



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 06:13 PM EDT

PDB ID : 2POC
Title : The crystal structure of isomerase domain of glucosamine-6-phosphate synthase from *Candida albicans*
Authors : Raczynska, J.; Olchoway, J.; Milewski, S.; Rypniewski, W.
Deposited on : 2007-04-26
Resolution : 1.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

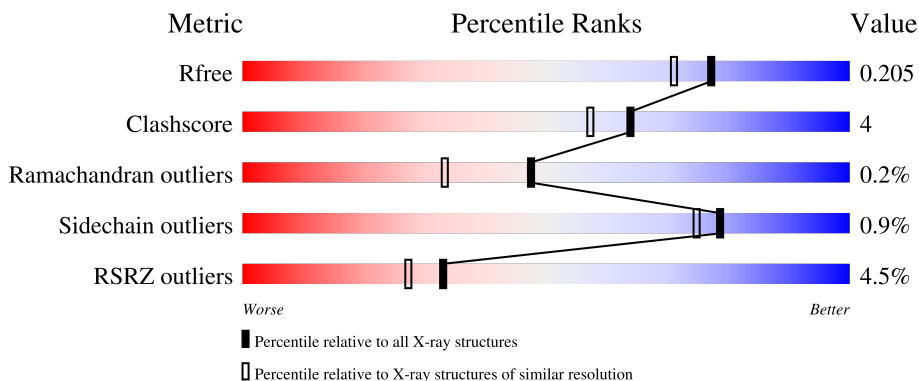
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	367	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	B	367	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>
1	C	367	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>
1	D	367	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>

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	BG6	C	713	X	-	-	-
2	BG6	D	713	X	-	-	-

2 Entry composition [i](#)

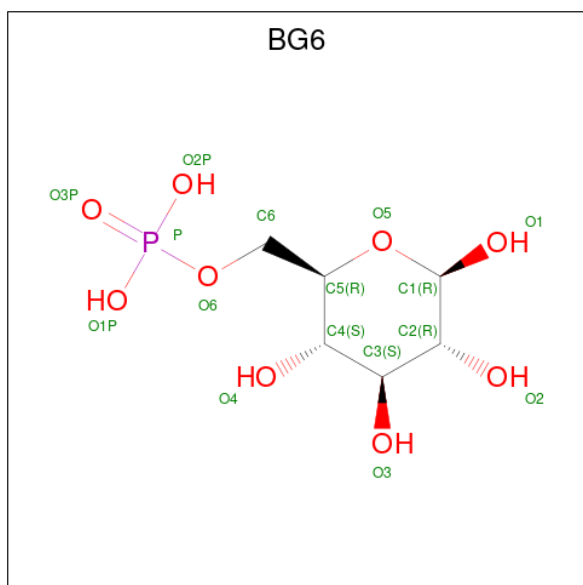
There are 6 unique types of molecules in this entry. The entry contains 11928 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	339	Total 2647	C 1671	N 462	O 497	S 17	0	4	0
1	B	352	Total 2753	C 1740	N 473	O 522	S 18	0	6	0
1	C	352	Total 2739	C 1729	N 473	O 519	S 18	0	2	0
1	D	340	Total 2665	C 1681	N 461	O 506	S 17	0	5	0

- Molecule 2 is 6-O-phosphono-beta-D-glucopyranose (three-letter code: BG6) (formula: C₆H₁₃O₉P).



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

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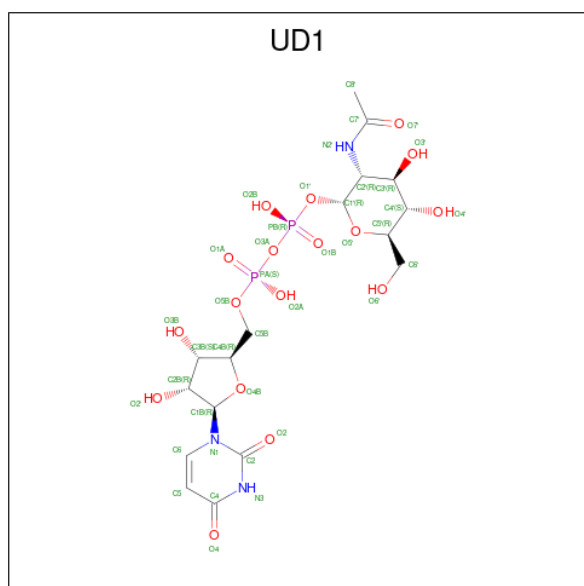
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



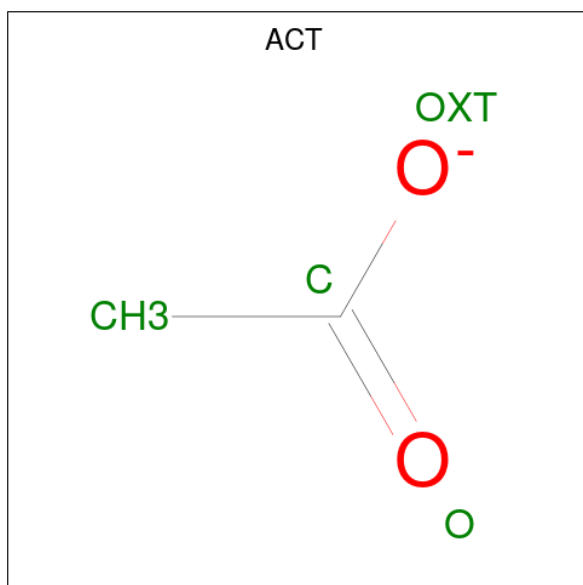
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	C O	0	0
			4	2 2		
5	C	1	Total	C O	0	0
			4	2 2		

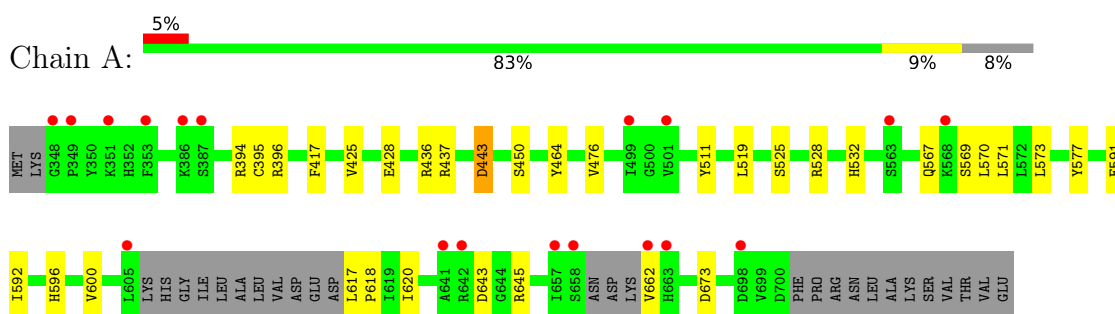
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	199	Total	O	0	0
			199	199		
6	B	234	Total	O	0	0
			234	234		
6	C	231	Total	O	0	0
			231	231		
6	D	228	Total	O	0	0
			228	228		

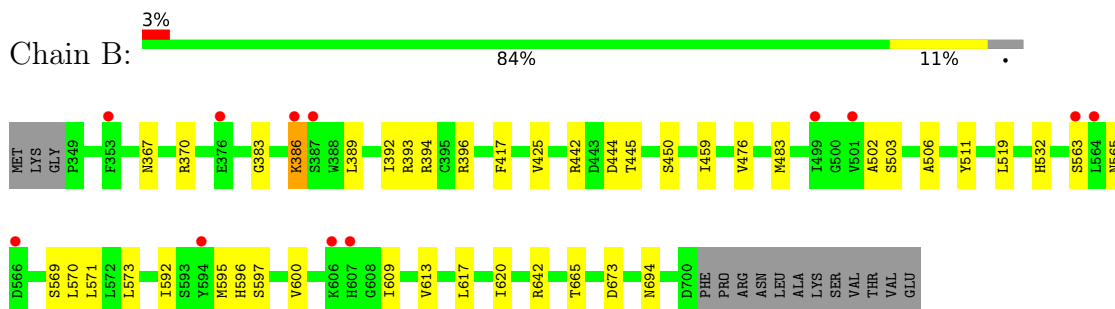
3 Residue-property plots [i](#)

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

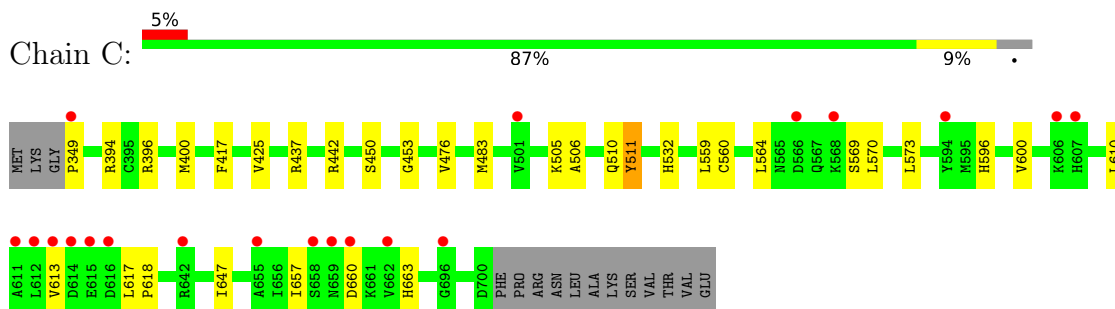
- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)




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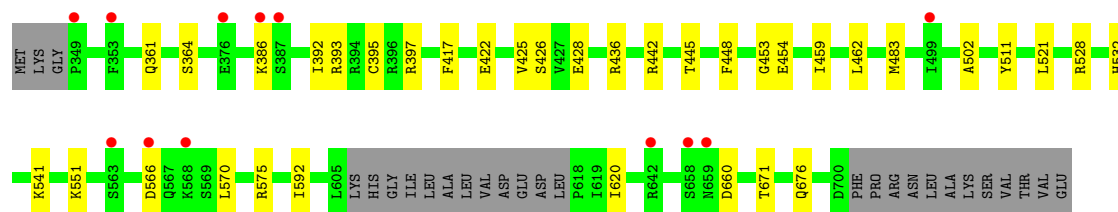


- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)



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

Chain D:  3% 83% 10% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.98Å 117.83Å 99.71Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	19.94 – 1.80 19.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-1.80) 99.9 (19.93-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.175 , 0.206 0.174 , 0.205	Depositor DCC
R_{free} test set	2819 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11928	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: BG6, NA, ACT, UD1

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	0.82	1/2704 (0.0%)	0.82	2/3652 (0.1%)
1	B	0.75	0/2819	0.79	2/3810 (0.1%)
1	C	0.77	0/2787	0.79	2/3766 (0.1%)
1	D	0.82	0/2721	0.83	2/3674 (0.1%)
All	All	0.79	1/11031 (0.0%)	0.81	8/14902 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	TYR	CD1-CE1	5.09	1.47	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	D	575	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	673	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	570	LEU	CA-CB-CG	5.68	128.35	115.30
1	A	443	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	673	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	575	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	511	TYR	CB-CG-CD2	-5.15	117.91	121.00

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	2647	0	2689	24	0
1	B	2753	0	2807	32	0
1	C	2739	0	2794	22	0
1	D	2665	0	2718	20	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
2	C	16	0	11	0	0
2	D	16	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	39	0	25	1	0
4	B	39	0	25	0	0
4	C	39	0	25	0	0
4	D	39	0	25	1	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
6	A	199	0	0	2	0
6	B	234	0	0	4	0
6	C	231	0	0	10	0
6	D	228	0	0	4	0
All	All	11928	0	11158	94	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 4.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459[A]:ILE:HD13	1:B:483[A]:MET:SD	1.98	1.02
1:C:400:MET:SD	6:C:5190:HOH:O	2.41	0.78
1:A:596[B]:HIS:NE2	1:B:609:ILE:HD12	1.98	0.78
1:B:459[A]:ILE:CD1	1:B:483[A]:MET:SD	2.74	0.76
1:B:571:LEU:HG	1:B:617:LEU:HD21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:OE1	1:A:436[A]:ARG:NH2	2.21	0.73
1:D:428:GLU:OE1	1:D:436:ARG:NH2	2.22	0.72
1:D:426:SER:HB3	6:D:5220:HOH:O	1.90	0.70
1:A:571:LEU:HD11	1:A:617:LEU:HD21	1.75	0.68
1:C:394:ARG:HB2	6:C:5210:HOH:O	1.94	0.68
1:C:349:PRO:N	6:C:5153:HOH:O	2.27	0.67
1:D:502:ALA:HB2	1:D:592:ILE:HD11	1.76	0.67
1:A:395:CYS:HB3	1:C:442[B]:ARG:NH2	2.09	0.66
1:C:505:LYS:HB3	6:C:5234:HOH:O	1.96	0.65
1:B:367:ASN:OD1	1:B:370:ARG:NH2	2.30	0.64
1:D:502:ALA:CB	1:D:592:ILE:HD11	2.28	0.64
1:A:643:ASP:HB2	6:A:5193:HOH:O	1.99	0.62
1:D:393:ARG:HD2	1:D:521:LEU:O	2.00	0.62
1:A:443:ASP:CG	6:A:5200:HOH:O	2.38	0.61
1:D:453:GLY:O	1:D:483:MET:HG3	2.01	0.61
1:B:389:LEU:O	1:B:393:ARG:HG3	2.02	0.60
1:A:596[B]:HIS:HE2	1:B:609:ILE:HD12	1.67	0.59
1:B:613:VAL:O	1:B:642:ARG:NH2	2.34	0.58
1:A:569:SER:O	1:A:618:PRO:HD2	2.04	0.57
1:B:459[A]:ILE:HD11	1:B:483[A]:MET:HG2	1.87	0.57
1:C:394:ARG:HB3	6:C:5151:HOH:O	2.04	0.57
1:A:591:GLU:HG3	1:A:592:ILE:HG12	1.85	0.56
1:B:396:ARG:HD3	6:B:5071:HOH:O	2.04	0.56
1:B:502:ALA:CB	1:B:592:ILE:HD11	2.35	0.56
1:D:551:LYS:HE3	6:D:5161:HOH:O	2.06	0.55
1:B:565:ASN:OD1	1:B:694:ASN:HB3	2.08	0.54
1:A:571:LEU:CD1	1:A:617:LEU:HD21	2.37	0.54
1:A:567:GLN:HG3	1:A:618:PRO:HG3	1.90	0.54
1:C:505:LYS:CB	6:C:5234:HOH:O	2.55	0.53
1:B:502:ALA:HB2	1:B:592:ILE:HD11	1.92	0.52
1:B:442[B]:ARG:NH2	1:D:395:CYS:HB3	2.24	0.52
1:C:657:ILE:HD12	1:C:663:HIS:CG	2.43	0.52
1:B:573:LEU:HD23	1:B:600:VAL:HB	1.91	0.52
1:B:503:SER:OG	1:B:506:ALA:HB3	2.10	0.51
1:C:417:PHE:HB3	1:C:425:VAL:HG21	1.92	0.51
1:A:570:LEU:C	1:A:570:LEU:HD23	2.32	0.50
1:B:571:LEU:HD21	1:B:609:ILE:HD11	1.95	0.48
1:A:519:LEU:O	1:A:532[A]:HIS:HE1	1.96	0.47
1:B:450:SER:O	1:B:476:VAL:HA	2.15	0.47
1:A:570:LEU:HD21	1:A:620:ILE:HD12	1.96	0.47
1:C:506:ALA:O	1:C:510:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:PHE:HB3	1:D:425:VAL:HG21	1.96	0.47
1:D:541:LYS:HE3	6:D:5127:HOH:O	2.14	0.47
1:B:442[B]:ARG:NH2	1:D:445:THR:OG1	2.37	0.47
1:B:665[A]:THR:HG21	6:B:5163:HOH:O	2.14	0.47
1:C:617:LEU:HD12	1:C:618:PRO:HD2	1.97	0.47
1:D:570:LEU:HD21	1:D:620:ILE:HD12	1.97	0.47
1:A:567:GLN:HG3	1:A:618:PRO:CG	2.45	0.46
1:A:643:ASP:OD2	1:A:645:ARG:NH1	2.49	0.46
1:A:450:SER:O	1:A:476:VAL:HA	2.16	0.45
4:A:5002:UD1:H8'2	4:A:5002:UD1:H5'2	1.98	0.45
1:C:613:VAL:HB	1:C:617:LEU:HD23	1.99	0.45
1:B:642:ARG:HG3	6:B:5154:HOH:O	2.16	0.45
1:A:525:SER:OG	1:A:528:ARG:HD3	2.17	0.44
1:B:444:ASP:O	1:D:442[B]:ARG:NH2	2.50	0.44
1:A:417:PHE:HB3	1:A:425:VAL:HG21	1.99	0.44
1:B:417:PHE:HB3	1:B:425:VAL:HG21	1.99	0.44
1:C:560:CYS:HA	1:C:564:LEU:HB2	1.98	0.44
1:C:573:LEU:HD23	1:C:600:VAL:HB	1.99	0.44
1:B:519:LEU:O	1:B:532:HIS:HE1	2.01	0.44
1:C:400:MET:HE1	6:C:5190:HOH:O	2.17	0.43
1:D:454:GLU:HA	1:D:459:ILE:HD11	2.00	0.43
1:C:559:LEU:HD21	1:C:647:ILE:HD13	2.01	0.43
1:B:392:ILE:HG23	1:B:445:THR:HG21	2.00	0.43
1:A:573:LEU:HD23	1:A:600:VAL:HB	2.01	0.43
1:B:570:LEU:HD21	1:B:620:ILE:HD12	2.00	0.43
1:B:665[A]:THR:HG23	6:B:5161:HOH:O	2.18	0.43
1:A:394:ARG:O	1:A:394:ARG:HG2	2.18	0.43
1:D:361:GLN:HA	1:D:364:SER:OG	2.19	0.43
1:C:453:GLY:O	1:C:483[B]:MET:HG2	2.18	0.42
1:A:645:ARG:HE	1:A:662:VAL:HG11	1.84	0.42
1:C:610:LEU:HA	1:C:613:VAL:HG13	2.02	0.42
1:D:660:ASP:O	6:D:5174:HOH:O	2.21	0.42
1:B:570:LEU:O	1:B:597:SER:HA	2.20	0.42
1:C:396:ARG:HD3	6:C:5029:HOH:O	2.18	0.42
1:A:396:ARG:HD3	6:C:5155:HOH:O	2.19	0.42
1:B:609:ILE:O	1:B:613:VAL:HG13	2.19	0.41
1:A:437:ARG:HH21	1:A:464:TYR:HE2	1.68	0.41
1:D:392:ILE:HG23	1:D:445:THR:HG21	2.03	0.41
1:B:383:GLY:O	1:B:386:LYS:HB2	2.20	0.41
4:D:5005:UD1:H8'2	4:D:5005:UD1:H5'2	2.01	0.41
1:D:671:THR:CG2	1:D:676:GLN:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:SER:HA	1:B:596:HIS:O	2.21	0.41
1:B:595:MET:HE2	1:B:595:MET:HB2	1.90	0.41
1:C:450:SER:O	1:C:476:VAL:HA	2.21	0.41
1:C:569:SER:HA	1:C:596:HIS:O	2.21	0.41
1:D:448:PHE:CZ	1:D:462:LEU:HA	2.56	0.40
1:D:422:GLU:OE2	1:D:528:ARG:NH2	2.52	0.40
1:C:400:MET:CE	6:C:5190:HOH:O	2.69	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	337/367 (92%)	332 (98%)	5 (2%)	0	100	100
1	B	356/367 (97%)	349 (98%)	5 (1%)	2 (1%)	25	12
1	C	352/367 (96%)	349 (99%)	3 (1%)	0	100	100
1	D	341/367 (93%)	337 (99%)	3 (1%)	1 (0%)	41	27
All	All	1386/1468 (94%)	1367 (99%)	16 (1%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	LYS
1	D	386	LYS
1	B	394	ARG

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/319 (93%)	297 (100%)	1 (0%)	92	91
1	B	312/319 (98%)	310 (99%)	2 (1%)	86	84
1	C	308/319 (97%)	304 (99%)	4 (1%)	69	62
1	D	301/319 (94%)	297 (99%)	4 (1%)	69	62
All	All	1219/1276 (96%)	1208 (99%)	11 (1%)	78	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	TYR
1	B	511	TYR
1	B	563	SER
1	C	437	ARG
1	C	511	TYR
1	C	532	HIS
1	C	660	ASP
1	D	397	ARG
1	D	511	TYR
1	D	532	HIS
1	D	566	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	ASN

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	B	713	-	16,16,16	0.88	1 (6%)	24,24,24	1.09	3 (12%)
4	UD1	C	5004	3	38,41,41	0.88	2 (5%)	57,62,62	1.36	7 (12%)
4	UD1	D	5005	3	38,41,41	0.78	0	57,62,62	1.32	8 (14%)
2	BG6	D	713	-	16,16,16	1.37	2 (12%)	24,24,24	0.75	0
4	UD1	B	5003	3	38,41,41	0.96	2 (5%)	57,62,62	1.57	7 (12%)
4	UD1	A	5002	3	38,41,41	0.82	2 (5%)	57,62,62	1.42	6 (10%)
2	BG6	A	713	-	16,16,16	1.08	2 (12%)	24,24,24	1.16	2 (8%)
5	ACT	C	714	-	3,3,3	0.80	0	3,3,3	1.31	0
5	ACT	B	714	-	3,3,3	0.84	0	3,3,3	1.37	0
2	BG6	C	713	-	16,16,16	1.17	2 (12%)	24,24,24	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BG6	B	713	-	1/1/6/6	0/6/26/26	0/1/1/1
4	UD1	C	5004	3	-	0/26/63/63	0/3/3/3
4	UD1	D	5005	3	-	1/26/63/63	0/3/3/3
2	BG6	D	713	-	1/1/6/6	0/6/26/26	0/1/1/1
4	UD1	B	5003	3	-	4/26/63/63	0/3/3/3
4	UD1	A	5002	3	-	0/26/63/63	0/3/3/3
2	BG6	A	713	-	1/1/6/6	0/6/26/26	0/1/1/1
2	BG6	C	713	-	1/1/6/6	0/6/26/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	713	BG6	P-O3P	3.58	1.62	1.50
2	D	713	BG6	O1-C1	3.10	1.49	1.39
2	C	713	BG6	P-O3P	2.97	1.60	1.50
2	C	713	BG6	O5-C1	2.85	1.50	1.42
4	B	5003	UD1	C6-C5	2.57	1.41	1.35
4	B	5003	UD1	C4-N3	-2.53	1.34	1.38
4	A	5002	UD1	C6-C5	2.49	1.40	1.35
4	C	5004	UD1	C4-N3	-2.27	1.34	1.38
2	B	713	BG6	O1-C1	2.24	1.46	1.39
2	A	713	BG6	P-O3P	2.18	1.57	1.50
4	C	5004	UD1	C5-C4	-2.12	1.38	1.43
4	A	5002	UD1	C5-C4	-2.10	1.39	1.43
2	A	713	BG6	P-O2P	2.03	1.62	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5002	UD1	C4-N3-C2	-4.77	120.29	126.58
4	B	5003	UD1	C5-C4-N3	4.73	121.92	114.84
4	B	5003	UD1	C4-N3-C2	-4.58	120.54	126.58
4	A	5002	UD1	N3-C2-N1	4.24	120.51	114.89
4	A	5002	UD1	O2-C2-N1	-3.78	117.77	122.79
4	A	5002	UD1	C5-C4-N3	3.73	120.41	114.84
4	B	5003	UD1	O4-C4-C5	-3.65	118.73	125.16
4	D	5005	UD1	C4-N3-C2	-3.62	121.81	126.58
4	C	5004	UD1	C5-C4-N3	3.53	120.12	114.84
4	D	5005	UD1	N3-C2-N1	3.45	119.46	114.89
4	B	5003	UD1	N3-C2-N1	3.44	119.46	114.89
4	B	5003	UD1	O5'-C5'-C4'	3.38	115.83	109.69
4	C	5004	UD1	O5'-C1'-O1'	-3.38	106.95	111.36
4	C	5004	UD1	C4-N3-C2	-3.31	122.22	126.58
4	C	5004	UD1	N3-C2-N1	3.28	119.25	114.89
4	B	5003	UD1	C3'-C4'-C5'	3.27	116.08	110.24
4	D	5005	UD1	O4-C4-C5	-3.10	119.71	125.16
4	B	5003	UD1	C4'-C3'-C2'	3.07	114.84	110.34
4	D	5005	UD1	C5-C4-N3	3.01	119.34	114.84
4	A	5002	UD1	O4-C4-C5	-2.87	120.11	125.16
2	B	713	BG6	O5-C1-C2	-2.69	105.48	110.28
4	C	5004	UD1	O4-C4-C5	-2.67	120.46	125.16
2	A	713	BG6	O1-C1-C2	-2.44	102.16	109.03
4	D	5005	UD1	O2-C2-N1	-2.41	119.58	122.79
4	A	5002	UD1	O4B-C1B-N1	-2.41	102.86	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5005	UD1	O5'-C5'-C4'	2.38	114.02	109.69
2	A	713	BG6	O1P-P-O6	2.38	113.07	106.73
4	D	5005	UD1	C2'-N2'-C7'	-2.15	117.94	123.18
2	B	713	BG6	C3-C4-C5	-2.12	106.45	110.24
4	C	5004	UD1	O2-C2-N1	-2.12	119.96	122.79
4	D	5005	UD1	C6'-C5'-C4'	-2.12	108.04	113.00
4	C	5004	UD1	O4B-C4B-C5B	-2.07	102.57	109.37
2	B	713	BG6	O2-C2-C1	2.06	113.95	109.16

All (4) chirality outliers are listed below:

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

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5003	UD1	C4'-C5'-C6'-O6'
4	B	5003	UD1	C8'-C7'-N2'-C2'
4	B	5003	UD1	O5'-C5'-C6'-O6'
4	B	5003	UD1	O7'-C7'-N2'-C2'
4	D	5005	UD1	C4'-C5'-C6'-O6'

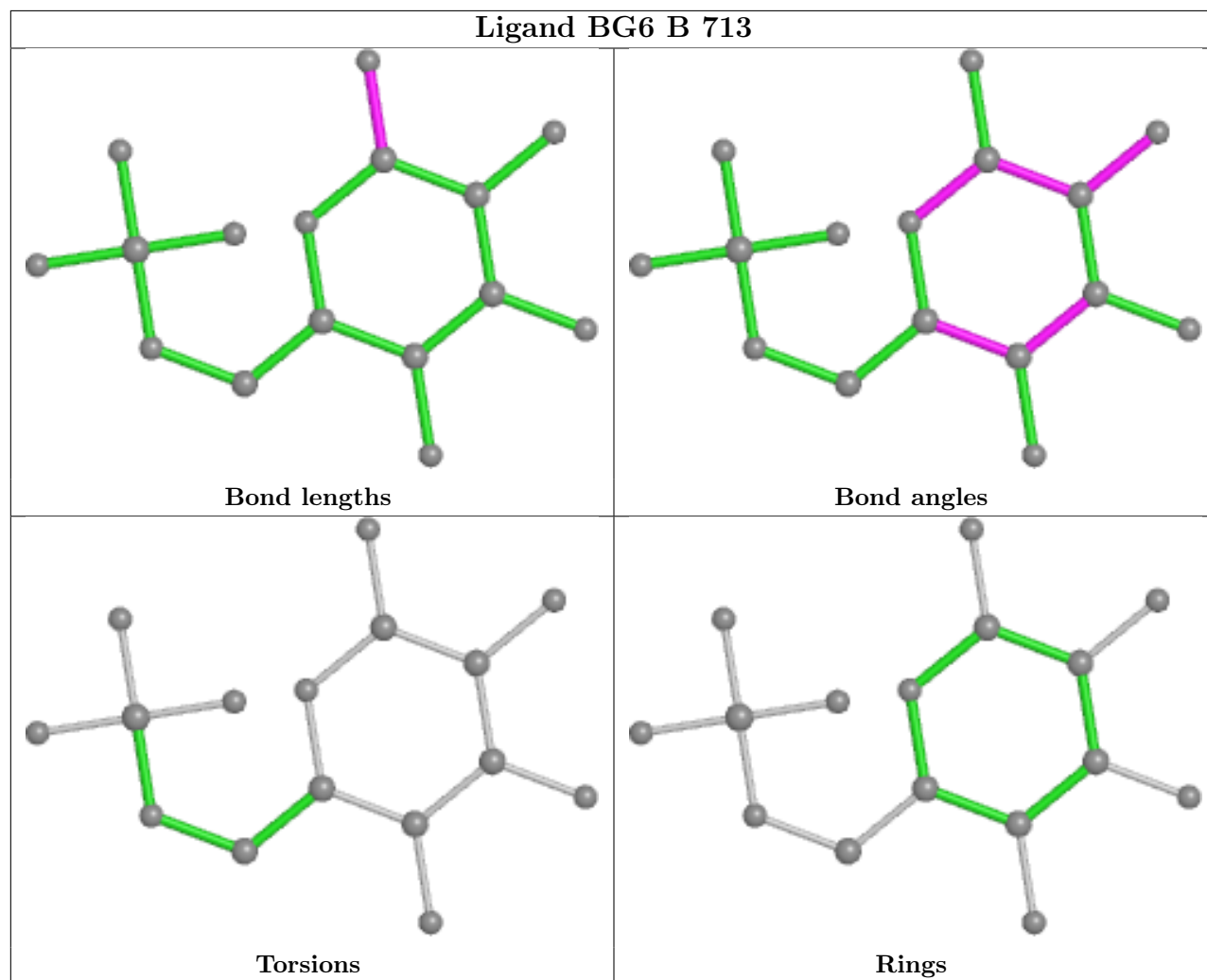
There are no ring outliers.

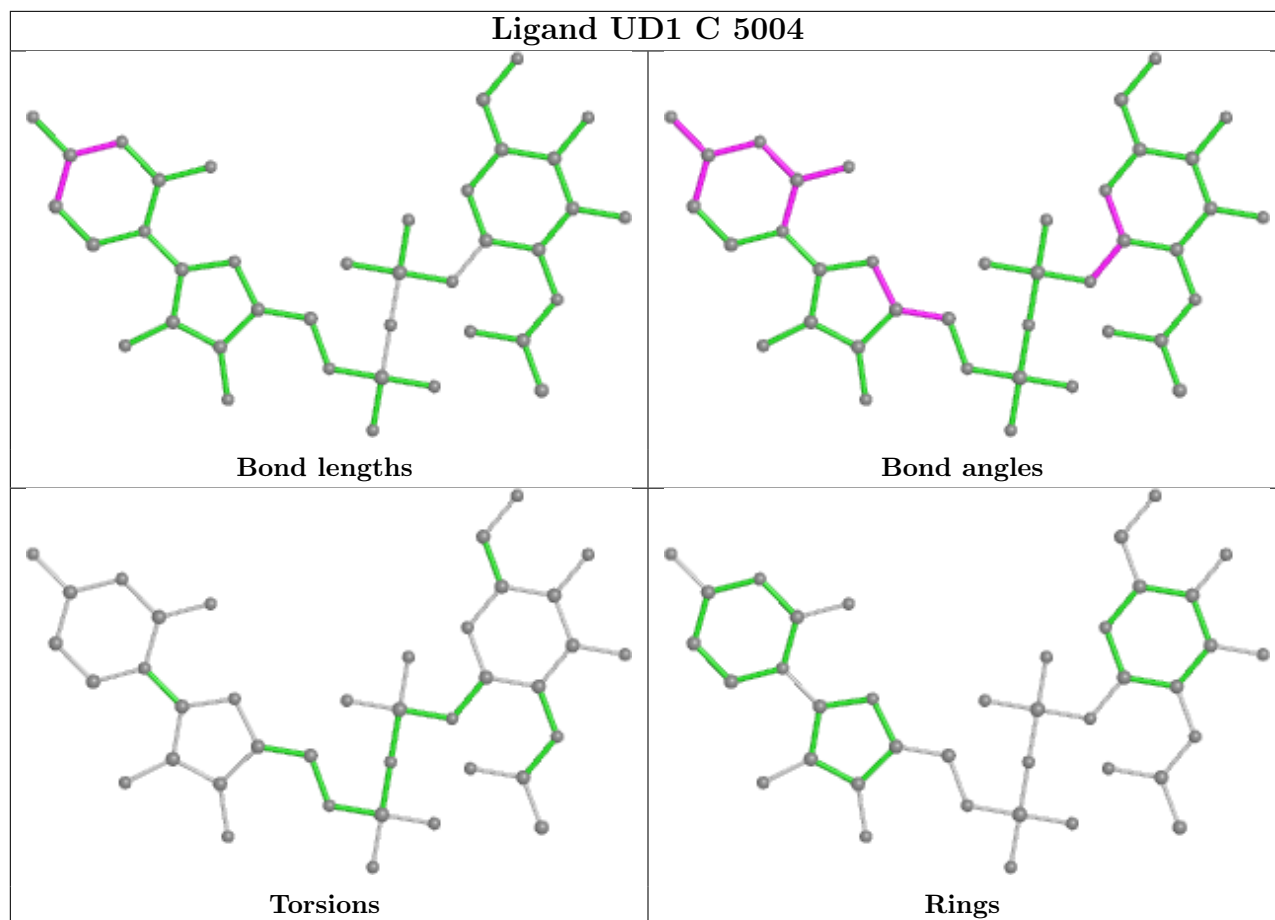
2 monomers are involved in 2 short contacts:

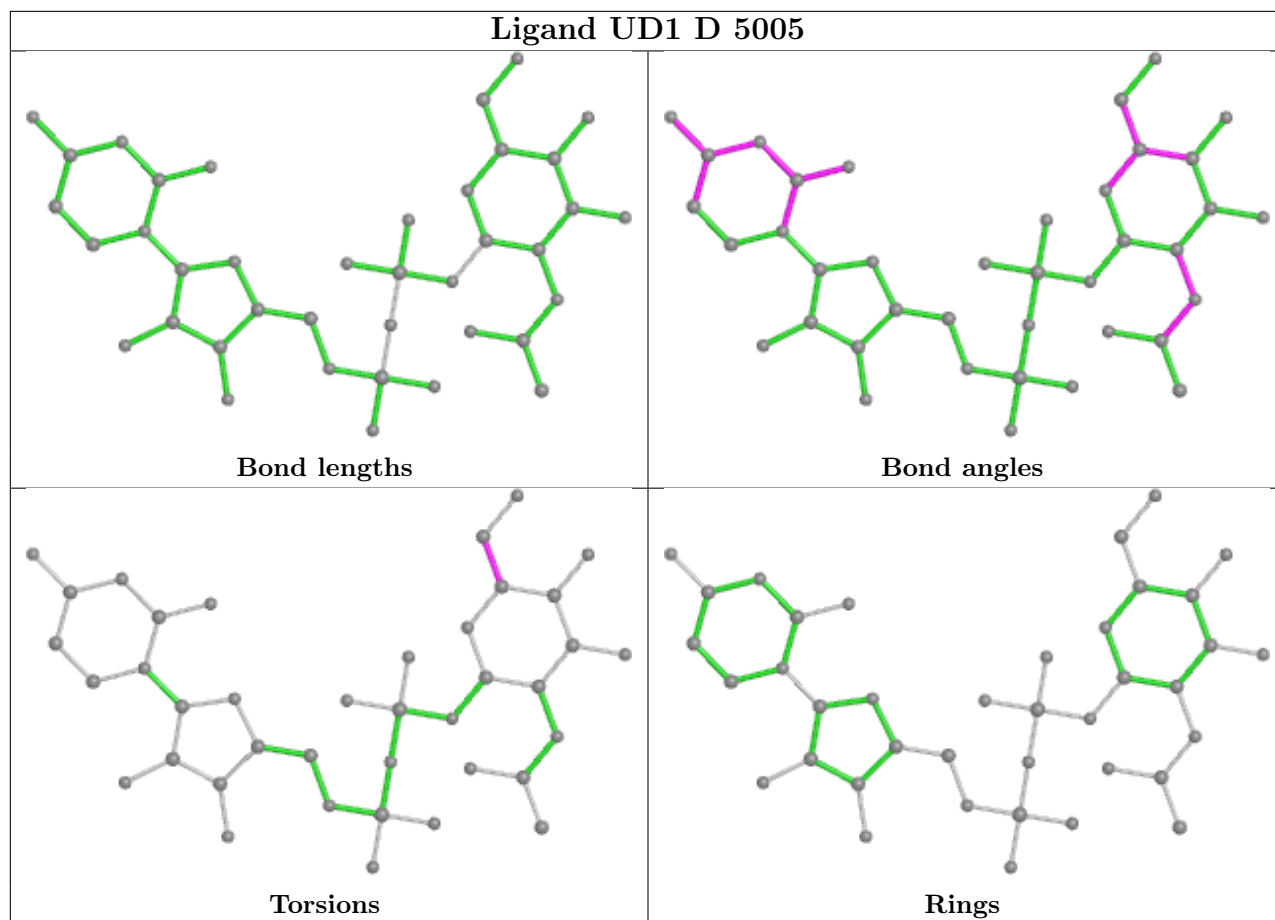
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5005	UD1	1	0
4	A	5002	UD1	1	0

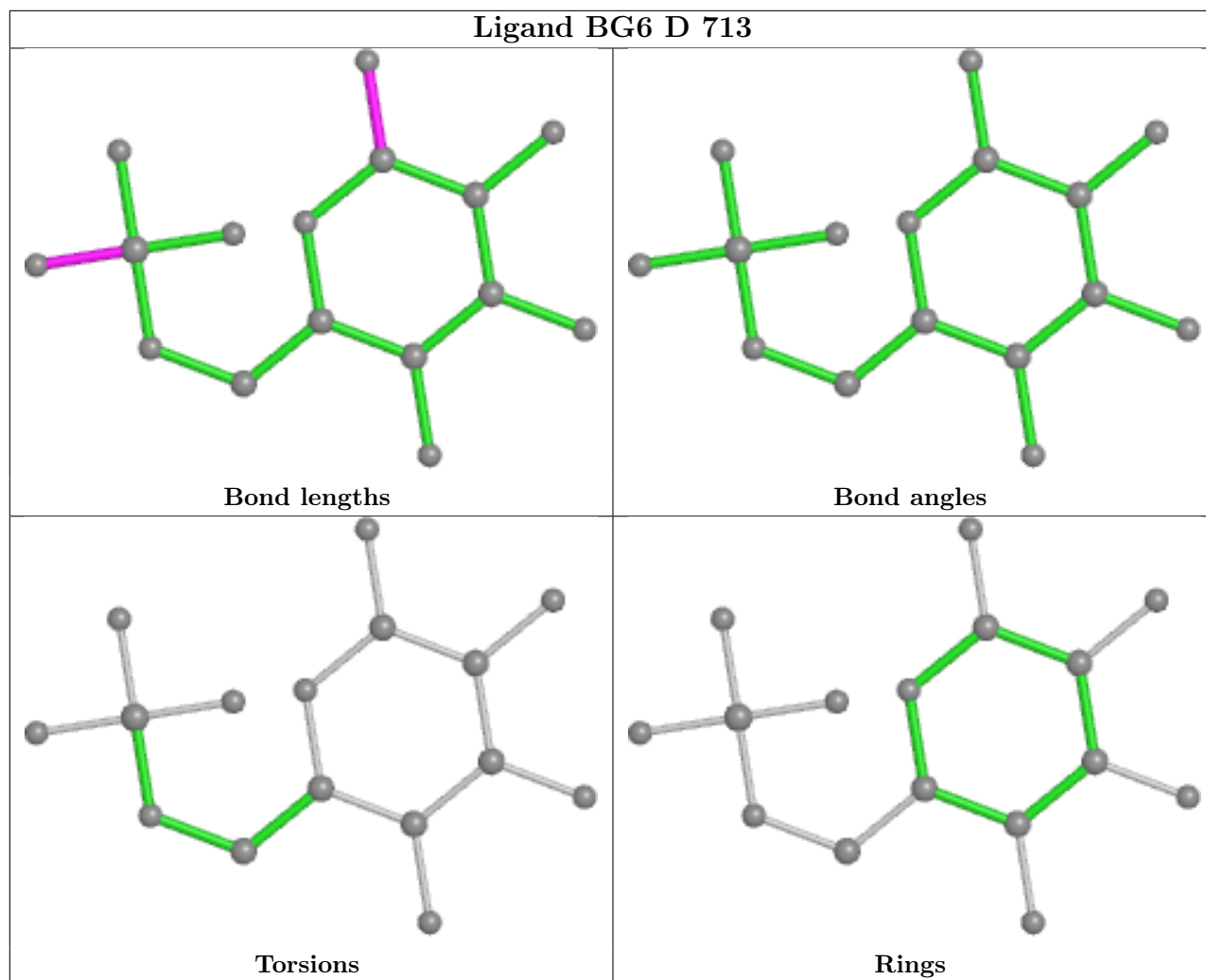
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

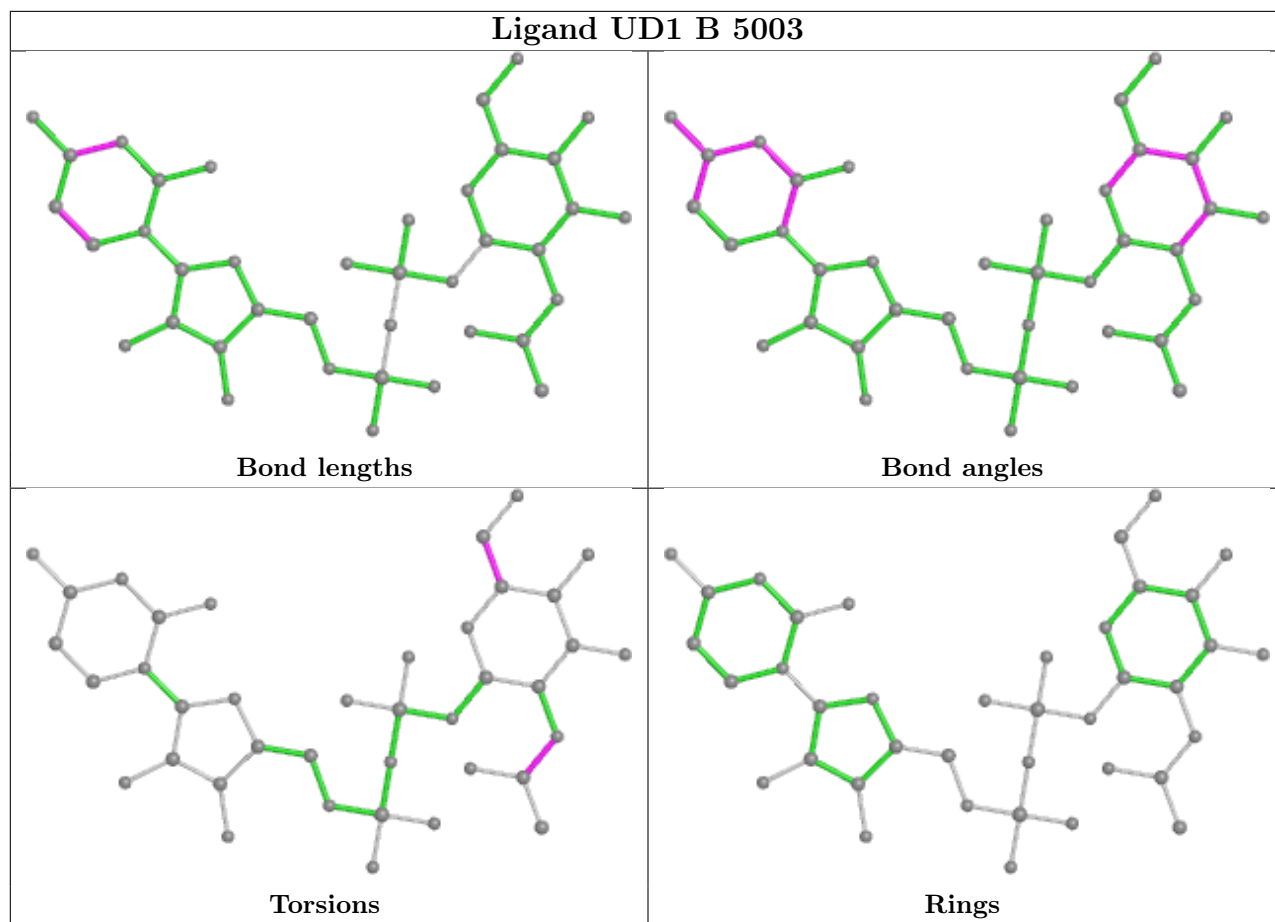
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

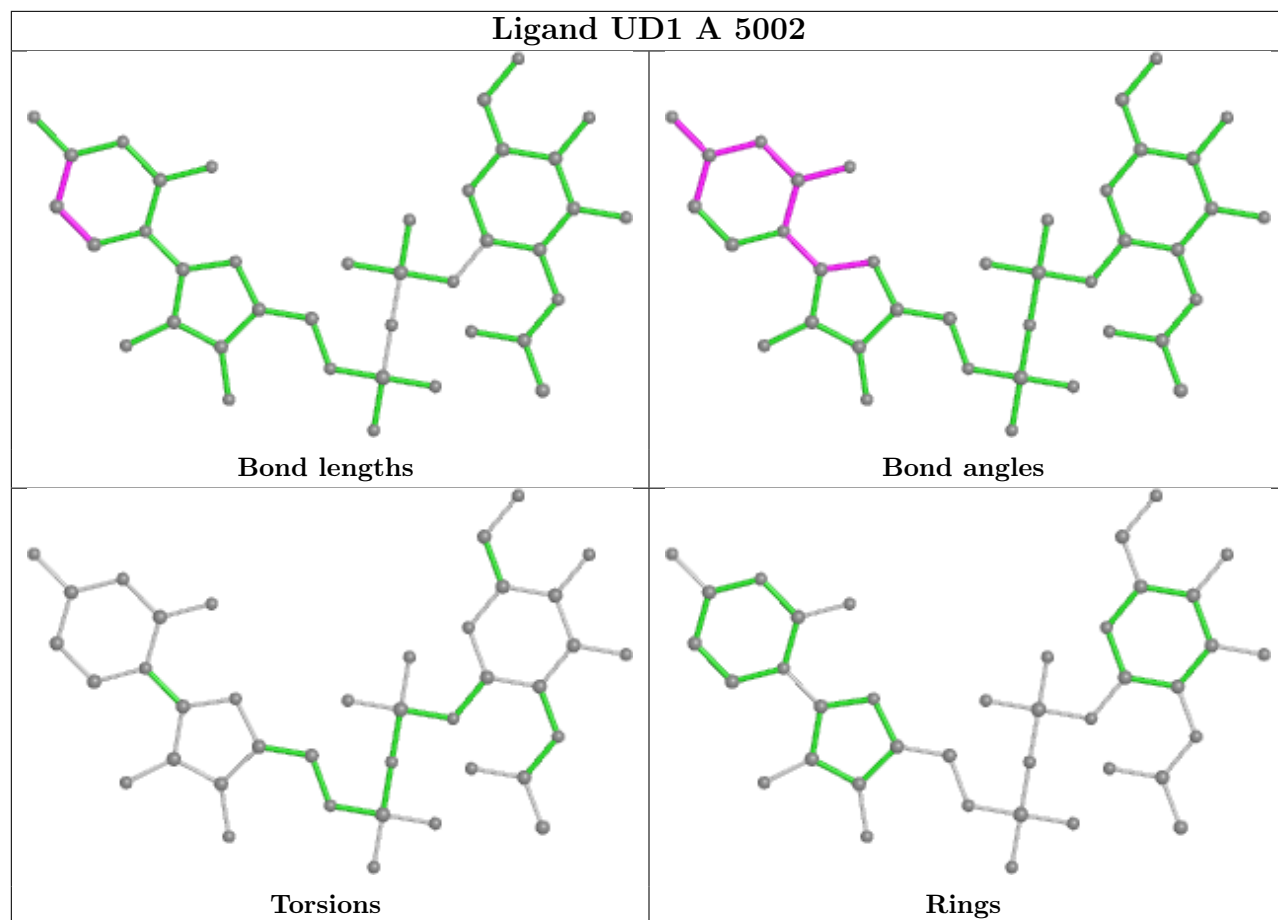


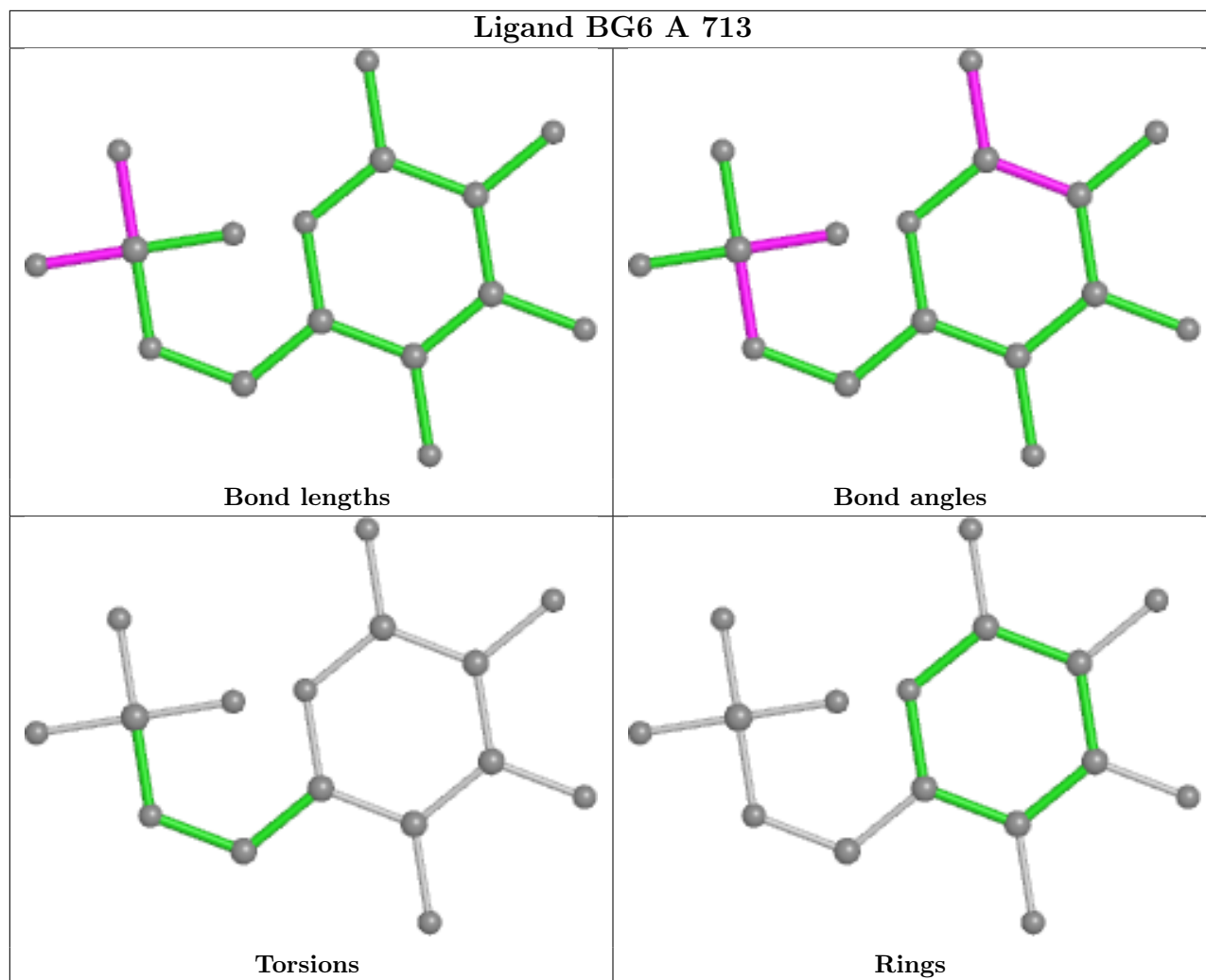


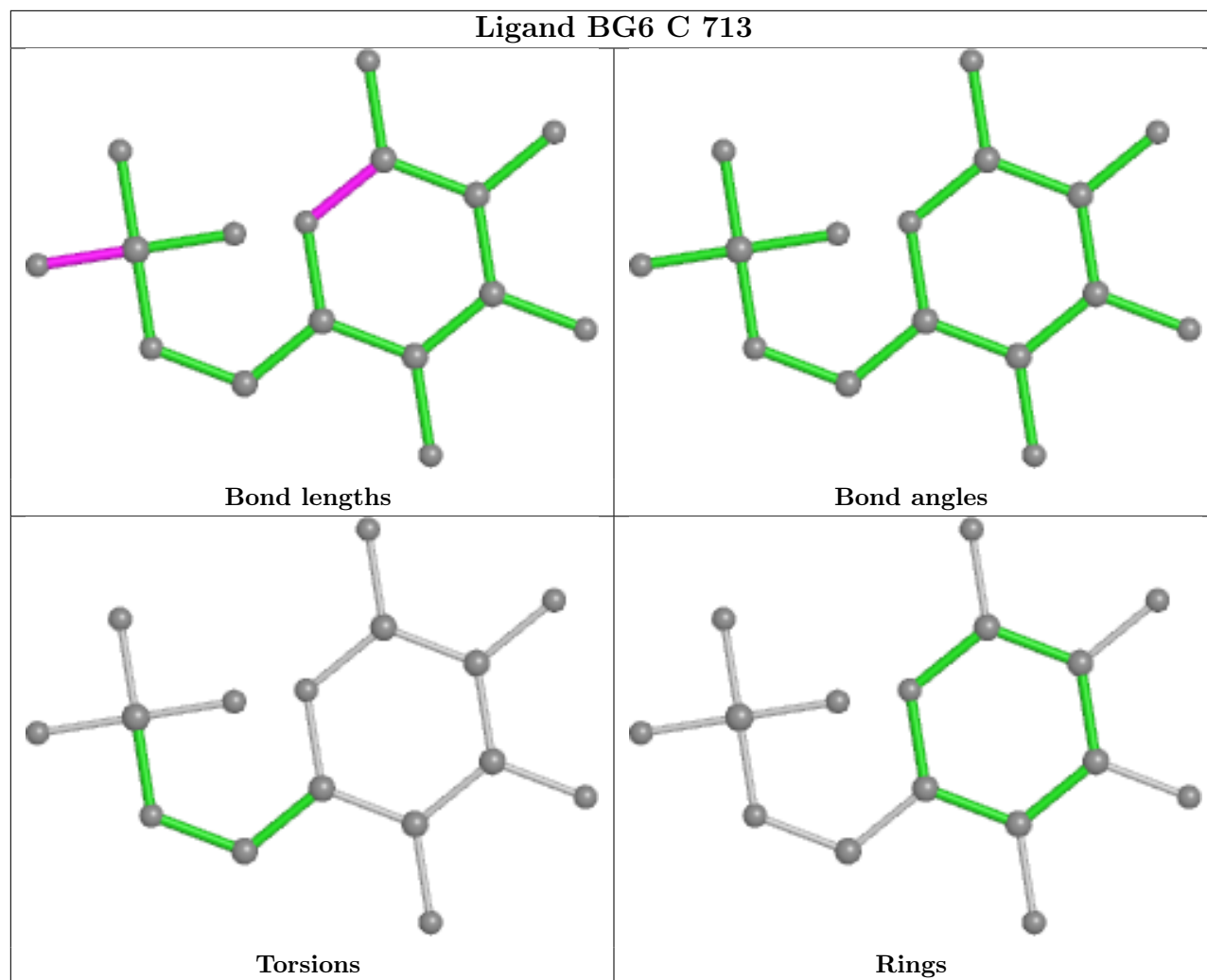












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/367 (92%)	-0.11	18 (5%) 26 21	14, 24, 41, 53	0
1	B	352/367 (95%)	-0.10	12 (3%) 45 39	15, 24, 47, 59	0
1	C	352/367 (95%)	0.03	20 (5%) 23 19	14, 25, 52, 65	0
1	D	340/367 (92%)	-0.12	12 (3%) 44 38	14, 24, 39, 49	0
All	All	1383/1468 (94%)	-0.07	62 (4%) 33 27	14, 24, 46, 65	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	659	ASN	6.5
1	B	563	SER	5.6
1	C	607	HIS	5.5
1	C	660	ASP	5.4
1	A	501	VAL	5.1
1	C	615	GLU	4.5
1	C	616	ASP	4.4
1	C	655	ALA	4.3
1	B	566	ASP	4.2
1	D	349	PRO	4.2
1	D	386	LYS	4.1
1	A	348	GLY	4.1
1	D	659	ASN	3.9
1	A	349	PRO	3.9
1	A	658	SER	3.7
1	C	662	VAL	3.6
1	B	607	HIS	3.6
1	C	349	PRO	3.5
1	D	376	GLU	3.5
1	C	606	LYS	3.5
1	A	499	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	642	ARG	3.4
1	B	594	TYR	3.4
1	C	613	VAL	3.4
1	A	353	PHE	3.4
1	C	594	TYR	3.3
1	C	611	ALA	3.3
1	D	658	SER	3.3
1	C	568	LYS	3.2
1	B	387	SER	3.1
1	B	386	LYS	3.1
1	D	387	SER	3.0
1	C	658	SER	3.0
1	A	563	SER	2.9
1	A	662	VAL	2.9
1	C	642	ARG	2.9
1	B	499	ILE	2.8
1	A	605	LEU	2.7
1	A	386	LYS	2.7
1	C	566	ASP	2.6
1	B	353	PHE	2.6
1	B	564	LEU	2.6
1	D	568	LYS	2.6
1	D	563	SER	2.5
1	A	351	LYS	2.5
1	D	353	PHE	2.4
1	C	612	LEU	2.4
1	B	606	LYS	2.4
1	C	696	GLY	2.4
1	B	376	GLU	2.3
1	D	566	ASP	2.3
1	A	387	SER	2.2
1	B	501	VAL	2.2
1	D	499	ILE	2.2
1	A	698	ASP	2.2
1	A	568	LYS	2.2
1	D	642	ARG	2.2
1	A	641	ALA	2.1
1	C	501	VAL	2.0
1	A	657	ILE	2.0
1	C	614	ASP	2.0
1	A	663	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

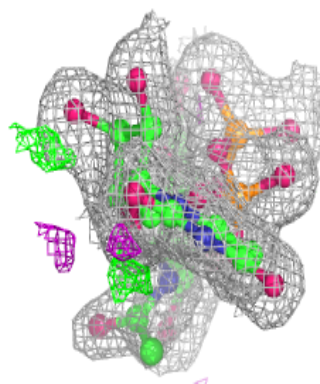
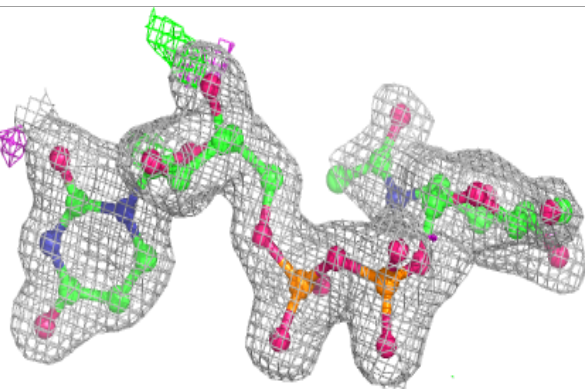
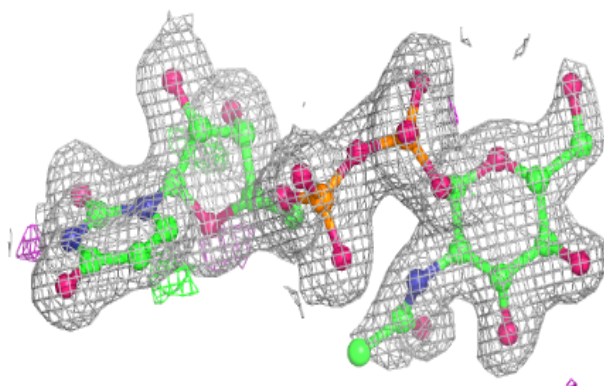
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ACT	B	714	4/4	0.89	0.10	34,35,35,35	0
5	ACT	C	714	4/4	0.92	0.13	40,40,41,41	0
4	UD1	A	5002	39/39	0.93	0.12	20,25,46,49	0
4	UD1	D	5005	39/39	0.93	0.13	21,26,47,51	0
4	UD1	B	5003	39/39	0.95	0.12	18,26,58,59	0
2	BG6	A	713	16/16	0.95	0.14	21,28,40,41	0
3	NA	A	5001	1/1	0.97	0.11	26,26,26,26	0
2	BG6	D	713	16/16	0.97	0.08	20,28,40,41	0
2	BG6	B	713	16/16	0.98	0.07	17,22,35,38	0
2	BG6	C	713	16/16	0.98	0.08	19,24,38,38	0
4	UD1	C	5004	39/39	0.98	0.07	18,21,28,33	0
3	NA	B	5002	1/1	0.98	0.04	21,21,21,21	0
3	NA	C	5003	1/1	0.98	0.04	21,21,21,21	0
3	NA	D	5004	1/1	0.98	0.06	27,27,27,27	0

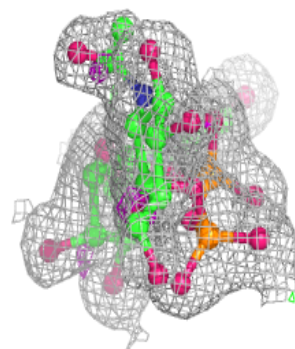
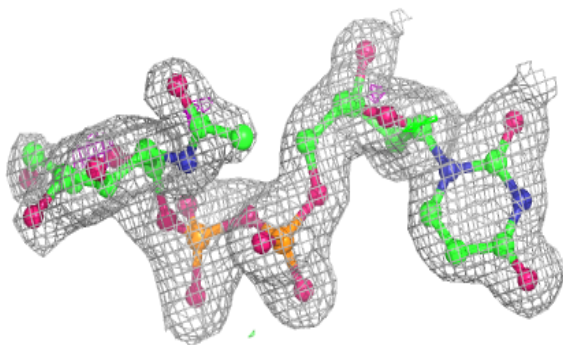
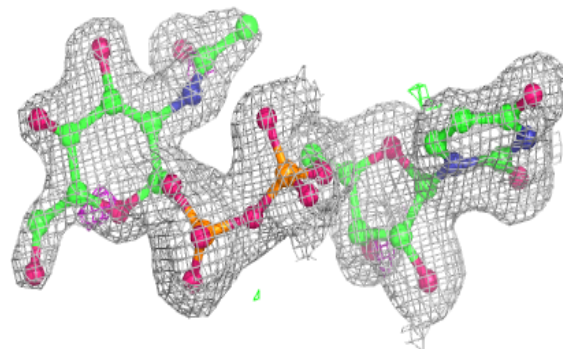
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD1 A 5002:

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

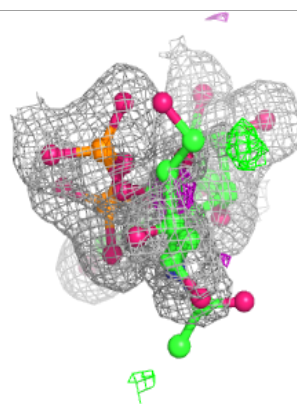
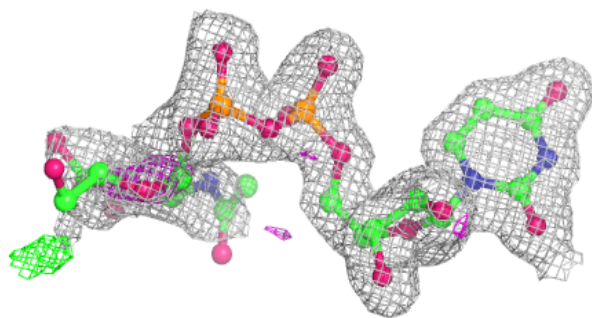
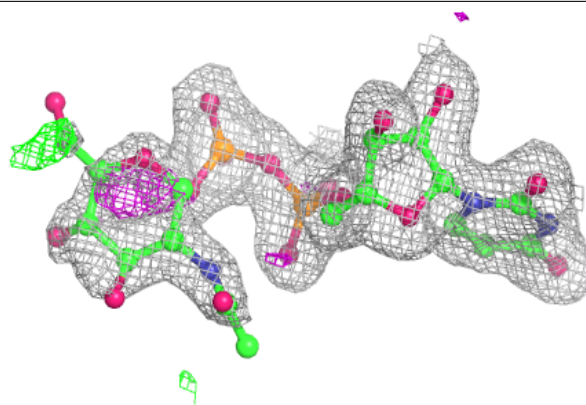
**Electron density around UD1 D 5005:**

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

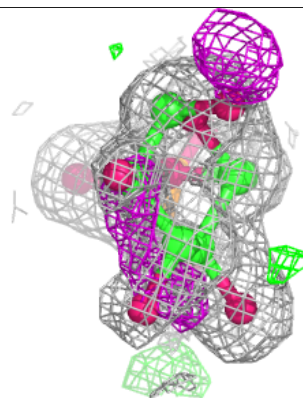
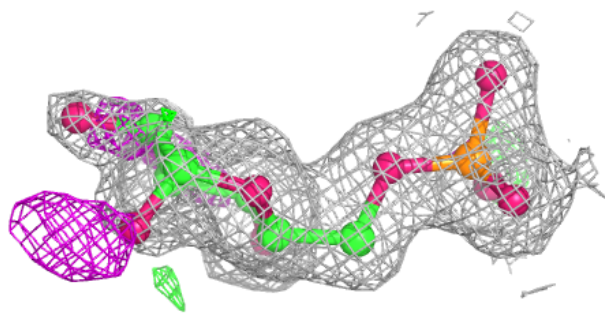
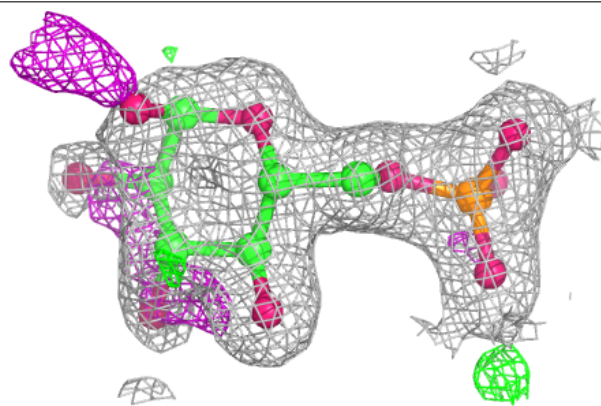


Electron density around UD1 B 5003:

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

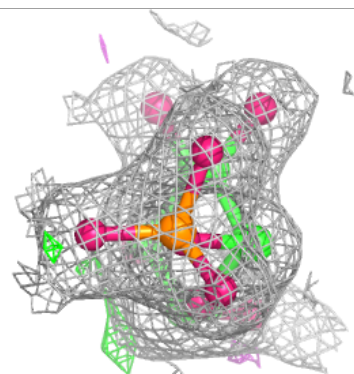
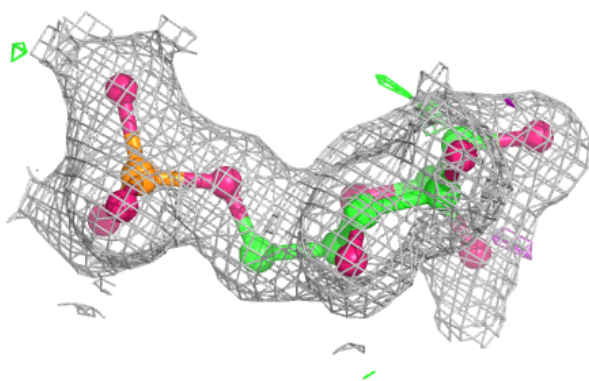
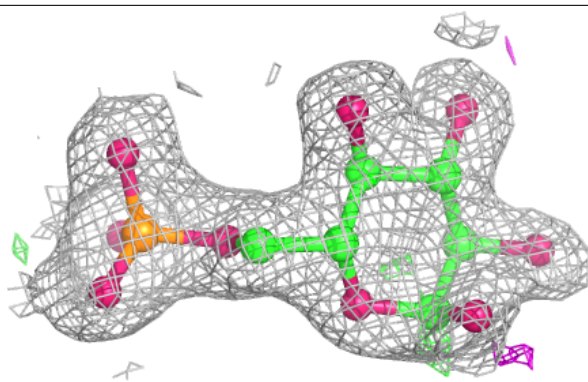
**Electron density around BG6 A 713:**

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

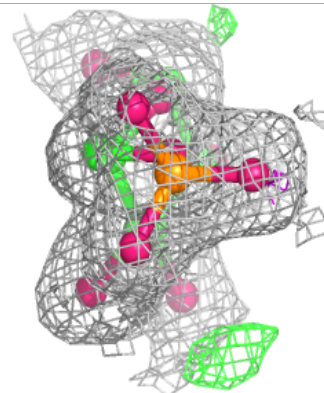
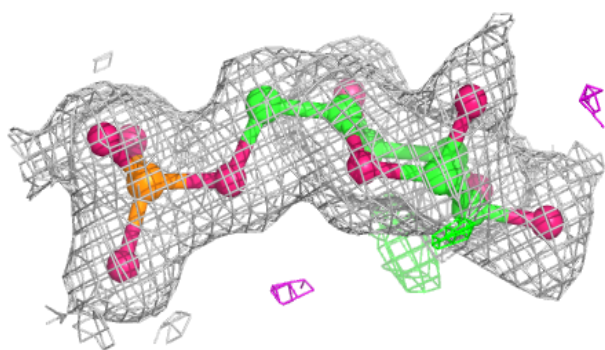
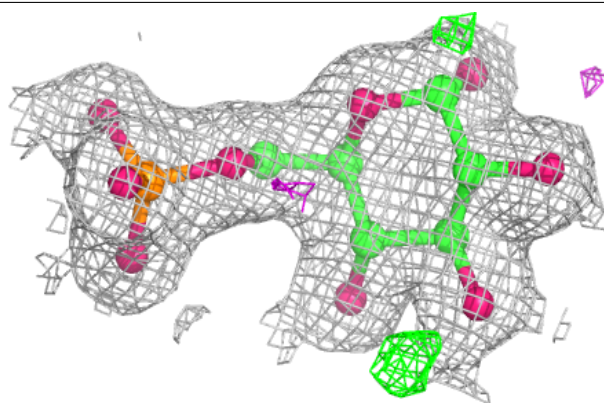


Electron density around BG6 D 713:

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

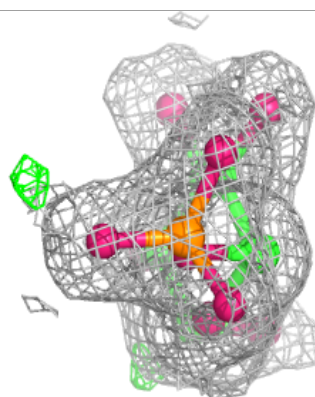
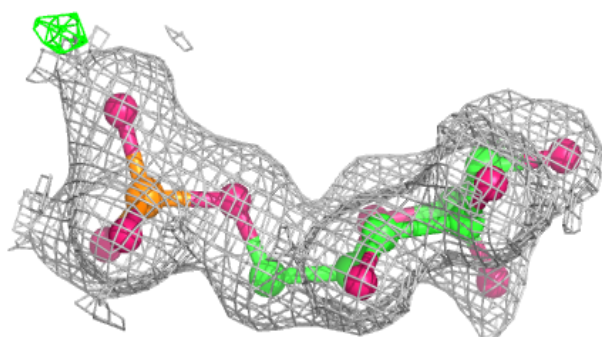
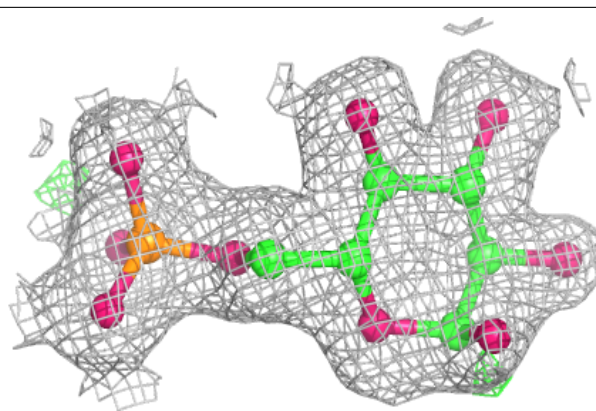
**Electron density around BG6 B 713:**

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

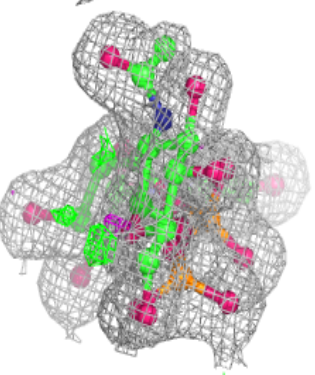
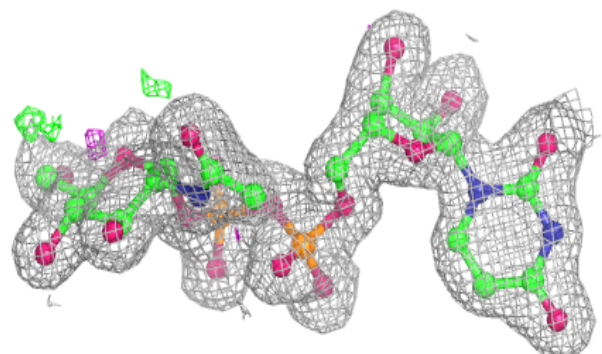
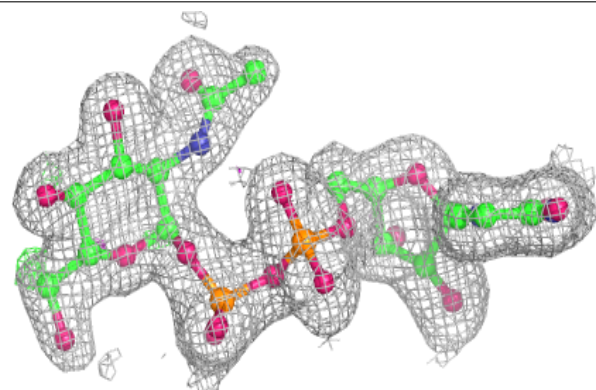


Electron density around BG6 C 713:

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

**Electron density around UD1 C 5004:**

$2mF_o-DF_c$ (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.