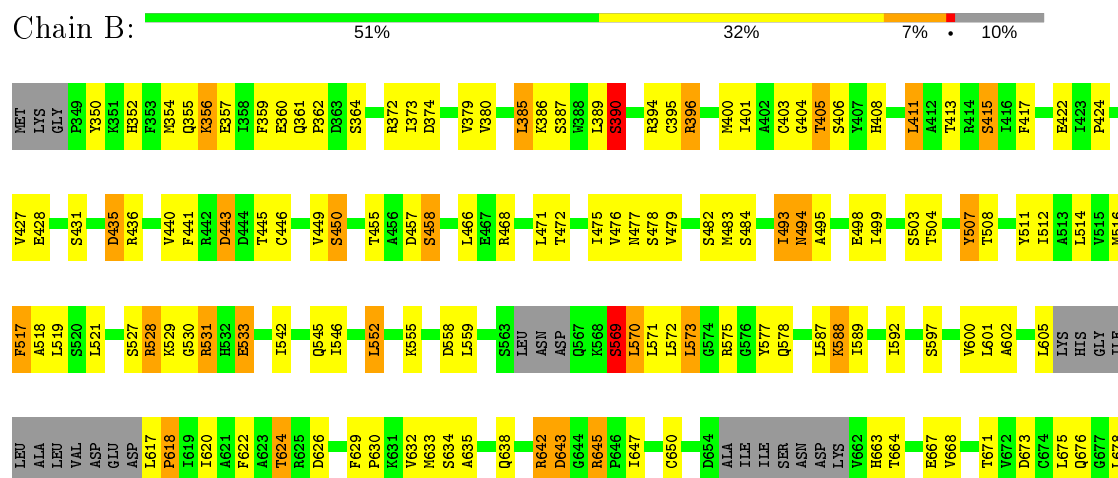
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)



- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)



I679	V699
M680	D700
V681	PHE
I682	PRO
P683	ARG
L684	ASN
	LEU
	ALA
	LYS
	SER
	VAL
	THR
	VAL
	GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.86Å 148.86Å 102.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.55 – 3.15 19.55 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.55-3.15) 99.8 (19.55-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.230 , 0.279 0.230 , 0.274	Depositor DCC
$R_{free}$ test set	399 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 15.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.269 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5235	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BG6, CL

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	0.64	0/2674	0.73	0/3611
1	B	0.67	2/2604 (0.1%)	0.75	1/3515 (0.0%)
All	All	0.65	2/5278 (0.0%)	0.74	1/7126 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	650	CYS	CB-SG	-5.46	1.73	1.81
1	B	446	CYS	CB-SG	-5.08	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	605	LEU	CA-CB-CG	5.07	126.97	115.30

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	2635	0	2675	102	0
1	B	2566	0	2609	95	0
2	A	16	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	5235	0	5306	197	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 (197) 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:357:GLU:HA	1:A:360:GLU:HB2	1.49	0.90
1:B:571:LEU:HD21	1:B:573:LEU:HD23	1.56	0.87
1:B:571:LEU:CD2	1:B:573:LEU:HD23	2.06	0.86
1:B:569:SER:O	1:B:570:LEU:HB2	1.75	0.85
1:B:588:LYS:HA	1:B:588:LYS:HE2	1.62	0.81
1:A:593:SER:HA	1:A:692:ALA:HB2	1.62	0.80
1:A:584:GLU:OE1	1:A:584:GLU:HA	1.84	0.78
1:B:571:LEU:HD21	1:B:573:LEU:CD2	2.14	0.76
1:B:396:ARG:HB2	1:B:443:ASP:HB2	1.67	0.75
1:B:518:ALA:HA	1:B:521:LEU:HD12	1.68	0.75
1:A:450:SER:O	1:A:476:VAL:HA	1.90	0.72
1:B:572:LEU:HD13	1:B:620:ILE:HB	1.70	0.72
1:A:528:ARG:CG	1:A:528:ARG:HH11	2.03	0.71
1:A:476:VAL:O	1:A:492:HIS:HA	1.91	0.70
1:A:503:SER:OG	1:A:506:ALA:HB3	1.90	0.70
1:B:359:PHE:O	1:B:362:PRO:HD2	1.91	0.70
1:B:356:LYS:O	1:B:356:LYS:HE2	1.92	0.69
1:A:536:ILE:O	1:A:539:LEU:HB2	1.93	0.68
1:A:536:ILE:HA	1:A:539:LEU:HD12	1.76	0.68
1:B:411:LEU:HD23	1:B:427:VAL:HG11	1.76	0.67
1:B:405:THR:HG23	1:B:507:TYR:HD1	1.59	0.67
1:A:510:GLN:O	1:A:513:ALA:HB3	1.95	0.67
1:A:541:LYS:O	1:A:545:GLN:HG3	1.96	0.65
1:B:528:ARG:HG2	1:B:528:ARG:HH11	1.62	0.65
1:A:531:ARG:HG3	1:A:531:ARG:O	1.96	0.65
1:B:552:LEU:HD11	1:B:667:GLU:O	1.97	0.63
1:B:477:ASN:HA	1:B:493:ILE:HG12	1.81	0.63
1:B:572:LEU:HD11	1:B:684:LEU:HD11	1.81	0.62
1:B:408:HIS:CE1	1:B:587:LEU:HD22	2.35	0.62
1:A:369:MET:HB3	1:A:373:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:HA	1:B:360:GLU:HB2	1.82	0.61
1:B:466:LEU:HG	1:B:472:THR:HG21	1.84	0.60
1:B:570:LEU:O	1:B:597:SER:HA	2.01	0.60
1:A:455:THR:OG1	2:A:713:BG6:O3P	2.18	0.60
1:B:528:ARG:CG	1:B:528:ARG:HH11	2.14	0.60
1:B:645:ARG:HB3	1:B:645:ARG:HH11	1.66	0.60
1:B:531:ARG:HG3	1:B:531:ARG:O	2.01	0.59
1:A:508:THR:O	1:A:511:TYR:HB3	2.02	0.59
1:B:516:MET:HA	1:B:519:LEU:HD12	1.84	0.59
1:A:434:LEU:HD11	1:A:460:LEU:HB2	1.84	0.58
1:A:448:PHE:CZ	1:A:462:LEU:HA	2.38	0.58
1:A:575:ARG:HG3	1:A:575:ARG:HH11	1.69	0.58
1:B:626:ASP:HB2	1:B:673:ASP:HB2	1.85	0.57
1:B:571:LEU:HD22	1:B:573:LEU:HD23	1.86	0.57
1:B:624:THR:HG21	1:B:680:ASN:HD21	1.68	0.57
1:B:559:LEU:HD21	1:B:647:ILE:HG12	1.86	0.56
1:B:624:THR:CG2	1:B:680:ASN:HD21	2.18	0.56
1:A:454:GLU:OE2	1:A:481:SER:HA	2.06	0.56
1:A:651:ASN:HA	1:A:668:VAL:O	2.06	0.55
1:A:552:LEU:HD11	1:A:667:GLU:H	1.71	0.55
1:B:530:GLY:O	1:B:533:GLU:HG2	2.06	0.55
1:A:645:ARG:HG2	1:A:662:VAL:HG13	1.88	0.55
1:A:620:ILE:HG21	1:A:684:LEU:HD21	1.88	0.55
1:B:633:MET:CE	1:B:633:MET:HA	2.36	0.55
1:B:403:CYS:HB2	2:B:713:BG6:HC62	1.89	0.54
1:A:399:ILE:HD12	1:A:399:ILE:H	1.72	0.54
1:A:578:GLN:HG3	1:A:680:ASN:HD22	1.72	0.54
1:B:528:ARG:CG	1:B:528:ARG:NH1	2.71	0.54
1:A:528:ARG:HH11	1:A:528:ARG:HG2	1.72	0.54
1:A:585:GLY:O	1:A:589:ILE:HG12	2.07	0.53
1:B:372:ARG:HH22	1:B:494:ASN:CB	2.21	0.53
1:B:570:LEU:HD21	1:B:620:ILE:CG1	2.38	0.53
1:B:634:SER:O	1:B:638:GLN:HB2	2.08	0.53
1:A:375:PHE:CE1	1:A:540:GLN:HB2	2.44	0.53
1:A:406:SER:HB3	1:A:449:VAL:HG12	1.91	0.53
1:A:549:VAL:O	1:A:552:LEU:HB2	2.08	0.53
1:A:689:TYR:CE1	1:A:699:VAL:HG21	2.43	0.53
1:A:399:ILE:HD12	1:A:399:ILE:N	2.24	0.53
1:B:512:ILE:O	1:B:516:MET:HG3	2.08	0.53
1:A:544:GLU:O	1:A:547:LYS:HB2	2.09	0.53
1:A:355:GLN:HB2	1:A:689:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:CG	1:A:528:ARG:NH1	2.68	0.52
1:A:390:SER:HA	1:A:393:ARG:HD2	1.92	0.52
1:A:508:THR:O	1:A:512:ILE:HG13	2.10	0.52
1:B:645:ARG:NH1	1:B:645:ARG:HB3	2.24	0.52
1:A:449:VAL:HG22	1:A:475:ILE:HB	1.91	0.52
1:A:491:VAL:HG12	1:A:492:HIS:N	2.25	0.52
1:B:570:LEU:HD21	1:B:620:ILE:HG12	1.92	0.52
1:A:528:ARG:HH11	1:A:528:ARG:HG3	1.74	0.51
1:B:396:ARG:HB2	1:B:443:ASP:CB	2.39	0.51
1:A:645:ARG:CG	1:A:662:VAL:HG13	2.40	0.51
1:A:689:TYR:HE1	1:A:699:VAL:HG21	1.74	0.51
1:B:617:LEU:N	1:B:618:PRO:HD3	2.26	0.51
1:A:511:TYR:OH	1:A:674:CYS:O	2.21	0.50
1:B:372:ARG:HH22	1:B:494:ASN:HB3	1.76	0.50
1:A:667:GLU:OE1	1:A:667:GLU:HA	2.12	0.49
1:B:415:SER:HB2	1:B:577:TYR:CE1	2.47	0.49
1:A:382:LEU:HB2	1:A:385:LEU:HD12	1.93	0.49
1:A:567:GLN:O	1:A:695:ARG:NH2	2.45	0.49
1:B:450:SER:O	1:B:476:VAL:HA	2.13	0.49
1:A:594:TYR:HB2	1:A:697:ILE:HD13	1.95	0.49
1:A:551:LYS:C	1:A:553:GLU:H	2.16	0.48
1:B:642:ARG:HA	1:B:642:ARG:CZ	2.44	0.48
1:B:395:CYS:HB2	1:B:443:ASP:O	2.13	0.48
1:A:372:ARG:HG3	1:A:381:THR:O	2.14	0.48
1:B:542:ILE:HD11	1:B:675:LEU:HB3	1.94	0.48
1:A:514:LEU:O	1:A:517:PHE:HB3	2.13	0.47
1:A:661:LYS:O	1:A:663:HIS:ND1	2.46	0.47
1:B:396:ARG:NH2	1:B:441:PHE:HB2	2.29	0.47
1:B:642:ARG:O	1:B:643:ASP:HB2	2.14	0.47
1:A:417:PHE:HB3	1:A:425:VAL:HG21	1.97	0.47
1:A:511:TYR:O	1:A:512:ILE:C	2.52	0.47
1:B:588:LYS:O	1:B:589:ILE:C	2.52	0.47
1:A:405:THR:HG23	1:A:507:TYR:HD1	1.80	0.47
1:B:431:SER:O	1:B:435:ASP:OD1	2.33	0.47
1:B:361:GLN:HA	1:B:364:SER:OG	2.14	0.47
1:B:675:LEU:O	1:B:678:LEU:HB2	2.14	0.47
1:A:452:SER:O	1:A:478:SER:HB2	2.15	0.47
1:A:548:GLN:HE21	1:A:548:GLN:N	2.13	0.47
1:B:413:THR:OG1	1:B:514:LEU:HD13	2.15	0.47
1:A:559:LEU:HD13	1:A:664:THR:HG21	1.96	0.47
1:B:542:ILE:O	1:B:546:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:NH1	1:A:528:ARG:HG3	2.28	0.46
1:A:694:ASN:C	1:A:696:GLY:H	2.18	0.46
1:B:354:MET:HE3	1:B:592:ILE:HG12	1.97	0.46
1:A:366:PHE:HE2	1:A:370:ARG:HD3	1.80	0.46
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.78	0.46
1:A:472:THR:O	1:A:488:HIS:HB2	2.15	0.46
1:B:403:CYS:O	1:B:404:GLY:C	2.54	0.46
1:B:401:ILE:HA	1:B:428:GLU:O	2.16	0.46
1:B:357:GLU:HA	1:B:360:GLU:CB	2.45	0.46
1:A:361:GLN:C	1:A:363:ASP:H	2.20	0.45
1:B:406:SER:HB3	1:B:449:VAL:O	2.16	0.45
1:B:385:LEU:C	1:B:387:SER:N	2.67	0.45
1:B:546:ILE:HD12	1:B:682:ILE:HD11	1.98	0.45
1:A:559:LEU:HD21	1:A:647:ILE:HG12	1.98	0.45
1:B:350:TYR:HB3	1:B:355:GLN:OE1	2.17	0.45
1:A:468:ARG:HH11	1:A:468:ARG:HG3	1.82	0.45
1:B:508:THR:O	1:B:511:TYR:HB3	2.17	0.45
1:B:630:PRO:O	1:B:633:MET:HB2	2.17	0.45
1:A:697:ILE:H	1:A:697:ILE:HG13	1.49	0.45
1:B:483:MET:O	1:B:484:SER:C	2.55	0.44
1:A:636:ILE:O	1:A:637:GLU:C	2.56	0.44
1:B:372:ARG:NH2	1:B:494:ASN:HB3	2.33	0.44
1:B:389:LEU:O	1:B:390:SER:C	2.56	0.44
1:A:361:GLN:C	1:A:363:ASP:N	2.71	0.44
1:A:351:LYS:HG3	1:A:352:HIS:ND1	2.32	0.44
1:B:572:LEU:HD12	1:B:622:PHE:CZ	2.53	0.44
1:A:366:PHE:CE2	1:A:370:ARG:HD3	2.52	0.44
1:A:617:LEU:HB2	1:A:618:PRO:HD2	1.99	0.44
1:A:642:ARG:NE	1:A:642:ARG:O	2.51	0.44
1:A:403:CYS:O	1:A:404:GLY:C	2.56	0.44
1:A:626:ASP:HB3	1:A:673:ASP:CB	2.49	0.43
1:A:507:TYR:O	1:A:510:GLN:HB2	2.18	0.43
1:A:546:ILE:HD13	1:A:679:LEU:HD23	2.00	0.43
1:B:575:ARG:HA	1:B:601:LEU:HD12	2.00	0.43
1:A:375:PHE:CD1	1:A:540:GLN:HB2	2.54	0.43
1:A:546:ILE:HD13	1:A:679:LEU:CD2	2.48	0.43
1:B:373:ILE:HD11	1:B:516:MET:SD	2.58	0.43
1:A:584:GLU:CA	1:A:584:GLU:OE1	2.61	0.43
1:B:352:HIS:CD2	1:B:699:VAL:HB	2.54	0.43
1:B:681:VAL:O	1:B:684:LEU:HB2	2.19	0.43
1:A:567:GLN:CD	1:A:568:LYS:H	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:HD2	1:A:632:VAL:HG23	2.00	0.42
1:A:361:GLN:HG2	1:A:505:LYS:HA	2.02	0.42
1:A:572:LEU:CD1	1:A:597:SER:OG	2.67	0.42
1:A:407:TYR:CE1	1:A:427:VAL:HG12	2.54	0.42
1:B:405:THR:HG23	1:B:507:TYR:CD1	2.45	0.42
1:A:575:ARG:NH1	1:A:575:ARG:HG3	2.33	0.42
1:B:380:VAL:HG11	1:B:516:MET:HB3	2.01	0.42
1:A:389:LEU:O	1:A:391:THR:N	2.52	0.42
1:A:440:VAL:HG12	1:A:470:ALA:HB2	2.02	0.42
1:A:453:GLY:HA3	1:A:481:SER:HB2	2.01	0.42
1:B:445:THR:HG23	1:B:471:LEU:CD2	2.50	0.42
1:B:498:GLU:OE2	1:B:503:SER:HA	2.20	0.42
1:B:671:THR:HG22	1:B:676:GLN:OE1	2.20	0.42
1:B:373:ILE:HG12	1:B:380:VAL:HG13	2.02	0.42
1:B:449:VAL:HA	1:B:475:ILE:HB	2.01	0.42
1:A:641:ALA:C	1:A:643:ASP:H	2.24	0.42
1:A:546:ILE:HD12	1:A:682:ILE:HD11	2.01	0.42
1:B:355:GLN:O	1:B:359:PHE:HD2	2.03	0.42
1:A:552:LEU:O	1:A:556:ILE:HD12	2.20	0.41
1:B:632:VAL:O	1:B:635:ALA:HB3	2.19	0.41
1:A:389:LEU:C	1:A:391:THR:N	2.74	0.41
1:B:482:SER:O	1:B:483:MET:C	2.56	0.41
1:B:455:THR:HB	1:B:458:SER:HB2	2.01	0.41
1:B:589:ILE:HB	1:B:597:SER:HB2	2.02	0.41
1:B:629:PHE:HB2	1:B:632:VAL:HG23	2.01	0.41
1:A:392:ILE:HG23	1:A:445:THR:HG21	2.01	0.41
1:B:555:LYS:O	1:B:558:ASP:HB3	2.21	0.41
1:A:635:ALA:O	1:A:639:VAL:HG23	2.20	0.41
1:A:545:GLN:O	1:A:549:VAL:HG23	2.21	0.41
1:B:477:ASN:OD1	1:B:495:ALA:HB3	2.21	0.41
1:A:556:ILE:HG23	1:A:687:ILE:HG12	2.03	0.41
1:B:671:THR:CG2	1:B:676:GLN:HA	2.51	0.41
1:A:361:GLN:HA	1:A:364:SER:OG	2.20	0.40
1:A:398:ILE:HA	1:A:445:THR:O	2.21	0.40
1:B:396:ARG:CB	1:B:443:ASP:HB2	2.46	0.40
1:B:588:LYS:CE	1:B:588:LYS:HA	2.43	0.40
1:B:575:ARG:HB2	1:B:602:ALA:HB3	2.02	0.40
1:A:438:SER:HA	1:A:439:PRO:HD3	1.96	0.40
1:A:593:SER:HB3	1:A:688:SER:O	2.20	0.40
1:A:693:VAL:O	1:A:696:GLY:N	2.53	0.40
1:B:514:LEU:O	1:B:517:PHE:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PHE:C	1:B:361:GLN:H	2.24	0.40
1:B:682:ILE:HB	1:B:683:PRO:HD3	2.03	0.40
1:A:506:ALA:C	1:A:510:GLN:HE21	2.25	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	334/367 (91%)	287 (86%)	43 (13%)	4 (1%)	13	46
1	B	323/367 (88%)	263 (81%)	47 (15%)	13 (4%)	3	18
All	All	657/734 (90%)	550 (84%)	90 (14%)	17 (3%)	5	28

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	569	SER
1	B	570	LEU
1	A	404	GLY
1	A	481	SER
1	A	511	TYR
1	B	390	SER
1	B	415	SER
1	B	422	GLU
1	B	507	TYR
1	B	643	ASP
1	B	396	ARG
1	B	578	GLN
1	A	552	LEU
1	B	504	THR
1	B	588	LYS

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Mol	Chain	Res	Type
1	B	424	PRO
1	B	618	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	296/319 (93%)	259 (88%)	37 (12%)	4	19
1	B	288/319 (90%)	247 (86%)	41 (14%)	3	14
All	All	584/638 (92%)	506 (87%)	78 (13%)	4	17

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	PHE
1	A	360	GLU
1	A	372	ARG
1	A	379	VAL
1	A	386	LYS
1	A	395	CYS
1	A	409	SER
1	A	414	ARG
1	A	426	SER
1	A	442	ARG
1	A	443	ASP
1	A	450	SER
1	A	476	VAL
1	A	511	TYR
1	A	526	ILE
1	A	528	ARG
1	A	531	ARG
1	A	532	HIS
1	A	548	GLN
1	A	553	GLU
1	A	558	ASP

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Mol	Chain	Res	Type
1	A	567	GLN
1	A	570	LEU
1	A	581	THR
1	A	600	VAL
1	A	615	GLU
1	A	626	ASP
1	A	633	MET
1	A	642	ARG
1	A	643	ASP
1	A	645	ARG
1	A	659	ASN
1	A	660	ASP
1	A	664	THR
1	A	665	THR
1	A	684	LEU
1	A	697	ILE
1	B	356	LYS
1	B	374	ASP
1	B	379	VAL
1	B	385	LEU
1	B	386	LYS
1	B	390	SER
1	B	394	ARG
1	B	400	MET
1	B	405	THR
1	B	411	LEU
1	B	417	PHE
1	B	435	ASP
1	B	436	ARG
1	B	440	VAL
1	B	443	ASP
1	B	450	SER
1	B	457	ASP
1	B	458	SER
1	B	468	ARG
1	B	478	SER
1	B	479	VAL
1	B	493	ILE
1	B	494	ASN
1	B	499	ILE
1	B	517	PHE
1	B	527	SER

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Mol	Chain	Res	Type
1	B	528	ARG
1	B	529	LYS
1	B	531	ARG
1	B	533	GLU
1	B	545	GLN
1	B	552	LEU
1	B	569	SER
1	B	573	LEU
1	B	600	VAL
1	B	624	THR
1	B	642	ARG
1	B	645	ARG
1	B	663	HIS
1	B	664	THR
1	B	668	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	GLN
1	A	545	GLN
1	A	548	GLN
1	A	651	ASN
1	B	463	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	BG6	A	713	-	16,16,16	1.54	3 (18%)	24,24,24	1.32	2 (8%)
2	BG6	B	713	-	16,16,16	1.66	3 (18%)	24,24,24	1.24	4 (16%)

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	BG6	A	713	-	1/1/6/6	6/6/26/26	0/1/1/1
2	BG6	B	713	-	1/1/6/6	2/6/26/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	713	BG6	P-O3P	4.83	1.66	1.50
2	A	713	BG6	P-O3P	3.39	1.61	1.50
2	A	713	BG6	O5-C1	2.19	1.48	1.42
2	B	713	BG6	C3-C2	2.15	1.57	1.52
2	A	713	BG6	O5-C5	2.09	1.49	1.44
2	B	713	BG6	P-O2P	2.09	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	713	BG6	O1P-P-O6	3.44	115.89	106.73
2	B	713	BG6	C4-C3-C2	3.36	116.69	110.82
2	A	713	BG6	O5-C5-C6	2.63	111.98	106.67
2	B	713	BG6	C3-C4-C5	2.29	114.33	110.24
2	B	713	BG6	O1P-P-O6	2.17	112.50	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	713	BG6	C1-C2-C3	2.00	114.47	110.31

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	713	BG6	C1
2	B	713	BG6	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	713	BG6	C4-C5-C6-O6
2	A	713	BG6	C6-O6-P-O1P
2	A	713	BG6	C6-O6-P-O2P
2	A	713	BG6	C6-O6-P-O3P
2	B	713	BG6	C4-C5-C6-O6
2	B	713	BG6	O5-C5-C6-O6
2	A	713	BG6	C5-C6-O6-P
2	A	713	BG6	O5-C5-C6-O6

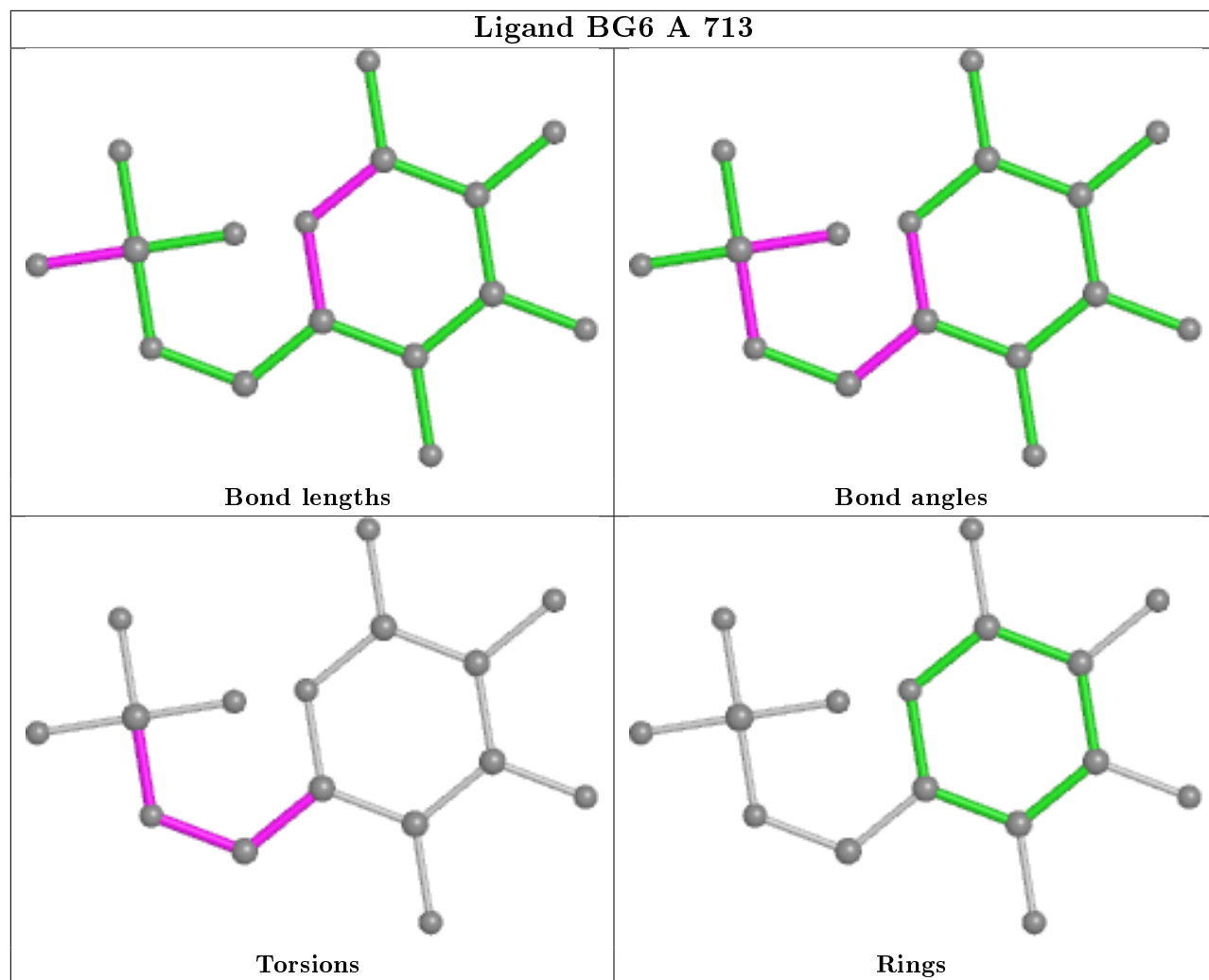
There are no ring outliers.

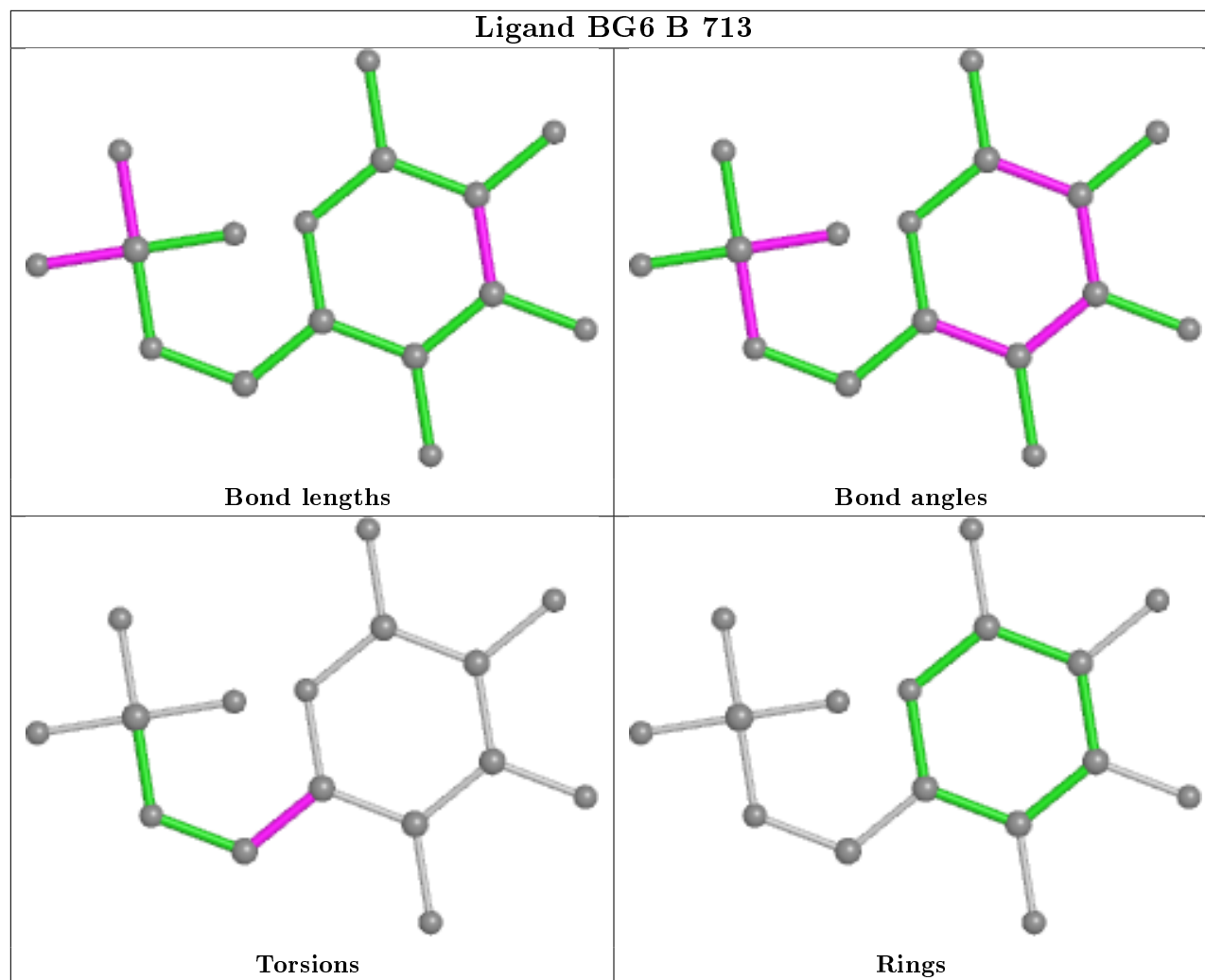
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	713	BG6	1	0
2	B	713	BG6	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 BG6 A 713





## 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	340/367 (92%)	-0.26	0 100 100	27, 51, 73, 81	0
1	B	331/367 (90%)	-0.28	0 100 100	30, 49, 74, 82	0
All	All	671/734 (91%)	-0.27	0 100 100	27, 50, 74, 82	0

There are no RSRZ outliers to report.

### 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.

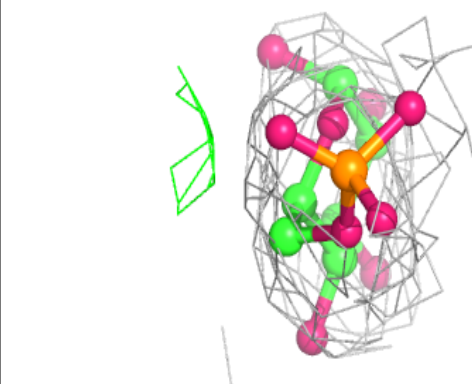
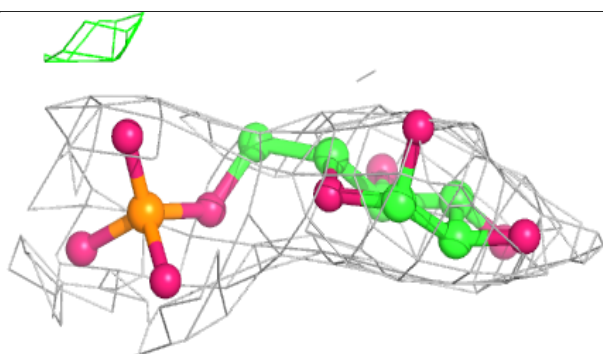
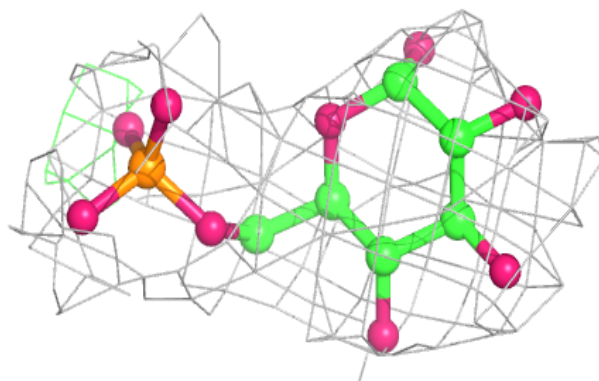
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BG6	A	713	16/16	0.94	0.20	67,80,81,81	0
3	CL	A	714	1/1	0.95	0.11	37,37,37,37	0
2	BG6	B	713	16/16	0.95	0.17	64,67,69,69	0
3	CL	B	714	1/1	0.97	0.13	47,47,47,47	0

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.

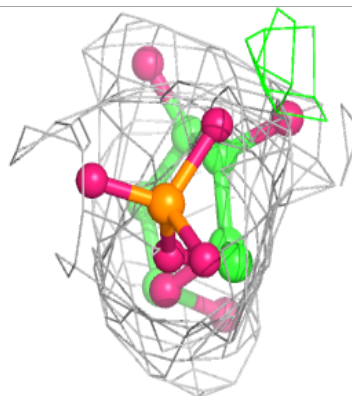
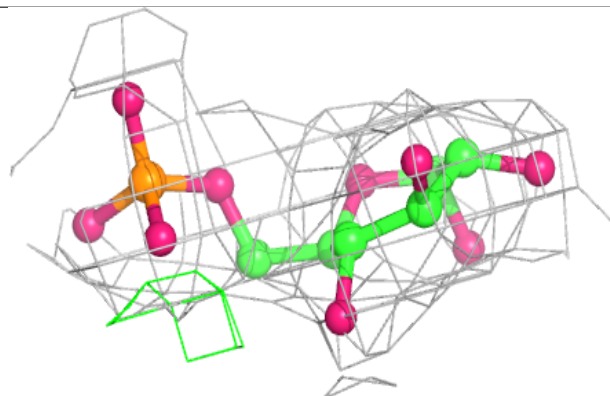
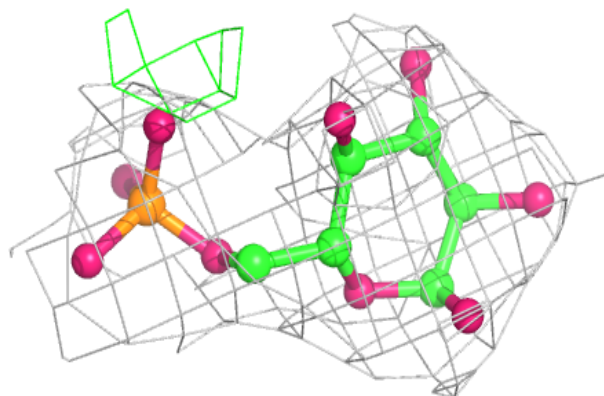
**Electron density around BG6 A 713:**

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



**Electron density around BG6 B 713:**

$2mF_o-DF_c$  (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.