



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:56 pm BST

PDB ID : 4OP1  
Title : GKRP bound to AMG0556 and Sorbitol-6-Phosphate  
Authors : Jordan, S.R.; Chmait, S.  
Deposited on : 2014-02-04  
Resolution : 2.39 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 : 2.11  
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) : 2.11

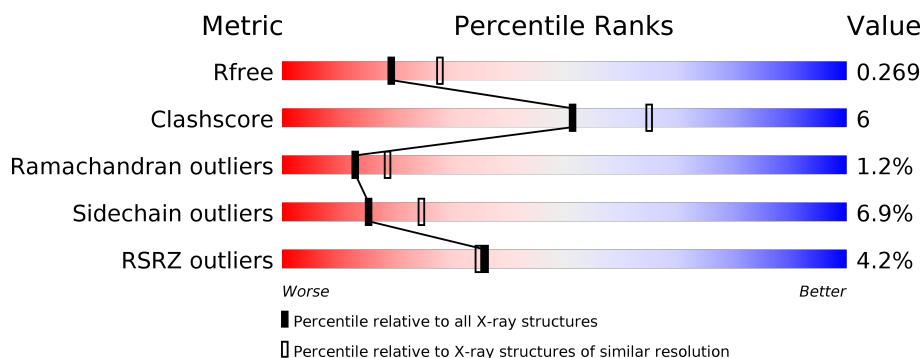
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	638	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	638	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>8%</div> </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
4	IOD	B	713	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9368 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 Glucokinase Regulatory Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4521	2882	774	841	24			
1	B	590	Total	C	N	O	S	0	0	0
			4554	2901	781	848	24			

There are 26 discrepancies between the modelled and reference sequences:

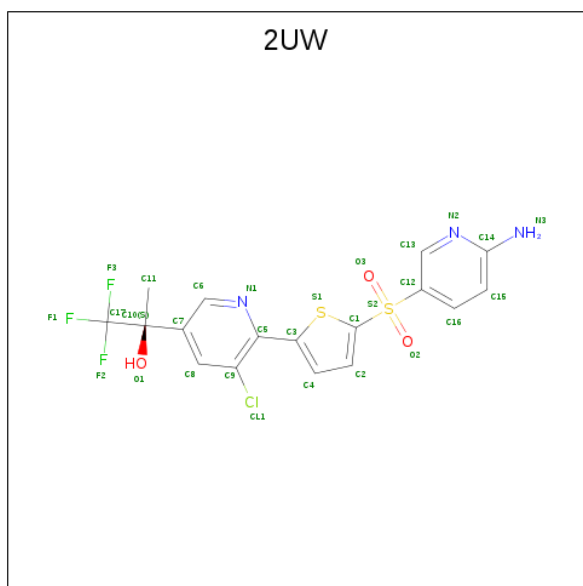
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q14397
A	-10	ALA	-	EXPRESSION TAG	UNP Q14397
A	-9	HIS	-	EXPRESSION TAG	UNP Q14397
A	-8	HIS	-	EXPRESSION TAG	UNP Q14397
A	-7	HIS	-	EXPRESSION TAG	UNP Q14397
A	-6	HIS	-	EXPRESSION TAG	UNP Q14397
A	-5	HIS	-	EXPRESSION TAG	UNP Q14397
A	-4	HIS	-	EXPRESSION TAG	UNP Q14397
A	-3	ASP	-	EXPRESSION TAG	UNP Q14397
A	-2	GLU	-	EXPRESSION TAG	UNP Q14397
A	-1	VAL	-	EXPRESSION TAG	UNP Q14397
A	0	ASP	-	EXPRESSION TAG	UNP Q14397
A	626	GLY	-	EXPRESSION TAG	UNP Q14397
B	-11	MET	-	EXPRESSION TAG	UNP Q14397
B	-10	ALA	-	EXPRESSION TAG	UNP Q14397
B	-9	HIS	-	EXPRESSION TAG	UNP Q14397
B	-8	HIS	-	EXPRESSION TAG	UNP Q14397
B	-7	HIS	-	EXPRESSION TAG	UNP Q14397
B	-6	HIS	-	EXPRESSION TAG	UNP Q14397
B	-5	HIS	-	EXPRESSION TAG	UNP Q14397
B	-4	HIS	-	EXPRESSION TAG	UNP Q14397
B	-3	ASP	-	EXPRESSION TAG	UNP Q14397
B	-2	GLU	-	EXPRESSION TAG	UNP Q14397
B	-1	VAL	-	EXPRESSION TAG	UNP Q14397
B	0	ASP	-	EXPRESSION TAG	UNP Q14397

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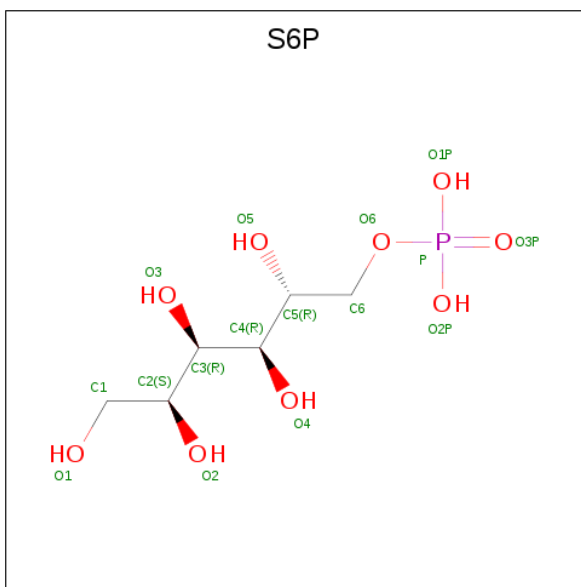
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	EXPRESSION TAG	UNP Q14397

- Molecule 2 is (2S)-2-(6-[(6-aminopyridin-3-yl)sulfonyl]thiophen-2-yl)-5-chloropyridin-3-yl)-1,1,1-trifluoropropan-2-ol (three-letter code: 2UW) (formula:  $C_{17}H_{13}ClF_3N_3O_3S_2$ ).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			29	17	1	3	3	3	2		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			29	17	1	3	3	3	2		

- Molecule 3 is D-SORBITOL-6-PHOSPHATE (three-letter code: S6P) (formula:  $C_6H_{15}O_9P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	15	Total	I	0	0
			15	15		
4	A	13	Total	I	0	0
			13	13		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

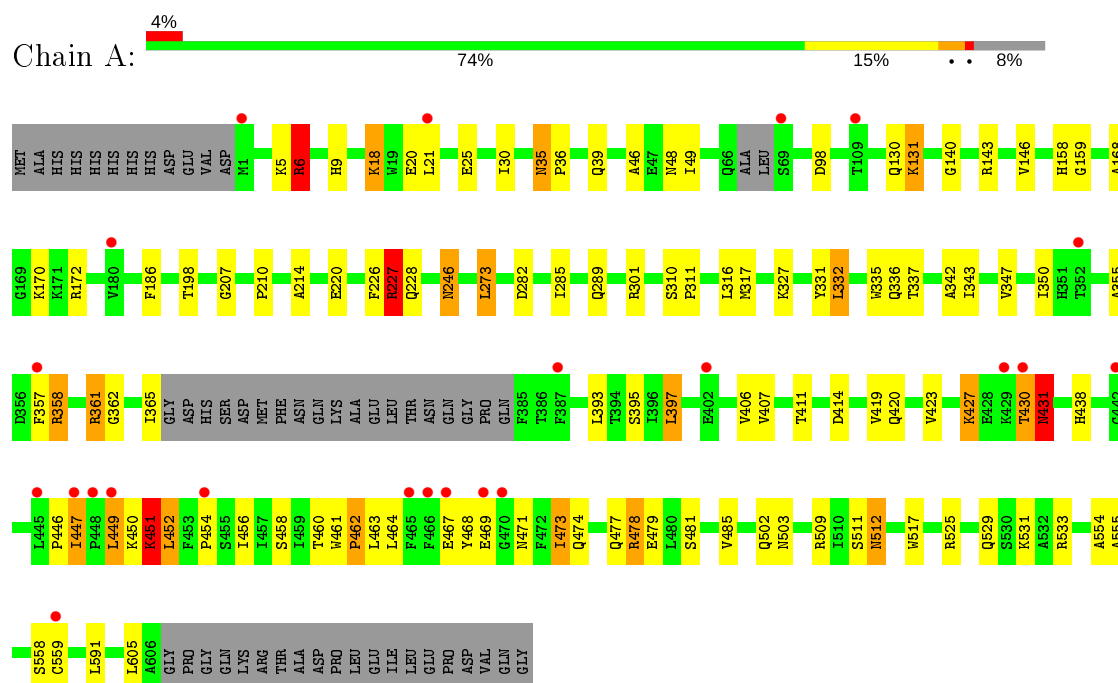
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	62	Total 62	O 62	0	0
7	B	97	Total 97	O 97	0	0



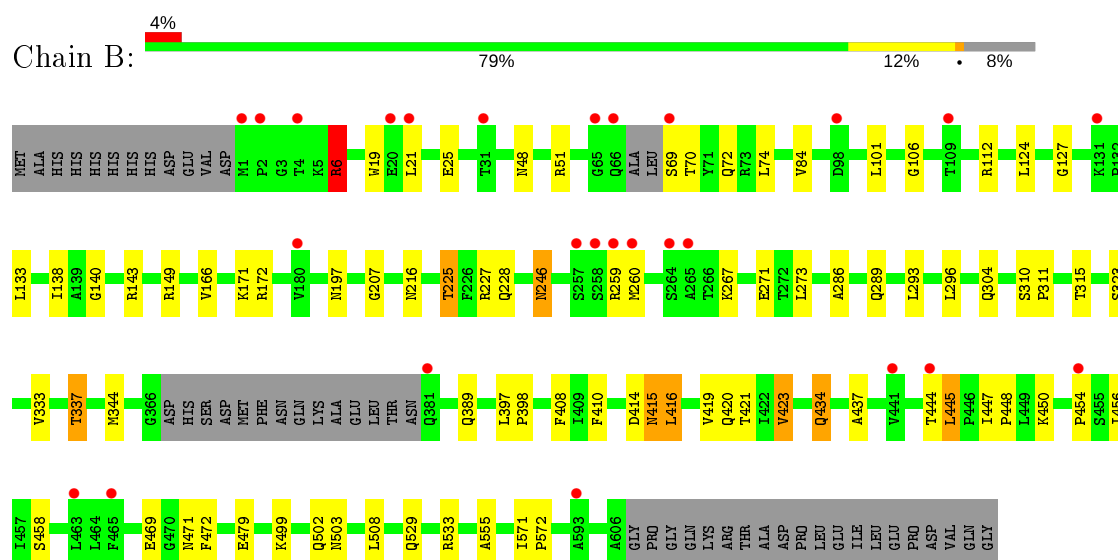
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Glucokinase Regulatory Protein



#### • Molecule 1: Glucokinase Regulatory Protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.18Å 149.18Å 132.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.39 37.92 – 2.39	Depositor EDS
% Data completeness (in resolution range)	86.9 (50.00-2.39) 86.9 (37.92-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.208 , 0.268 0.214 , 0.269	Depositor DCC
$R_{free}$ test set	2904 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IOD, SO4, S6P, 2UW

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	0.71	0/4603	0.86	8/6228 (0.1%)
1	B	0.74	0/4637	0.88	5/6274 (0.1%)
All	All	0.72	0/9240	0.87	13/12502 (0.1%)

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

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	B	259	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	478	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	227	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	227	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	6	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	6	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	361	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	301	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	6	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	358	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	273	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	273	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	LYS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4618	60	0
1	B	4554	0	4647	41	0
2	A	29	0	13	1	0
2	B	29	0	12	1	0
3	A	16	0	13	1	0
3	B	16	0	13	0	0
4	A	13	0	0	3	0
4	B	15	0	0	7	0
5	B	6	0	8	0	0
6	B	10	0	0	0	0
7	A	62	0	0	2	0
7	B	97	0	0	0	0
All	All	9368	0	9324	104	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 6.

All (104) 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:25:GLU:OE2	4:B:711:IOD:I	2.64	0.86
1:A:220:GLU:OE2	1:A:558:SER:OG	2.00	0.79
2:A:701:2UW:CL1	2:A:701:2UW:S1	2.77	0.79
1:B:502:GLN:NE2	4:B:717:IOD:I	2.86	0.78
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.16	0.77
1:A:140:GLY:H	1:A:158:HIS:HE1	1.34	0.76
1:B:216:ASN:OD1	1:B:225:THR:HG21	1.90	0.72
1:A:430:THR:O	1:A:431:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:O	1:A:423:VAL:HG23	1.97	0.64
1:B:447:ILE:HG22	1:B:450:LYS:HE3	1.81	0.62
1:A:512:ASN:C	1:A:512:ASN:HD22	2.02	0.62
1:B:337:THR:HG21	1:B:479:GLU:OE1	2.00	0.61
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.66	0.61
1:A:447:ILE:O	1:A:450:LYS:HB2	2.01	0.60
1:A:36:PRO:O	1:A:39:GLN:HG2	2.01	0.60
1:A:130:GLN:O	1:A:131:LYS:HB2	2.02	0.60
1:B:469:GLU:HG2	4:B:716:IOD:I	2.72	0.59
1:B:389:GLN:OE1	1:B:421:THR:HG21	2.03	0.59
1:B:420:GLN:HA	1:B:423:VAL:HG13	1.85	0.59
1:A:332:LEU:HB3	1:A:342:ALA:HB1	1.84	0.58
1:A:25:GLU:OE2	1:A:525:ARG:NH2	2.34	0.57
1:A:474:GLN:O	1:A:478:ARG:HD3	2.04	0.57
1:A:146:VAL:O	1:A:146:VAL:CG1	2.53	0.57
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.53	0.56
1:A:140:GLY:H	1:A:158:HIS:CE1	2.20	0.56
1:A:6:ARG:HD2	1:A:554:ALA:O	2.04	0.55
1:A:446:PRO:O	1:A:450:LYS:HB2	2.07	0.55
1:A:146:VAL:O	1:A:347:VAL:HG21	2.07	0.54
1:B:445:LEU:HG	4:B:713:IOD:I	2.77	0.54
2:B:701:2UW:CL1	2:B:701:2UW:S1	3.02	0.54
1:B:267:LYS:NZ	1:B:271:GLU:OE1	2.41	0.54
1:B:48:ASN:HD22	1:B:51:ARG:HH21	1.54	0.54
1:A:343:ILE:HA	1:A:362:GLY:HA3	1.90	0.53
1:B:414:ASP:O	1:B:416:LEU:HD13	2.08	0.53
1:A:49:ILE:HD12	1:A:317:MET:HE1	1.90	0.53
1:A:6:ARG:HD3	1:A:555:ALA:O	2.09	0.52
4:A:712:IOD:I	4:B:714:IOD:I	3.67	0.52
1:B:112:ARG:HD3	1:B:344:MET:HG2	1.91	0.52
1:A:35:ASN:HD22	1:A:35:ASN:C	2.13	0.52
1:A:146:VAL:HG12	1:A:146:VAL:O	2.10	0.51
1:A:531:LYS:NZ	4:A:711:IOD:I	3.11	0.51
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.59	0.50
1:B:207:GLY:O	1:B:246:ASN:HA	2.11	0.50
1:A:350:ILE:HA	1:A:355:ALA:O	2.12	0.50
1:A:331:TYR:HB2	1:A:406:VAL:HG13	1.94	0.49
1:A:48:ASN:ND2	7:A:815:HOH:O	2.46	0.49
1:B:48:ASN:ND2	1:B:51:ARG:HH21	2.09	0.49
1:A:393:LEU:O	1:A:397:LEU:HB3	2.12	0.49
1:B:140:GLY:O	1:B:149:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:H	1:A:452:LEU:HD12	1.77	0.49
1:A:450:LYS:C	1:A:452:LEU:H	2.17	0.48
1:A:365:ILE:HD12	1:A:365:ILE:N	2.28	0.48
1:A:411:THR:HG22	1:A:438:HIS:HB2	1.95	0.47
1:A:140:GLY:N	1:A:158:HIS:HE1	2.09	0.47
1:A:46:ALA:HA	1:A:317:MET:HE1	1.97	0.47
1:A:337:THR:HG21	1:A:479:GLU:OE2	2.15	0.46
3:A:702:S6P:O1P	7:A:847:HOH:O	2.21	0.46
1:A:18:LYS:HD2	1:A:18:LYS:O	2.16	0.46
1:A:246:ASN:N	1:A:246:ASN:HD22	2.13	0.46
1:B:419:VAL:O	1:B:423:VAL:HG12	2.16	0.46
1:B:529:GLN:HE22	1:B:533:ARG:HH21	1.63	0.46
1:B:508:LEU:C	1:B:508:LEU:HD12	2.36	0.46
1:A:529:GLN:NE2	1:A:533:ARG:HE	2.14	0.46
1:A:214:ALA:O	1:A:227:ARG:HD3	2.16	0.46
1:A:529:GLN:HE22	1:A:533:ARG:HH21	1.64	0.45
1:B:333:VAL:O	1:B:408:PHE:HA	2.16	0.45
1:A:130:GLN:O	1:A:131:LYS:CB	2.61	0.45
1:A:46:ALA:HA	1:A:317:MET:CE	2.46	0.45
1:A:447:ILE:HG22	1:A:449:LEU:HB3	1.99	0.45
1:B:458:SER:HB3	4:B:713:IOD:I	2.87	0.45
1:A:481:SER:O	1:A:485:VAL:HG23	2.17	0.44
1:A:332:LEU:HD12	1:A:407:VAL:HB	1.97	0.44
1:A:461:TRP:O	1:A:462:PRO:O	2.36	0.44
1:B:6:ARG:HD3	1:B:555:ALA:O	2.18	0.44
1:B:315:THR:HG22	1:B:434:GLN:NE2	2.33	0.44
1:A:207:GLY:O	1:A:246:ASN:HA	2.18	0.43
1:A:468:TYR:HB2	4:A:703:IOD:I	2.88	0.43
1:B:410:PHE:O	1:B:437:ALA:HA	2.19	0.43
1:B:571:ILE:HB	1:B:572:PRO:HD3	2.00	0.43
1:B:124:LEU:HD12	1:B:472:PHE:CD2	2.54	0.43
1:B:310:SER:N	1:B:311:PRO:CD	2.81	0.43
1:B:19:TRP:O	1:B:25:GLU:HG3	2.18	0.43
1:B:106:GLY:O	1:B:138:ILE:HA	2.19	0.42
1:A:30:ILE:HD12	1:A:210:PRO:HD3	2.01	0.42
1:A:427:LYS:HE2	1:A:427:LYS:O	2.19	0.42
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.80	0.42
1:B:437:ALA:HB3	1:B:456:ILE:HD11	2.00	0.42
1:B:529:GLN:NE2	1:B:533:ARG:HE	2.17	0.42
1:A:473:ILE:O	1:A:477:GLN:HG3	2.20	0.42
1:A:310:SER:HB2	1:A:311:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.84	0.41
1:B:458:SER:CB	4:B:713:IOD:I	3.38	0.41
1:B:293:LEU:HA	1:B:293:LEU:HD12	1.93	0.41
1:B:74:LEU:HD21	1:B:296:LEU:HD22	2.03	0.41
1:A:473:ILE:HD13	1:A:473:ILE:O	2.21	0.41
1:A:509:ARG:HG2	1:A:511:SER:OG	2.20	0.41
1:A:159:GLY:HA2	1:A:186:PHE:CE1	2.56	0.41
1:B:101:LEU:HD12	1:B:133:LEU:O	2.20	0.41
1:A:9:HIS:HE1	1:A:517:TRP:CH2	2.39	0.41
1:A:335:TRP:CZ2	1:A:419:VAL:HG22	2.56	0.40
1:A:591:LEU:HA	1:A:591:LEU:HD12	1.85	0.40
1:B:246:ASN:HD22	1:B:246:ASN:N	2.18	0.40
1:B:397:LEU:N	1:B:398:PRO:CD	2.85	0.40
1:B:447:ILE:N	1:B:448:PRO:HD2	2.37	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	579/638 (91%)	539 (93%)	30 (5%)	10 (2%)	9	11
1	B	584/638 (92%)	561 (96%)	19 (3%)	4 (1%)	22	32
All	All	1163/1276 (91%)	1100 (95%)	49 (4%)	14 (1%)	13	19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	LYS
1	A	456	ILE
1	B	415	ASN
1	A	431	ASN

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Mol	Chain	Res	Type
1	A	454	PRO
1	A	462	PRO
1	B	127	GLY
1	A	131	LYS
1	A	469	GLU
1	A	168	ALA
1	A	447	ILE
1	B	260	MET
1	A	502	GLN
1	B	454	PRO

### 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	498/542 (92%)	454 (91%)	44 (9%)	10	15
1	B	501/542 (92%)	476 (95%)	25 (5%)	24	40
All	All	999/1084 (92%)	930 (93%)	69 (7%)	15	25

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	ARG
1	A	18	LYS
1	A	20	GLU
1	A	21	LEU
1	A	35	ASN
1	A	98	ASP
1	A	143	ARG
1	A	170	LYS
1	A	172	ARG
1	A	198	THR
1	A	226	PHE
1	A	227	ARG

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Mol	Chain	Res	Type
1	A	246	ASN
1	A	273	LEU
1	A	282	ASP
1	A	285	ILE
1	A	289	GLN
1	A	316	LEU
1	A	327	LYS
1	A	332	LEU
1	A	357	PHE
1	A	358	ARG
1	A	361	ARG
1	A	395	SER
1	A	397	LEU
1	A	420	GLN
1	A	427	LYS
1	A	430	THR
1	A	431	ASN
1	A	449	LEU
1	A	451	LYS
1	A	452	LEU
1	A	458	SER
1	A	460	THR
1	A	463	LEU
1	A	464	LEU
1	A	467	GLU
1	A	471	ASN
1	A	473	ILE
1	A	503	ASN
1	A	512	ASN
1	A	559	CYS
1	A	605	LEU
1	B	6	ARG
1	B	21	LEU
1	B	69	SER
1	B	70	THR
1	B	72	GLN
1	B	84	VAL
1	B	143	ARG
1	B	166	VAL
1	B	171	LYS
1	B	197	ASN
1	B	225	THR

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Mol	Chain	Res	Type
1	B	227	ARG
1	B	246	ASN
1	B	304	GLN
1	B	323	SER
1	B	337	THR
1	B	415	ASN
1	B	416	LEU
1	B	423	VAL
1	B	434	GLN
1	B	444	THR
1	B	445	LEU
1	B	471	ASN
1	B	499	LYS
1	B	503	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	35	ASN
1	A	48	ASN
1	A	91	GLN
1	A	123	GLN
1	A	130	GLN
1	A	158	HIS
1	A	190	GLN
1	A	196	ASN
1	A	246	ASN
1	A	289	GLN
1	A	309	GLN
1	A	329	HIS
1	A	420	GLN
1	A	471	ASN
1	A	477	GLN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN
1	B	39	GLN
1	B	48	ASN
1	B	55	GLN
1	B	197	ASN
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	246	ASN
1	B	289	GLN
1	B	304	GLN
1	B	309	GLN
1	B	384	GLN
1	B	415	ASN
1	B	425	GLN
1	B	434	GLN
1	B	471	ASN
1	B	503	ASN
1	B	529	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 28 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	S6P	B	702	-	15,15,15	1.46	1 (6%)	21,21,21	0.85	0
6	SO4	B	720	-	4,4,4	0.15	0	6,6,6	0.30	0
5	GOL	B	718	-	5,5,5	0.60	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2UW	B	701	-	28,31,31	2.51	7 (25%)	29,49,49	2.30	11 (37%)
6	SO4	B	719	-	4,4,4	0.48	0	6,6,6	0.34	0
3	S6P	A	702	-	15,15,15	1.58	4 (26%)	21,21,21	1.12	2 (9%)
2	2UW	A	701	-	28,31,31	1.70	4 (14%)	29,49,49	1.90	8 (27%)

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	2UW	A	701	-	-	4/21/31/31	0/3/3/3
3	S6P	A	702	-	-	1/20/20/20	-
5	GOL	B	718	-	-	2/4/4/4	-
3	S6P	B	702	-	-	0/20/20/20	-
2	2UW	B	701	-	-	13/21/31/31	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2UW	C17-C10	-6.76	1.44	1.53
2	B	701	2UW	C1-S2	-6.16	1.66	1.76
2	B	701	2UW	C1-S1	-5.69	1.62	1.72
2	A	701	2UW	C1-S2	-5.68	1.67	1.76
2	B	701	2UW	O1-C10	-4.48	1.36	1.43
3	B	702	S6P	P-O3P	4.42	1.64	1.50
2	A	701	2UW	C5-C3	-3.90	1.40	1.49
2	B	701	2UW	F2-C17	3.81	1.46	1.33
3	A	702	S6P	P-O3P	3.54	1.62	1.50
2	A	701	2UW	C17-C10	-3.33	1.49	1.53
3	A	702	S6P	P-O2P	2.70	1.65	1.54
2	B	701	2UW	C5-C3	-2.57	1.43	1.49
2	B	701	2UW	O3-S2	2.17	1.48	1.44
3	A	702	S6P	C6-C5	2.03	1.54	1.51
3	A	702	S6P	P-O1P	-2.01	1.47	1.54
2	A	701	2UW	O1-C10	-2.01	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2UW	F3-C17-F2	6.59	127.67	107.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2UW	O3-S2-C12	-6.57	100.57	107.97
2	B	701	2UW	C8-C7-C10	-3.80	115.73	120.43
2	B	701	2UW	F1-C17-F2	3.57	118.44	107.53
2	B	701	2UW	O3-S2-C1	3.50	113.79	107.96
2	B	701	2UW	C3-C5-N1	3.31	120.06	114.61
2	A	701	2UW	C8-C9-C5	-3.27	119.03	122.00
2	A	701	2UW	O3-S2-C1	3.21	113.31	107.96
2	B	701	2UW	O3-S2-O2	-3.05	113.41	119.23
2	B	701	2UW	O1-C10-C7	3.03	114.11	108.01
2	B	701	2UW	C6-N1-C5	2.86	123.12	117.95
2	B	701	2UW	F1-C17-F3	-2.70	99.28	107.53
2	B	701	2UW	C7-C6-N1	-2.66	120.81	123.34
2	B	701	2UW	C8-C9-CL1	-2.47	114.50	118.49
2	A	701	2UW	C15-C14-N3	-2.32	117.11	121.14
3	A	702	S6P	O1-C1-C2	-2.32	106.01	111.07
2	A	701	2UW	C1-S2-C12	2.26	108.47	105.28
2	A	701	2UW	O1-C10-C11	2.14	113.72	108.47
3	A	702	S6P	O6-P-O3P	2.05	112.23	106.47
2	A	701	2UW	F1-C17-F2	2.04	113.78	107.53
2	A	701	2UW	C7-C6-N1	-2.04	121.39	123.34

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	2UW	C17-C10-C7-C8
2	B	701	2UW	O1-C10-C7-C8
2	B	701	2UW	C11-C10-C7-C6
2	B	701	2UW	C7-C10-C17-F1
2	B	701	2UW	C11-C10-C17-F2
2	B	701	2UW	C11-C10-C17-F1
2	B	701	2UW	O1-C10-C17-F2
2	B	701	2UW	O1-C10-C17-F3
2	B	701	2UW	O1-C10-C17-F1
5	B	718	GOL	O1-C1-C2-C3
5	B	718	GOL	O1-C1-C2-O2
2	B	701	2UW	C17-C10-C7-C6
2	B	701	2UW	O1-C10-C7-C6
2	B	701	2UW	C7-C10-C17-F2
2	A	701	2UW	C17-C10-C7-C6
2	A	701	2UW	C17-C10-C7-C8
2	B	701	2UW	C11-C10-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	701	2UW	C11-C10-C7-C6
2	A	701	2UW	C11-C10-C7-C8
3	A	702	S6P	C1-C2-C3-O3

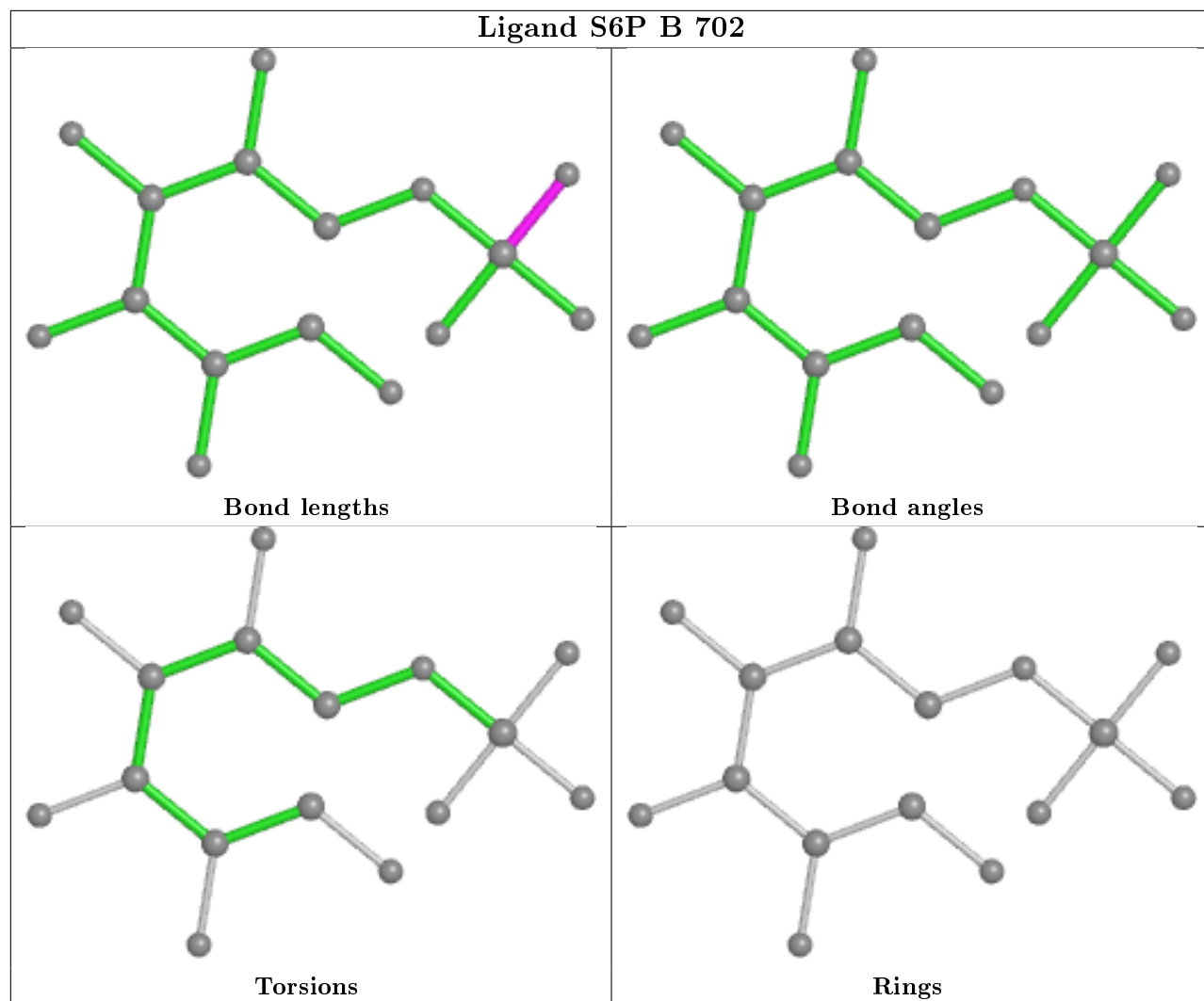
There are no ring outliers.

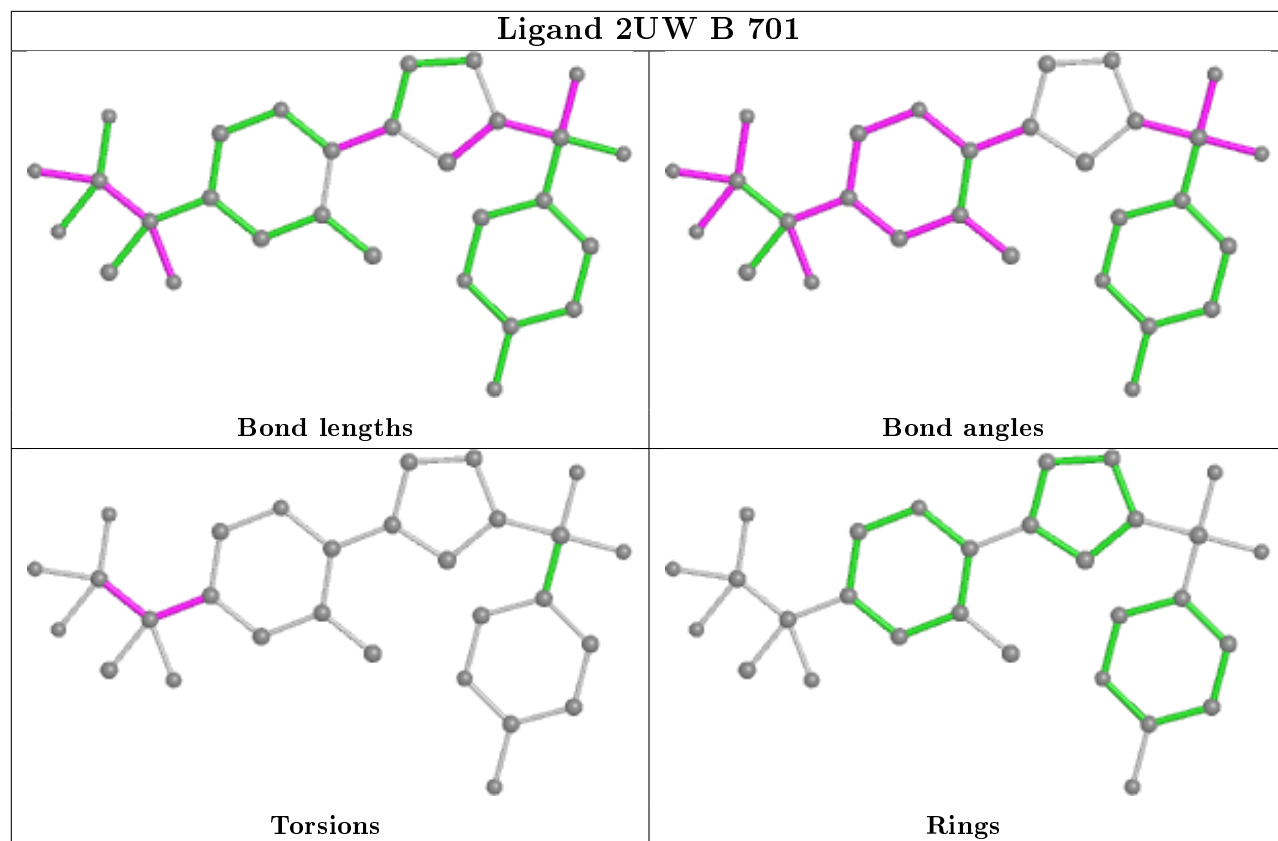
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	2UW	1	0
3	A	702	S6P	1	0
2	A	701	2UW	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.

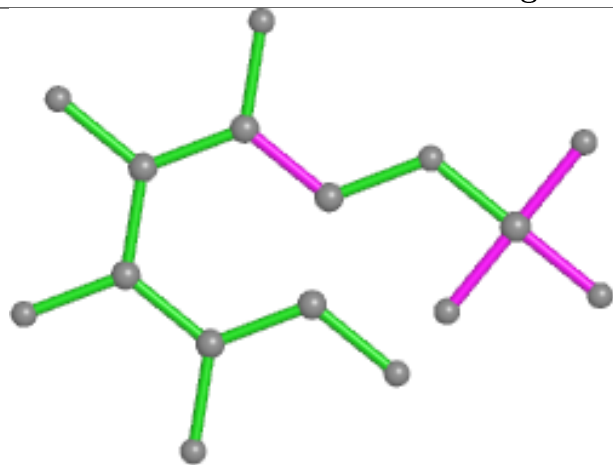
## Ligand S6P B 702



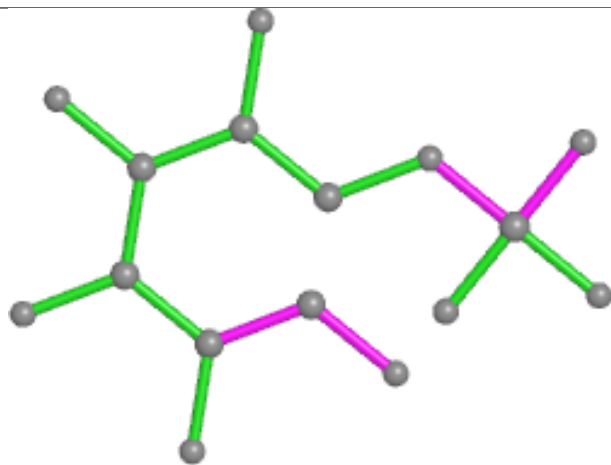




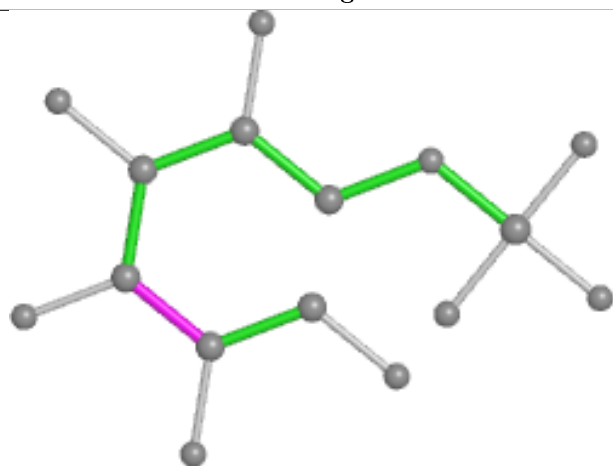
## Ligand S6P A 702



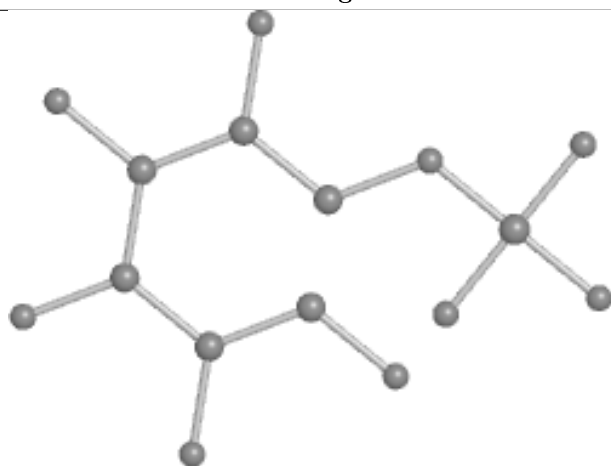
Bond lengths



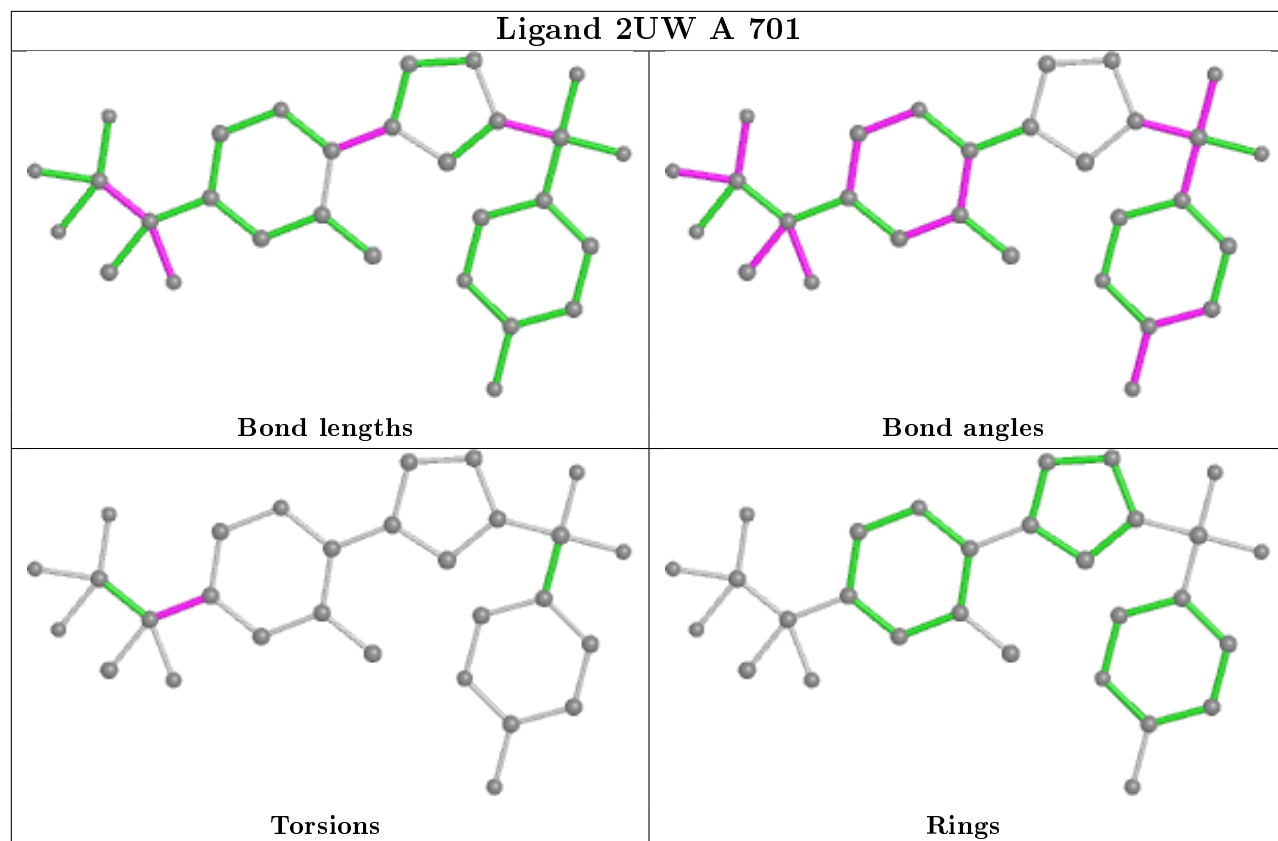
Bond angles



Torsions



Rings



## 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, 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	585/638 (91%)	0.12	23 (3%)	39 38	26, 46, 83, 127	0
1	B	590/638 (92%)	0.02	26 (4%)	34 33	23, 40, 69, 111	0
All	All	1175/1276 (92%)	0.07	49 (4%)	36 35	23, 43, 78, 127	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LEU	5.9
1	B	1	MET	4.7
1	B	21	LEU	4.0
1	B	2	PRO	4.0
1	A	465	PHE	3.8
1	A	469	GLU	3.8
1	A	21	LEU	3.6
1	B	4	THR	3.5
1	A	357	PHE	3.4
1	A	387	PHE	3.4
1	B	66	GLN	3.4
1	B	463	LEU	3.3
1	A	470	GLY	3.2
1	A	447	ILE	3.1
1	A	69	SER	3.0
1	A	448	PRO	3.0
1	A	466	PHE	3.0
1	B	180	VAL	2.9
1	B	260	MET	2.9
1	B	131	LYS	2.9
1	B	265	ALA	2.7
1	B	465	PHE	2.6
1	A	1	MET	2.6
1	A	454	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	444	THR	2.6
1	A	445	LEU	2.5
1	B	257	SER	2.5
1	B	381	GLN	2.5
1	A	180	VAL	2.5
1	B	20	GLU	2.5
1	B	109	THR	2.4
1	A	442	GLY	2.4
1	B	98	ASP	2.4
1	A	109	THR	2.4
1	B	441	VAL	2.4
1	B	69	SER	2.3
1	A	467	GLU	2.3
1	A	430	THR	2.3
1	B	264	SER	2.3
1	B	454	PRO	2.3
1	A	402	GLU	2.2
1	B	259	ARG	2.2
1	B	258	SER	2.2
1	A	429	LYS	2.2
1	B	593	ALA	2.2
1	B	65	GLY	2.1
1	B	31	THR	2.0
1	A	352	THR	2.0
1	A	559	CYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

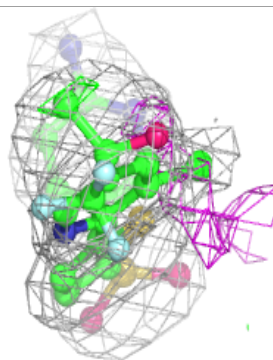
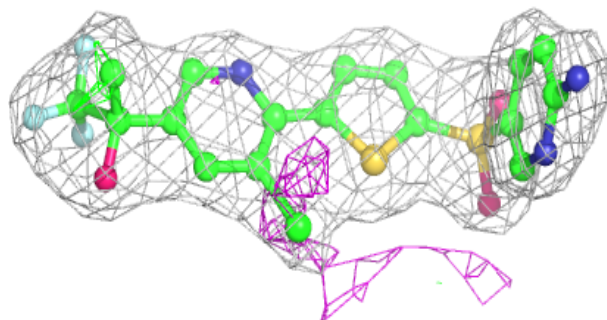
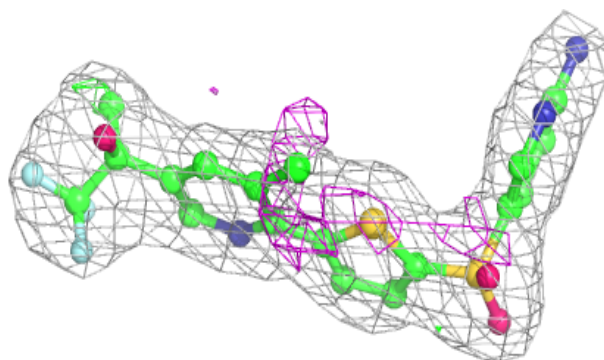
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	719	5/5	0.72	0.24	83,85,95,103	0
4	IOD	B	712	1/1	0.72	0.32	100,100,100,100	1
4	IOD	A	715	1/1	0.83	0.11	76,76,76,76	1
5	GOL	B	718	6/6	0.89	0.13	47,48,53,53	0
4	IOD	A	712	1/1	0.93	0.09	70,70,70,70	1
4	IOD	B	715	1/1	0.93	0.05	75,75,75,75	1
4	IOD	A	709	1/1	0.93	0.11	94,94,94,94	1
4	IOD	B	708	1/1	0.94	0.05	51,51,51,51	1
4	IOD	B	717	1/1	0.94	0.08	83,83,83,83	1
4	IOD	B	713	1/1	0.94	0.08	83,83,83,83	1
4	IOD	A	703	1/1	0.95	0.05	64,64,64,64	0
4	IOD	A	708	1/1	0.95	0.06	77,77,77,77	1
4	IOD	B	710	1/1	0.95	0.15	103,103,103,103	1
2	2UW	A	701	29/29	0.96	0.13	30,36,63,72	0
4	IOD	B	714	1/1	0.96	0.07	66,66,66,66	1
4	IOD	A	706	1/1	0.96	0.06	82,82,82,82	0
4	IOD	B	703	1/1	0.96	0.08	50,50,50,50	0
2	2UW	B	701	29/29	0.96	0.14	26,35,50,74	0
4	IOD	B	716	1/1	0.96	0.14	79,79,79,79	1
4	IOD	A	714	1/1	0.97	0.08	63,63,63,63	1
4	IOD	B	706	1/1	0.97	0.10	45,45,45,45	1
4	IOD	B	709	1/1	0.97	0.10	79,79,79,79	1
4	IOD	A	710	1/1	0.97	0.05	63,63,63,63	1
4	IOD	A	707	1/1	0.97	0.06	55,55,55,55	1
6	SO4	B	720	5/5	0.97	0.17	37,37,38,38	5
4	IOD	A	711	1/1	0.98	0.13	94,94,94,94	1
4	IOD	A	713	1/1	0.98	0.05	63,63,63,63	1
4	IOD	B	711	1/1	0.99	0.06	66,66,66,66	1
4	IOD	B	705	1/1	0.99	0.08	46,46,46,46	1
4	IOD	A	705	1/1	0.99	0.07	46,46,46,46	1
3	S6P	B	702	16/16	0.99	0.22	20,22,24,24	0
4	IOD	A	704	1/1	0.99	0.04	60,60,60,60	0
3	S6P	A	702	16/16	0.99	0.17	24,29,33,37	0
4	IOD	B	707	1/1	0.99	0.04	68,68,68,68	0
4	IOD	B	704	1/1	0.99	0.06	48,48,48,48	0

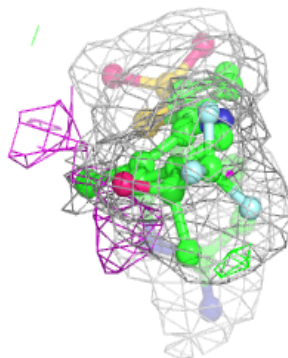
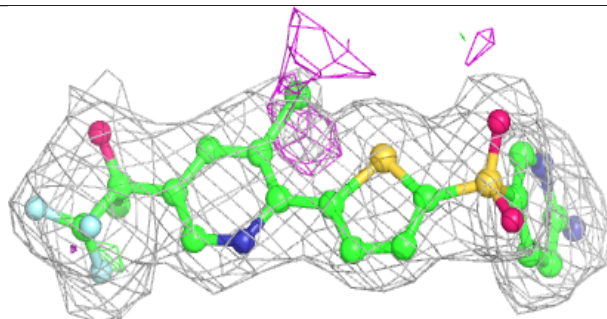
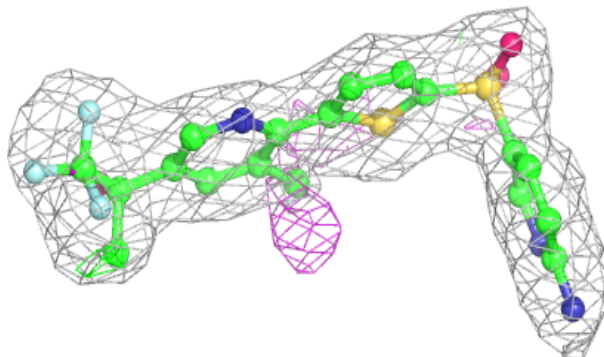
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2UW A 701:**

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

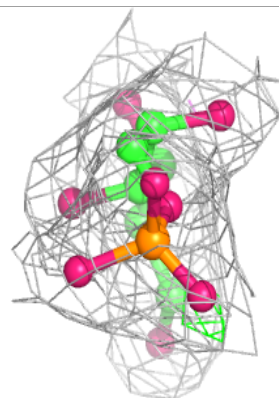
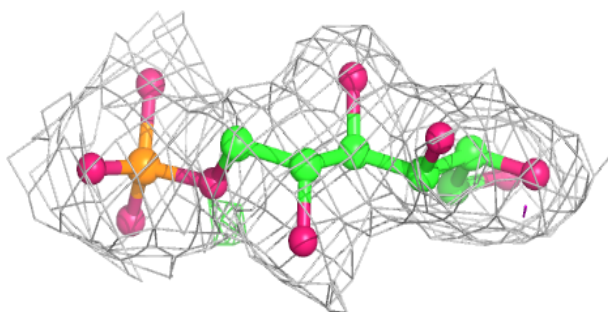
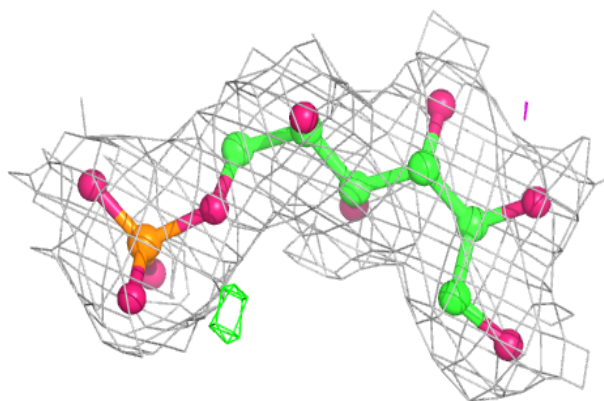
**Electron density around 2UW B 701:**

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

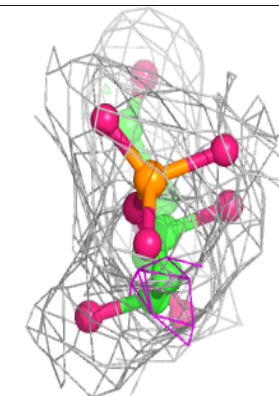
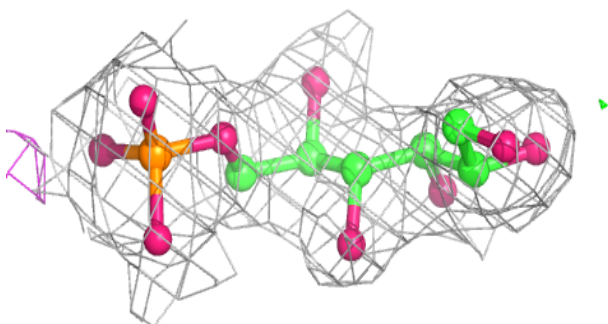
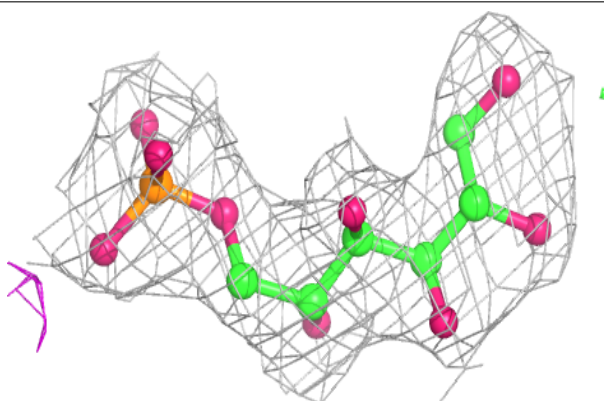


**Electron density around S6P B 702:**

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

**Electron density around S6P A 702:**

$2mF_o-DF_c$  (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.