



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 12:16 AM UTC

PDB ID : 4OHO / pdb\_00004oho  
Title : Human GKRP bound to AMG-2668  
Authors : Jordan, S.R.; Chmait, S.  
Deposited on : 2014-01-17  
Resolution : 2.58 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

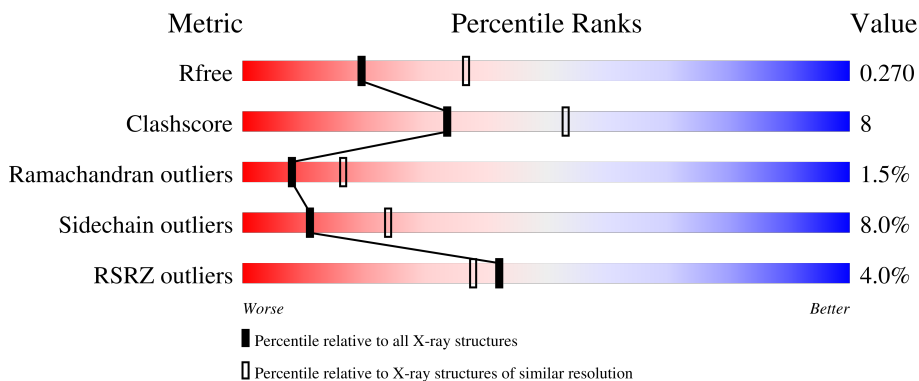
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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))
$R_{free}$	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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  $\geq 3$ , 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	
1	B	638	

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	A	709	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 9343 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
			Total	C	N	O	S			
1	A	585	4521	2882	774	841	24	0	0	0
1	B	590	4554	2901	781	848	24	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

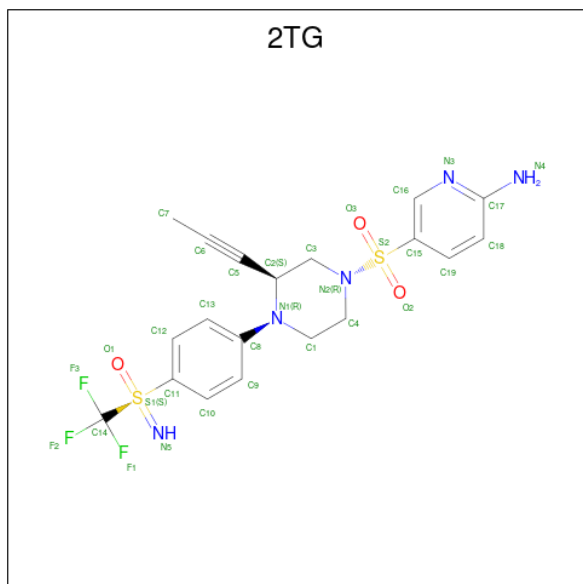
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q14397
A	-10	ALA	-	expression tag	UNP Q14397
A	-9	HIS	-	expression tag	UNP Q14397
A	-8	HIS	-	expression tag	UNP Q14397
A	-7	HIS	-	expression tag	UNP Q14397
A	-6	HIS	-	expression tag	UNP Q14397
A	-5	HIS	-	expression tag	UNP 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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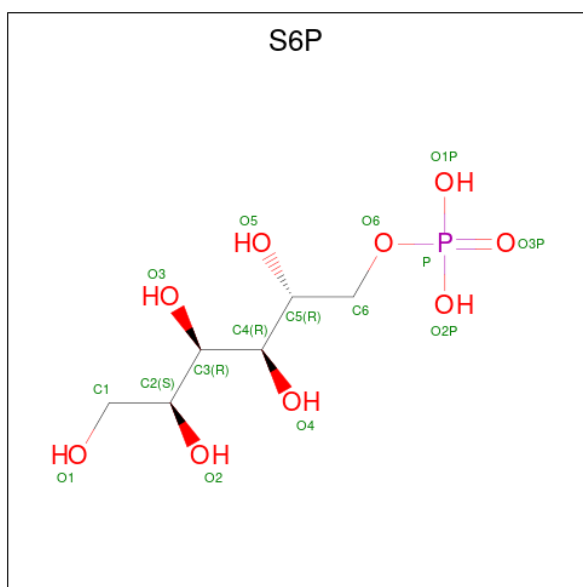
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	expression tag	UNP Q14397

- Molecule 2 is 5-{{(3S)-3-(prop-1-yn-1-yl)-4-{{4-[S-(trifluoromethyl)sulfonimidoyl]phenyl}piperazin-1-yl}sulfonyl}pyridin-2-amine (CCD ID: 2TG) (formula: C<sub>19</sub>H<sub>20</sub>F<sub>3</sub>N<sub>5</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	32	19	3	5	3	2	0	0
2	B	1	32	19	3	5	3	2	0	0

- Molecule 3 is D-SORBITOL-6-PHOSPHATE (CCD ID: S6P) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>9</sub>P).



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 (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	I	0	0
			12	12		
4	B	13	Total	I	0	0
			13	13		

- Molecule 5 is GLYCEROL (CCD ID: 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 (CCD ID: SO4) (formula: O<sub>4</sub>S).

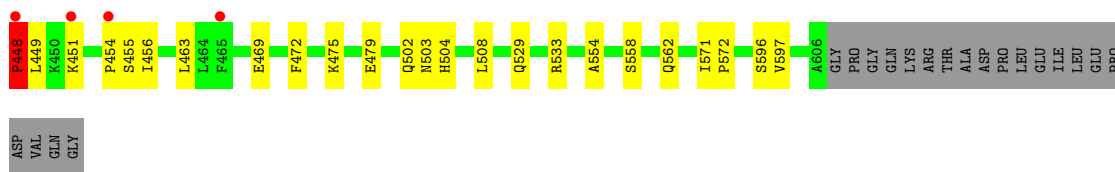


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total 53	O 53	0	0
7	B	73	Total 73	O 73	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.92Å 148.92Å 132.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 2.58 29.59 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.59-2.58) 99.5 (29.59-2.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.57Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.207 , 0.269 0.213 , 0.270	Depositor DCC
$R_{free}$ test set	2666 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 26.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: GOL, S6P, SO4, 2TG, IOD

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	0.97	3/4603 (0.1%)	1.09	5/6228 (0.1%)
1	B	0.99	0/4637	1.06	8/6274 (0.1%)
All	All	0.98	3/9240 (0.0%)	1.08	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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	PHE	C-O	-5.70	1.17	1.24
1	A	430	THR	N-CA	5.24	1.52	1.46
1	A	247	PRO	C-O	-5.05	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ILE	N-CA-C	-6.28	103.77	110.36
1	A	389	GLN	N-CA-C	6.16	118.53	111.02
1	B	434	GLN	N-CA-C	-5.99	99.62	108.79
1	B	475	LYS	N-CA-C	-5.62	105.06	111.07
1	B	48	ASN	N-CA-C	5.61	117.47	111.36
1	B	447	ILE	N-CA-CB	5.61	115.77	109.99
1	A	414	ASP	N-CA-C	5.60	120.23	112.45
1	B	246	ASN	N-CA-C	5.46	117.43	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	GLN	N-CA-C	5.40	118.18	110.24
1	A	430	THR	N-CA-C	5.37	122.23	110.80
1	B	336	GLN	CB-CA-C	-5.27	108.96	116.34
1	A	515	LEU	N-CA-C	-5.21	105.66	112.23
1	B	227	ARG	N-CA-C	5.16	118.36	111.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	447	ILE	Peptide
1	B	448	PRO	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	81	0
1	B	4554	0	4647	61	0
2	A	32	0	20	2	0
2	B	32	0	20	2	0
3	A	16	0	13	2	0
3	B	16	0	13	1	0
4	A	12	0	0	4	0
4	B	13	0	0	3	0
5	B	6	0	8	0	0
6	B	15	0	0	0	0
7	A	53	0	0	1	0
7	B	73	0	0	2	0
All	All	9343	0	9339	142	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 8.

All (142) 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:216:ASN:OD1	1:B:225:THR:HG21	1.75	0.85
1:B:419:VAL:O	1:B:423:VAL:HG12	1.83	0.77
1:A:447:ILE:HG22	1:A:450:LYS:N	1.99	0.77
1:B:389:GLN:OE1	1:B:421:THR:HG21	1.85	0.76
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.23	0.72
1:B:5:LYS:HB2	4:B:710:IOD:I	2.60	0.70
1:A:447:ILE:HG22	1:A:449:LEU:C	2.16	0.70
1:A:337:THR:HG21	1:A:479:GLU:OE2	1.94	0.67
1:B:508:LEU:C	1:B:508:LEU:HD12	2.19	0.66
1:B:445:LEU:HG	4:B:713:IOD:I	2.65	0.66
1:B:529:GLN:NE2	1:B:533:ARG:HE	1.95	0.64
1:B:337:THR:HG21	1:B:479:GLU:OE1	1.98	0.63
1:A:146:VAL:O	1:A:347:VAL:HG21	1.99	0.62
3:A:702:S6P:O1P	7:A:843:HOH:O	2.16	0.62
1:A:125:MET:HE1	1:A:133:LEU:HG	1.83	0.61
1:A:44:ALA:HB1	1:A:48:ASN:HB3	1.82	0.60
1:A:5:LYS:HB2	4:A:709:IOD:I	2.70	0.60
1:B:389:GLN:HE21	1:B:418:GLU:HG3	1.67	0.60
1:B:236:MET:HE3	1:B:241:LYS:HB3	1.84	0.60
1:B:220:GLU:OE1	1:B:558:SER:OG	2.21	0.58
1:B:448:PRO:HD3	1:B:451:LYS:HB2	1.85	0.58
1:A:512:ASN:C	1:A:512:ASN:HD22	2.11	0.57
1:A:5:LYS:CB	4:A:709:IOD:I	3.24	0.55
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.72	0.55
1:A:339:GLY:O	1:A:342:ALA:HB3	2.07	0.55
1:A:414:ASP:O	1:A:415:ASN:CB	2.54	0.55
1:A:393:LEU:O	1:A:397:LEU:HB3	2.06	0.55
1:A:273:LEU:C	1:A:273:LEU:HD23	2.33	0.54
1:B:529:GLN:HE21	1:B:533:ARG:HE	1.55	0.54
1:A:140:GLY:H	1:A:158:HIS:HE1	1.55	0.54
1:A:444:THR:O	1:A:446:PRO:HD3	2.06	0.54
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.90	0.54
1:A:272:THR:HA	1:A:295:ILE:HG21	1.90	0.53
1:A:18:LYS:O	1:A:18:LYS:HG3	2.09	0.53
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.56	0.52
1:A:343:ILE:HA	1:A:362:GLY:HA3	1.91	0.52
1:B:6:ARG:HD2	1:B:554:ALA:O	2.11	0.51
1:B:469:GLU:HG2	7:B:803:HOH:O	2.10	0.51
1:A:207:GLY:O	1:A:246:ASN:HA	2.11	0.51
1:A:236:MET:HE2	1:A:242:ALA:HB2	1.93	0.51
1:A:124:LEU:HD12	1:A:472:PHE:CD2	2.46	0.50
1:B:259:ARG:NH2	1:B:345:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HB3	1:A:342:ALA:HB1	1.94	0.49
1:B:246:ASN:HD22	1:B:246:ASN:N	2.10	0.49
1:B:420:GLN:O	1:B:421:THR:C	2.55	0.49
1:A:535:ILE:O	1:A:539:LEU:HG	2.13	0.48
1:A:451:LYS:N	1:A:452:LEU:HB2	2.28	0.48
1:A:320:VAL:HG13	1:A:330:VAL:HG21	1.94	0.48
1:A:113:MET:HA	1:A:113:MET:HE2	1.96	0.48
1:B:401:THR:HG22	1:B:403:ILE:H	1.78	0.48
1:B:225:THR:H	1:B:228:GLN:HE21	1.62	0.48
1:A:416:LEU:N	1:A:416:LEU:HD12	2.29	0.48
1:A:323:SER:O	1:A:328:GLY:N	2.47	0.47
1:A:10:VAL:HB	1:A:531:LYS:HE3	1.95	0.47
1:B:389:GLN:NE2	1:B:418:GLU:HG3	2.29	0.47
1:A:414:ASP:O	1:A:415:ASN:HB2	2.14	0.47
1:A:180:VAL:HG11	1:A:258:SER:HB2	1.96	0.47
1:B:420:GLN:HA	1:B:423:VAL:CG1	2.44	0.47
1:A:101:LEU:HD21	1:A:166:VAL:HG13	1.96	0.47
1:A:474:GLN:OE1	1:A:478:ARG:NH1	2.47	0.47
1:A:49:ILE:CD1	1:A:317:MET:HE1	2.44	0.47
1:A:104:LEU:HD23	1:A:176:ILE:HB	1.95	0.47
1:A:315:THR:HG22	1:A:434:GLN:HE22	1.79	0.46
1:A:447:ILE:O	1:A:450:LYS:N	2.46	0.46
1:A:4:THR:O	1:A:8:GLN:HB2	2.15	0.46
1:A:267:LYS:O	1:A:268:ILE:C	2.58	0.46
1:A:504:HIS:CE1	2:A:701:2TG:F2	2.58	0.46
1:A:422:ILE:O	1:A:426:VAL:HG23	2.15	0.46
1:A:481:SER:O	1:A:485:VAL:HG23	2.16	0.46
1:B:214:ALA:O	1:B:227:ARG:HD3	2.16	0.45
1:B:331:TYR:CE1	1:B:400:LEU:HD23	2.51	0.45
1:B:397:LEU:HB3	1:B:398:PRO:HD3	1.98	0.45
1:B:101:LEU:HD12	1:B:133:LEU:O	2.15	0.45
1:A:49:ILE:HD12	1:A:317:MET:HE1	1.97	0.45
1:A:451:LYS:HA	1:A:453:PHE:N	2.32	0.45
1:A:332:LEU:HD12	1:A:407:VAL:HB	1.98	0.45
1:B:246:ASN:HD22	1:B:246:ASN:H	1.65	0.45
1:A:246:ASN:N	1:A:246:ASN:HD22	2.14	0.45
1:A:278:HIS:O	1:A:281:VAL:HG22	2.16	0.45
1:A:509:ARG:NH2	1:A:568:GLU:OE2	2.49	0.44
1:A:205:LEU:HB2	1:A:233:MET:HE1	2.00	0.44
1:A:350:ILE:HA	1:A:355:ALA:O	2.18	0.44
1:A:117:MET:HE1	1:A:270:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:HG	1:B:269:LEU:HD21	1.99	0.44
1:A:177:GLY:HA3	1:A:191:MET:HE3	2.00	0.43
1:A:416:LEU:N	1:A:416:LEU:CD1	2.81	0.43
1:B:12:GLU:OE2	1:B:13:THR:N	2.51	0.43
1:B:273:LEU:C	1:B:273:LEU:HD23	2.42	0.43
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.65	0.43
1:B:175:VAL:HG21	1:B:194:CYS:SG	2.59	0.43
1:A:179:SER:OG	3:A:702:S6P:O2P	2.34	0.43
1:A:365:ILE:N	1:A:365:ILE:HD12	2.32	0.43
1:A:512:ASN:ND2	1:A:515:LEU:H	2.17	0.43
1:B:444:THR:O	1:B:446:PRO:HD3	2.18	0.43
1:B:508:LEU:C	1:B:508:LEU:CD1	2.91	0.43
1:A:427:LYS:HE3	1:A:431:ASN:HA	2.00	0.43
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.84	0.43
1:A:5:LYS:HB3	4:A:709:IOD:I	2.89	0.43
1:B:32:GLU:OE1	2:B:701:2TG:H16	2.19	0.43
1:A:331:TYR:CD1	1:A:331:TYR:N	2.86	0.43
1:A:353:PHE:HA	1:A:505:MET:HE2	2.01	0.43
1:B:183:SER:O	1:B:185:PRO:HD3	2.19	0.43
1:A:450:LYS:HA	1:A:452:LEU:HD12	2.00	0.43
1:B:110:SER:HB3	1:B:178:ILE:HG22	2.01	0.43
1:B:179:SER:OG	3:B:702:S6P:O2P	2.35	0.43
1:A:303:HIS:HA	1:A:484:TRP:CZ3	2.54	0.43
1:B:331:TYR:CE1	1:B:400:LEU:CD2	3.02	0.42
1:B:596:SER:O	1:B:597:VAL:C	2.60	0.42
1:B:571:ILE:HB	1:B:572:PRO:HD3	2.02	0.42
1:A:183:SER:O	1:A:185:PRO:HD3	2.20	0.42
1:A:504:HIS:CE1	2:A:701:2TG:C14	3.01	0.42
1:A:540:ARG:CZ	1:A:548:LEU:HD12	2.50	0.42
1:A:42:ASP:N	1:A:42:ASP:OD1	2.51	0.42
1:B:106:GLY:O	1:B:138:ILE:HA	2.19	0.42
1:A:140:GLY:O	1:A:149:ARG:NH1	2.39	0.42
1:B:217:ASP:OD1	1:B:217:ASP:N	2.53	0.42
1:B:124:LEU:HD12	1:B:472:PHE:CD2	2.55	0.42
1:B:48:ASN:ND2	1:B:51:ARG:HE	2.18	0.42
1:A:121:PHE:O	1:A:125:MET:HG3	2.18	0.42
1:A:271:GLU:O	1:A:272:THR:C	2.62	0.42
1:A:468:TYR:HB2	4:A:703:IOD:I	2.90	0.42
1:B:448:PRO:HA	1:B:449:LEU:C	2.45	0.42
1:A:419:VAL:O	1:A:423:VAL:HG23	2.20	0.42
1:B:25:GLU:OE2	4:B:711:IOD:I	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:O	1:B:408:PHE:HA	2.20	0.42
1:B:504:HIS:CE1	2:B:701:2TG:C14	3.02	0.42
1:B:299:PHE:O	1:B:302:ALA:HB3	2.19	0.41
1:B:397:LEU:HD11	1:B:426:VAL:HA	2.02	0.41
1:A:35:ASN:HD22	1:A:37:LEU:H	1.68	0.41
1:B:447:ILE:HB	1:B:448:PRO:HD2	2.01	0.41
1:B:413:ASP:OD1	1:B:413:ASP:N	2.54	0.41
1:A:388:SER:OG	1:A:389:GLN:N	2.53	0.41
1:B:115:PHE:O	1:B:116:LEU:C	2.61	0.41
1:A:335:TRP:CZ2	1:A:419:VAL:HG22	2.56	0.41
1:B:259:ARG:HD3	7:B:849:HOH:O	2.20	0.41
1:B:304:GLN:O	1:B:305:VAL:C	2.58	0.41
1:B:421:THR:O	1:B:424:GLU:HB2	2.21	0.41
1:B:571:ILE:N	1:B:572:PRO:CD	2.84	0.41
1:A:136:TYR:O	1:A:137:LEU:HD23	2.20	0.40
1:B:100:GLY:HA2	1:B:172:ARG:O	2.22	0.40
1:A:449:LEU:C	1:A:451:LYS:N	2.80	0.40
1:B:410:PHE:O	1:B:437:ALA:HA	2.22	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%)	532 (92%)	36 (6%)	11 (2%)	<b>6</b> <b>12</b>
1	B	584/638 (92%)	558 (96%)	20 (3%)	6 (1%)	<b>12</b> <b>26</b>
All	All	1163/1276 (91%)	1090 (94%)	56 (5%)	17 (2%)	<b>8</b> <b>16</b>

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	LYS
1	A	388	SER
1	A	415	ASN
1	A	456	ILE
1	B	448	PRO
1	B	260	MET
1	B	415	ASN
1	A	431	ASN
1	A	452	LEU
1	A	336	GLN
1	B	454	PRO
1	B	502	GLN
1	A	168	ALA
1	A	260	MET
1	A	446	PRO
1	B	418	GLU
1	A	447	ILE

### 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%)	449 (90%)	49 (10%)	7	16
1	B	501/542 (92%)	470 (94%)	31 (6%)	16	34
All	All	999/1084 (92%)	919 (92%)	80 (8%)	11	24

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	THR
1	A	5	LYS
1	A	6	ARG
1	A	18	LYS
1	A	25	GLU
1	A	35	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	39	GLN
1	A	131	LYS
1	A	143	ARG
1	A	166	VAL
1	A	170	LYS
1	A	172	ARG
1	A	227	ARG
1	A	235	LYS
1	A	239	LYS
1	A	246	ASN
1	A	273	LEU
1	A	282	ASP
1	A	285	ILE
1	A	316	LEU
1	A	322	THR
1	A	327	LYS
1	A	332	LEU
1	A	336	GLN
1	A	347	VAL
1	A	358	ARG
1	A	361	ARG
1	A	402	GLU
1	A	417	THR
1	A	427	LYS
1	A	431	ASN
1	A	436	LEU
1	A	439	SER
1	A	444	THR
1	A	445	LEU
1	A	456	ILE
1	A	458	SER
1	A	463	LEU
1	A	464	LEU
1	A	467	GLU
1	A	473	ILE
1	A	474	GLN
1	A	478	ARG
1	A	500	ILE
1	A	503	ASN
1	A	512	ASN
1	A	577	SER
1	A	605	LEU

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Mol	Chain	Res	Type
1	B	6	ARG
1	B	11	ILE
1	B	47	GLU
1	B	69	SER
1	B	126	LYS
1	B	133	LEU
1	B	166	VAL
1	B	171	LYS
1	B	225	THR
1	B	227	ARG
1	B	235	LYS
1	B	241	LYS
1	B	246	ASN
1	B	281	VAL
1	B	304	GLN
1	B	337	THR
1	B	357	PHE
1	B	401	THR
1	B	402	GLU
1	B	413	ASP
1	B	415	ASN
1	B	416	LEU
1	B	423	VAL
1	B	434	GLN
1	B	445	LEU
1	B	447	ILE
1	B	455	SER
1	B	456	ILE
1	B	463	LEU
1	B	503	ASN
1	B	562	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	55	GLN
1	A	72	GLN
1	A	91	GLN
1	A	123	GLN
1	A	158	HIS
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	246	ASN
1	A	329	HIS
1	A	425	GLN
1	A	434	GLN
1	A	477	GLN
1	A	503	ASN
1	A	504	HIS
1	A	512	ASN
1	A	529	GLN
1	B	8	GLN
1	B	9	HIS
1	B	39	GLN
1	B	48	ASN
1	B	62	GLN
1	B	197	ASN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	304	GLN
1	B	336	GLN
1	B	384	GLN
1	B	425	GLN
1	B	431	ASN
1	B	434	GLN
1	B	471	ASN
1	B	503	ASN
1	B	504	HIS
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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 33 ligands modelled in this entry, 25 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	717	-	4,4,4	0.72	0	6,6,6	0.32	0
2	2TG	B	701	-	30,34,34	1.64	4 (13%)	42,52,52	2.63	14 (33%)
5	GOL	B	716	-	5,5,5	0.40	0	5,5,5	0.79	0
6	SO4	B	718	-	4,4,4	0.50	0	6,6,6	0.48	0
3	S6P	A	702	-	15,15,15	1.37	3 (20%)	20,21,21	1.16	3 (15%)
2	2TG	A	701	-	30,34,34	1.94	7 (23%)	42,52,52	2.63	11 (26%)
6	SO4	B	719	-	4,4,4	0.34	0	6,6,6	0.47	0
3	S6P	B	702	-	15,15,15	1.58	2 (13%)	20,21,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2TG	B	701	-	-	8/31/47/47	0/3/3/3
5	GOL	B	716	-	-	2/4/4/4	-
3	S6P	A	702	-	-	2/20/20/20	-
2	2TG	A	701	-	-	11/31/47/47	0/3/3/3
3	S6P	B	702	-	-	1/20/20/20	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	2TG	O3-S2	5.32	1.49	1.43
2	B	701	2TG	O3-S2	4.61	1.48	1.43
2	A	701	2TG	O2-S2	4.34	1.48	1.43
2	B	701	2TG	O1-S1	4.29	1.50	1.45
3	B	702	S6P	P-O3P	3.94	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	2TG	C11-S1	-3.67	1.72	1.78
2	B	701	2TG	C3-N2	-3.37	1.44	1.47
2	A	701	2TG	C4-N2	-3.06	1.44	1.47
2	A	701	2TG	O1-S1	2.97	1.49	1.45
2	A	701	2TG	S2-N2	-2.93	1.59	1.63
3	A	702	S6P	P-O3P	2.88	1.59	1.50
2	A	701	2TG	C2-C5	2.68	1.49	1.48
3	A	702	S6P	C6-C5	2.51	1.55	1.51
2	B	701	2TG	C2-C5	-2.40	1.46	1.48
3	A	702	S6P	C2-C3	-2.24	1.49	1.53
3	B	702	S6P	P-O1P	-2.01	1.47	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2TG	F1-C14-S1	-9.51	95.25	110.38
2	B	701	2TG	F3-C14-S1	-9.25	95.66	110.38
2	A	701	2TG	O3-S2-N2	6.63	112.92	106.69
2	B	701	2TG	C4-N2-S2	-6.29	105.36	117.06
2	B	701	2TG	F2-C14-S1	6.16	120.18	110.38
2	A	701	2TG	O3-S2-O2	-5.37	111.21	119.59
2	A	701	2TG	C3-N2-S2	-5.05	108.07	117.17
2	A	701	2TG	C4-N2-S2	-4.77	108.19	117.06
2	B	701	2TG	C4-N2-C3	-4.64	107.44	112.66
2	A	701	2TG	F2-C14-S1	4.16	116.99	110.38
2	B	701	2TG	C3-N2-S2	-3.73	110.44	117.17
2	A	701	2TG	C15-C16-N3	-3.59	118.82	123.19
2	B	701	2TG	C12-C11-S1	3.17	122.86	119.20
2	B	701	2TG	O2-S2-C15	-3.10	104.25	108.10
2	B	701	2TG	O2-S2-N2	3.07	109.57	106.69
2	B	701	2TG	O3-S2-O2	-2.96	114.97	119.59
2	A	701	2TG	C12-C11-S1	2.90	122.54	119.20
2	A	701	2TG	C1-N1-C2	2.68	120.01	111.59
2	B	701	2TG	F3-C14-F2	2.68	118.68	107.49
2	B	701	2TG	C1-N1-C2	2.64	119.91	111.59
2	B	701	2TG	O3-S2-C15	2.57	111.30	108.10
2	B	701	2TG	C15-S2-N2	2.49	110.28	107.28
3	A	702	S6P	O1-C1-C2	-2.34	106.25	111.16
2	B	701	2TG	C15-C16-N3	-2.27	120.42	123.19
3	A	702	S6P	O2P-P-O3P	-2.27	101.98	110.83
3	B	702	S6P	O1-C1-C2	-2.17	106.60	111.16
3	A	702	S6P	O2-C2-C1	-2.12	104.20	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2TG	C9-C10-C11	2.12	121.50	119.44
2	A	701	2TG	C15-S2-N2	2.01	109.71	107.28

There are no chirality outliers.

All (24) torsion outliers are listed below:

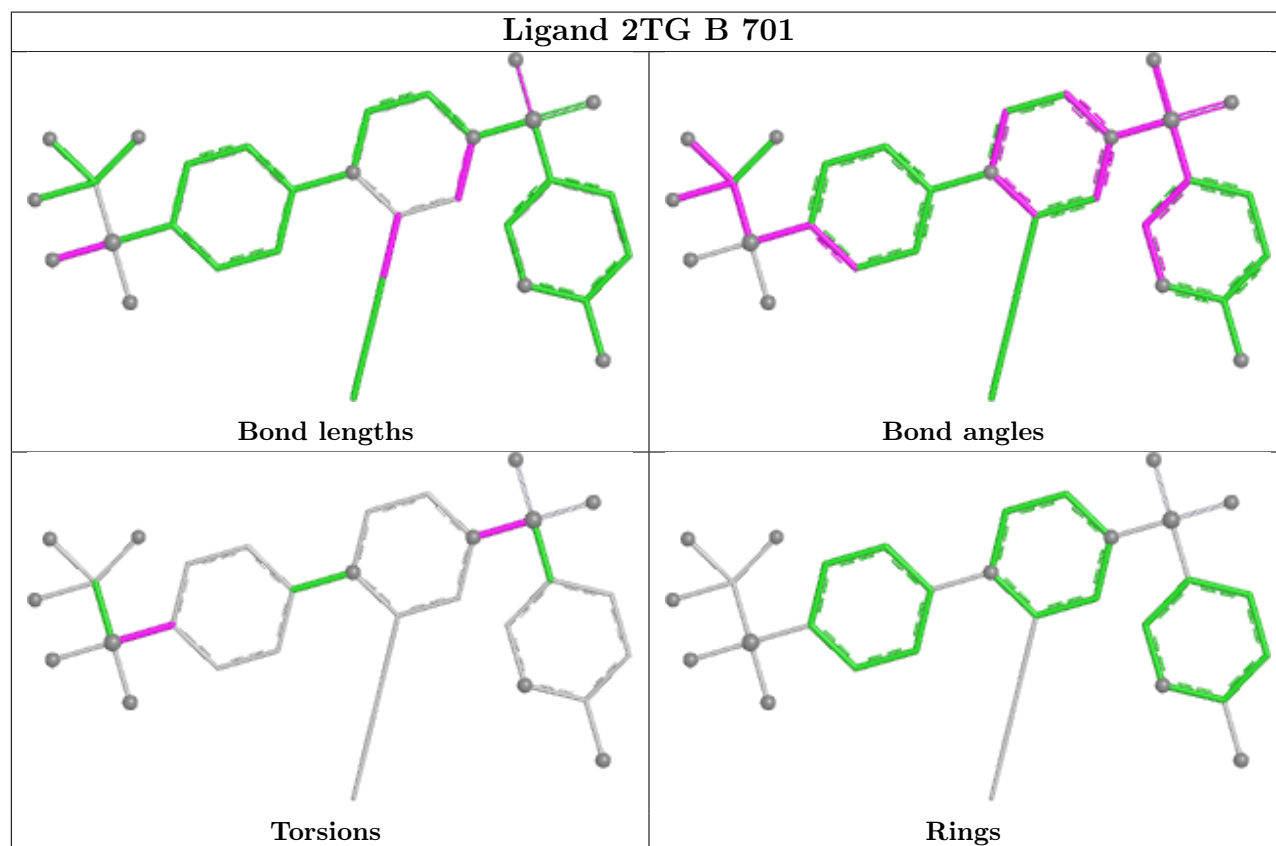
Mol	Chain	Res	Type	Atoms
2	A	701	2TG	C12-C11-S1-C14
2	A	701	2TG	C12-C11-S1-N5
2	A	701	2TG	C10-C11-S1-C14
2	A	701	2TG	C10-C11-S1-N5
2	B	701	2TG	C12-C11-S1-C14
2	B	701	2TG	C12-C11-S1-N5
2	B	701	2TG	C10-C11-S1-C14
2	B	701	2TG	C10-C11-S1-N5
2	A	701	2TG	C3-N2-S2-O2
5	B	716	GOL	O1-C1-C2-O2
5	B	716	GOL	O1-C1-C2-C3
2	A	701	2TG	C3-N2-S2-C15
2	A	701	2TG	C10-C11-S1-O1
2	A	701	2TG	F3-C14-S1-C11
2	B	701	2TG	C3-N2-S2-O2
3	B	702	S6P	O1-C1-C2-O2
2	A	701	2TG	F2-C14-S1-C11
3	A	702	S6P	O1-C1-C2-O2
3	A	702	S6P	O1-C1-C2-C3
2	B	701	2TG	C3-N2-S2-C15
2	A	701	2TG	C12-C11-S1-O1
2	B	701	2TG	C12-C11-S1-O1
2	B	701	2TG	C10-C11-S1-O1
2	A	701	2TG	F1-C14-S1-C11

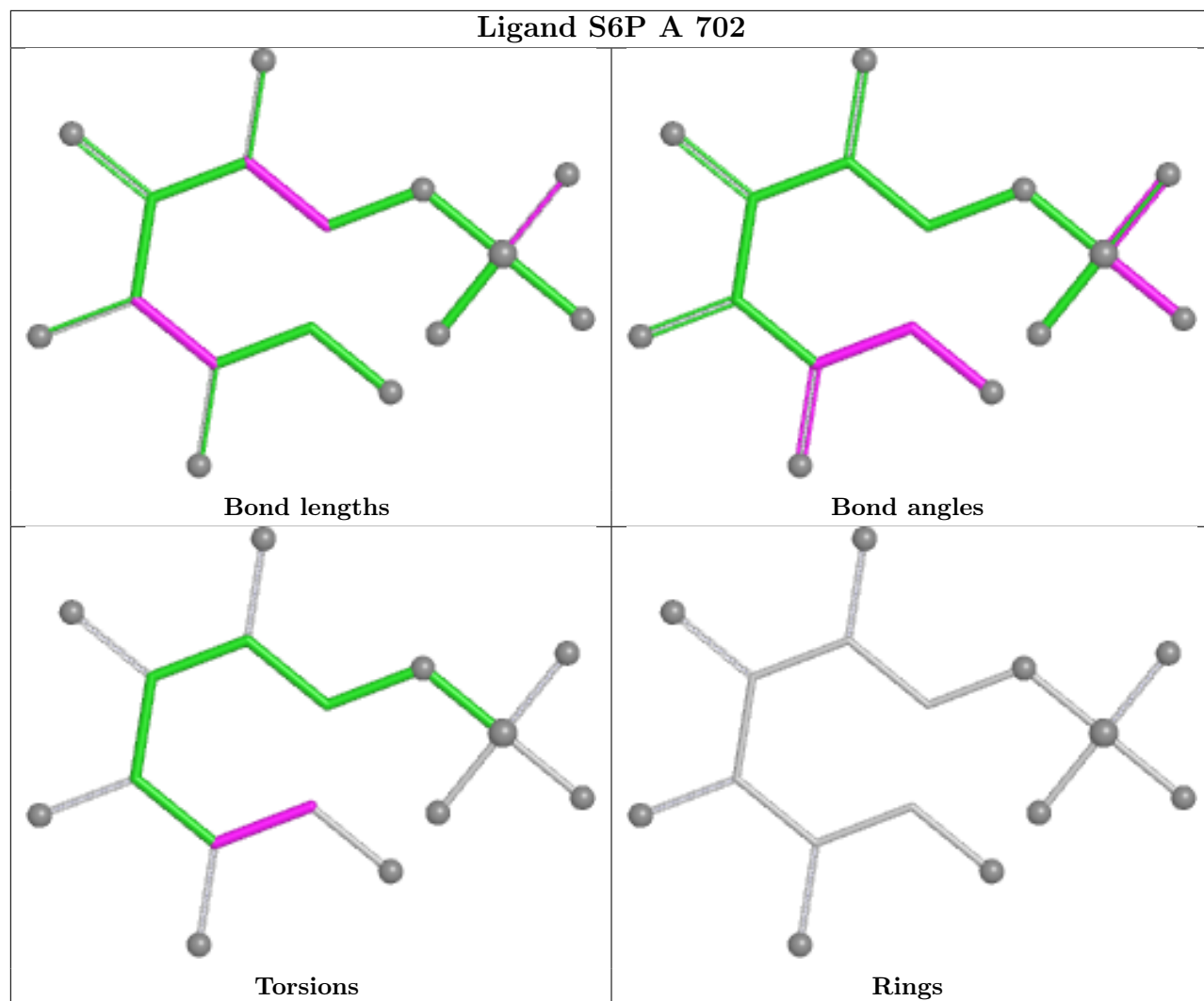
There are no ring outliers.

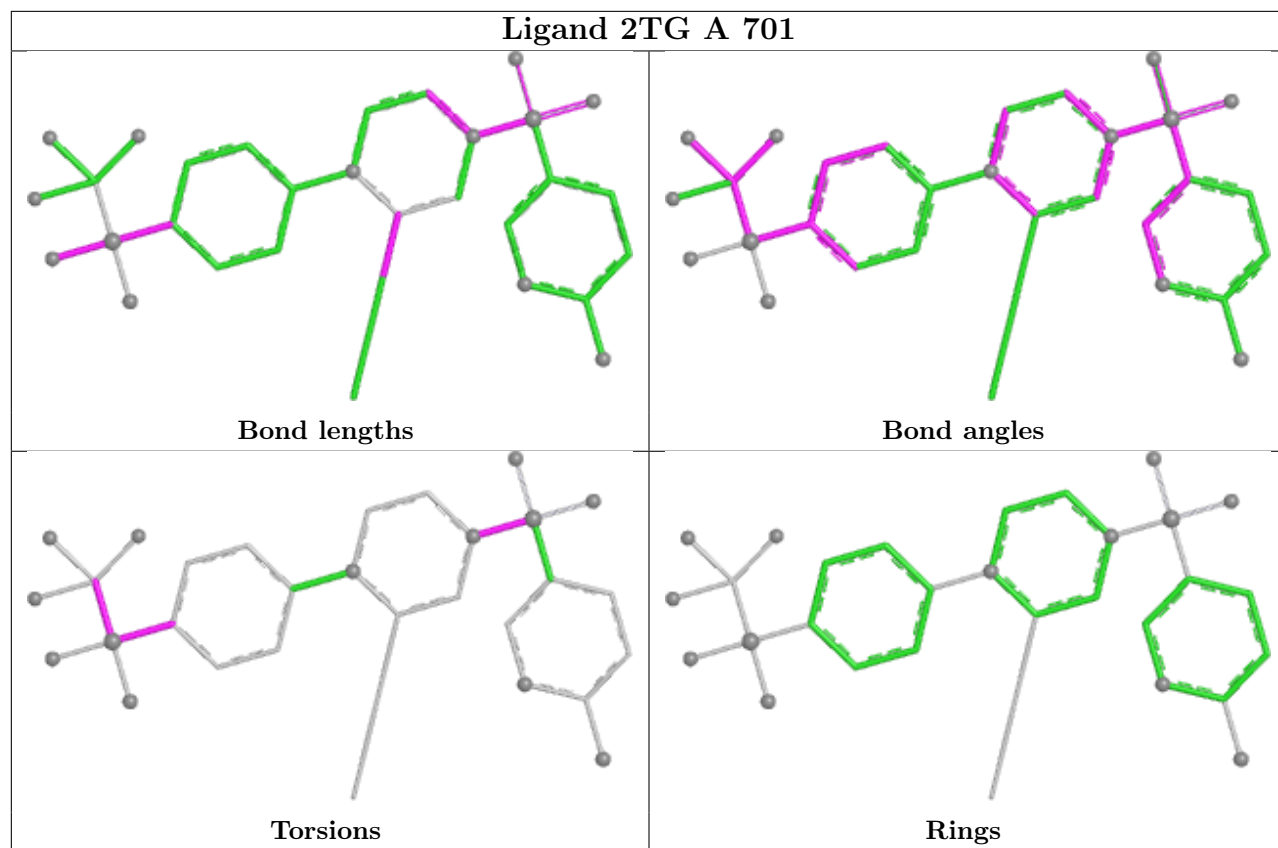
4 monomers are involved in 7 short contacts:

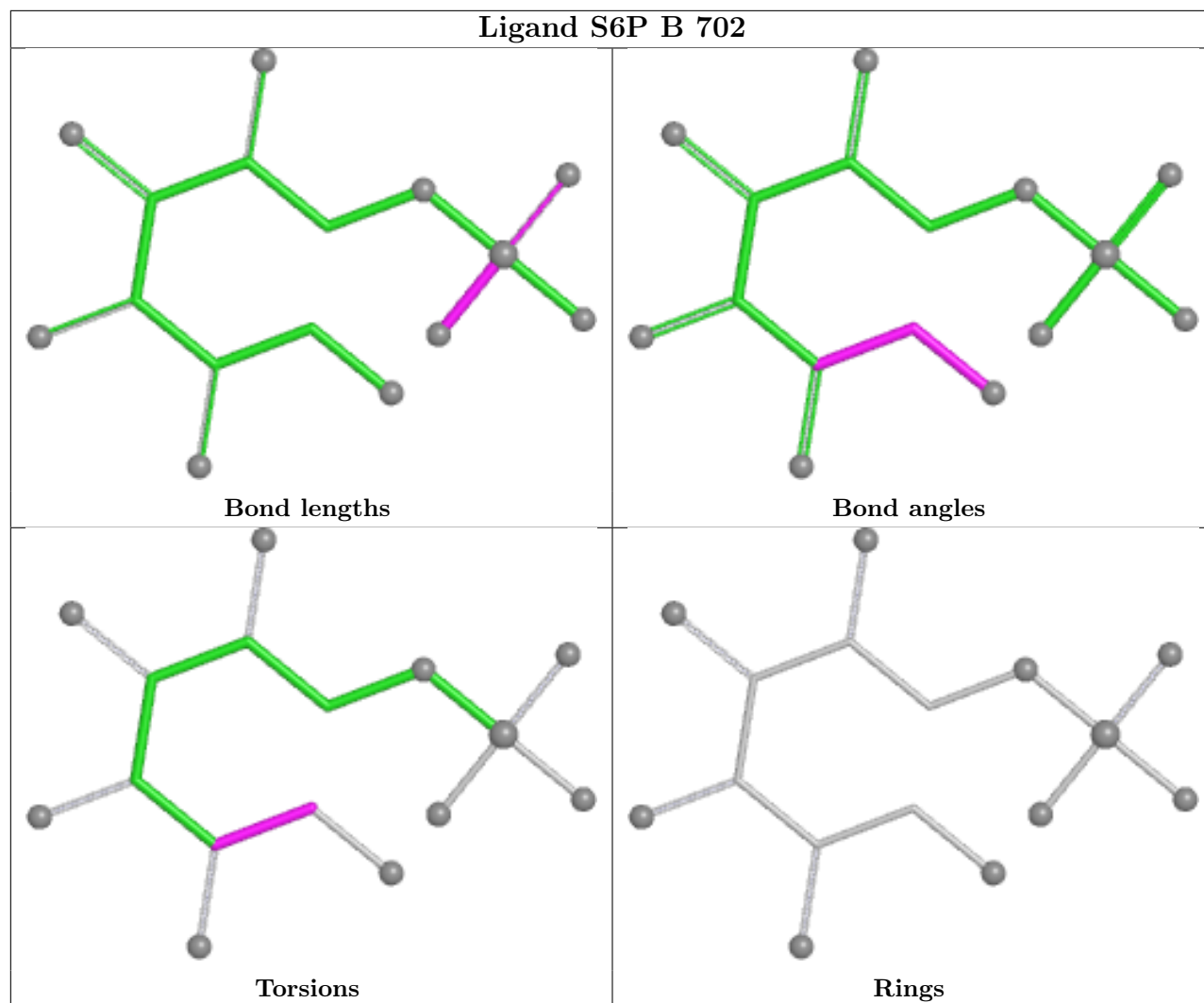
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	2TG	2	0
3	A	702	S6P	2	0
2	A	701	2TG	2	0
3	B	702	S6P	1	0

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, 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%)	0.30	31 (5%) 32 27	26, 49, 89, 128	0
1	B	590/638 (92%)	-0.02	16 (2%) 56 52	24, 44, 74, 124	0
All	All	1175/1276 (92%)	0.14	47 (4%) 42 38	24, 47, 81, 128	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LEU	6.6
1	A	387	PHE	5.2
1	A	465	PHE	5.0
1	A	464	LEU	4.1
1	B	448	PRO	4.0
1	B	447	ILE	3.8
1	A	430	THR	3.8
1	A	69	SER	3.7
1	B	366	GLY	3.7
1	B	5	LYS	3.5
1	B	465	PHE	3.3
1	A	429	LYS	3.2
1	A	400	LEU	3.1
1	A	447	ILE	3.1
1	A	357	PHE	3.1
1	B	454	PRO	3.1
1	B	1	MET	3.1
1	A	452	LEU	3.0
1	B	65	GLY	3.0
1	A	448	PRO	3.0
1	B	381	GLN	2.9
1	A	403	ILE	2.9
1	B	235	LYS	2.9
1	A	393	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	358	ARG	2.9
1	B	66	GLN	2.8
1	A	365	ILE	2.7
1	B	357	PHE	2.6
1	A	454	PRO	2.6
1	A	456	ILE	2.5
1	A	65	GLY	2.4
1	A	463	LEU	2.4
1	A	458	SER	2.4
1	A	1	MET	2.4
1	A	606	ALA	2.4
1	A	386	THR	2.4
1	A	469	GLU	2.4
1	A	385	PHE	2.3
1	B	21	LEU	2.3
1	B	70	THR	2.3
1	A	455	SER	2.2
1	A	235	LYS	2.2
1	B	451	LYS	2.2
1	A	283	GLN	2.2
1	B	69	SER	2.2
1	A	450	LYS	2.0
1	A	131	LYS	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 oligosaccharides 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.

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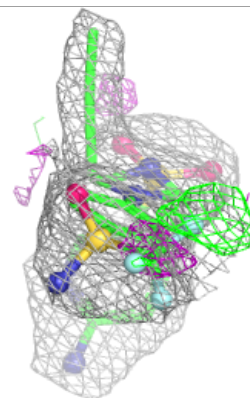
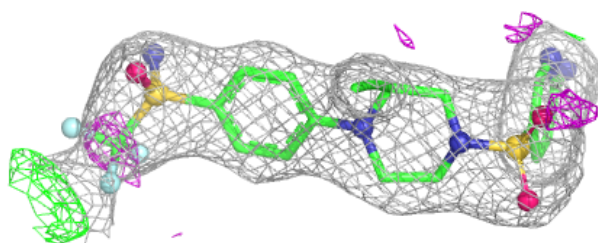
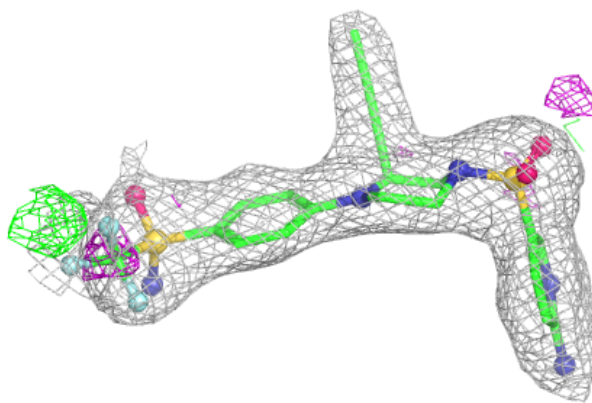
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	B	717	5/5	0.83	0.10	68,71,82,92	0
4	IOD	A	710	1/1	0.86	0.17	85,85,85,85	1
6	SO4	B	718	5/5	0.87	0.13	58,61,87,88	0
4	IOD	A	712	1/1	0.89	0.11	72,72,72,72	1
5	GOL	B	716	6/6	0.91	0.11	57,60,67,69	0
4	IOD	B	713	1/1	0.91	0.10	73,73,73,73	1
4	IOD	B	714	1/1	0.91	0.09	72,72,72,72	1
4	IOD	B	711	1/1	0.92	0.13	87,87,87,87	1
4	IOD	A	711	1/1	0.93	0.07	70,70,70,70	1
4	IOD	B	715	1/1	0.94	0.14	87,87,87,87	1
4	IOD	A	703	1/1	0.94	0.07	80,80,80,80	0
6	SO4	B	719	5/5	0.94	0.10	35,36,38,41	5
4	IOD	A	714	1/1	0.95	0.07	66,66,66,66	1
4	IOD	A	709	1/1	0.95	0.10	91,91,91,91	1
4	IOD	A	713	1/1	0.95	0.07	67,67,67,67	1
2	2TG	B	701	32/32	0.96	0.09	27,32,71,93	0
2	2TG	A	701	32/32	0.96	0.09	29,34,82,90	0
4	IOD	B	709	1/1	0.96	0.07	79,79,79,79	1
4	IOD	A	706	1/1	0.96	0.07	82,82,82,82	0
4	IOD	B	712	1/1	0.96	0.06	61,61,61,61	1
4	IOD	A	708	1/1	0.96	0.10	86,86,86,86	1
4	IOD	B	708	1/1	0.97	0.06	66,66,66,66	1
4	IOD	A	707	1/1	0.97	0.05	55,55,55,55	1
4	IOD	B	710	1/1	0.97	0.12	96,96,96,96	1
4	IOD	B	706	1/1	0.98	0.03	50,50,50,50	0
4	IOD	B	707	1/1	0.98	0.05	73,73,73,73	0
3	S6P	B	702	16/16	0.98	0.05	23,25,30,32	0
3	S6P	A	702	16/16	0.98	0.05	25,30,34,35	0
4	IOD	A	704	1/1	0.98	0.04	59,59,59,59	0
4	IOD	B	703	1/1	0.98	0.04	53,53,53,53	0
4	IOD	B	705	1/1	0.98	0.08	65,65,65,65	0
4	IOD	B	704	1/1	0.99	0.03	53,53,53,53	0
4	IOD	A	705	1/1	0.99	0.06	60,60,60,60	1

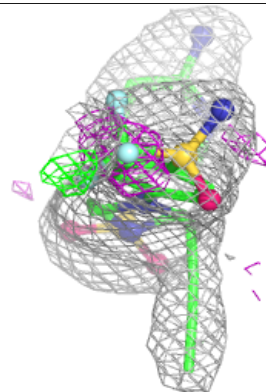
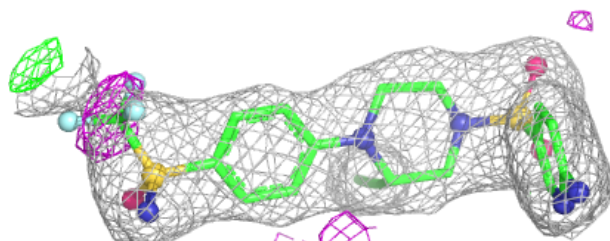
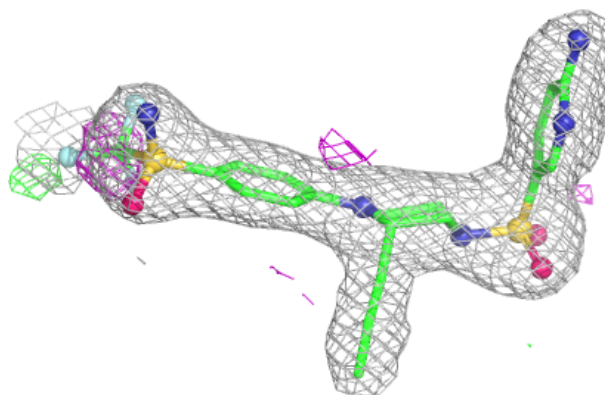
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2TG 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)

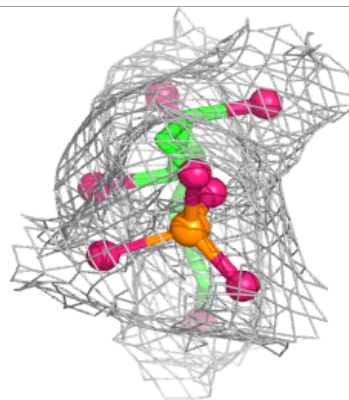
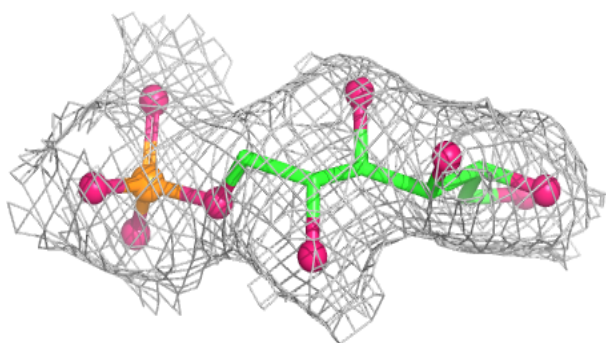
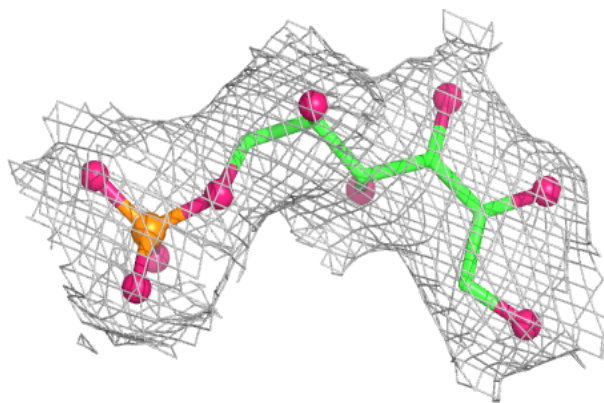
**Electron density around 2TG A 701:**

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

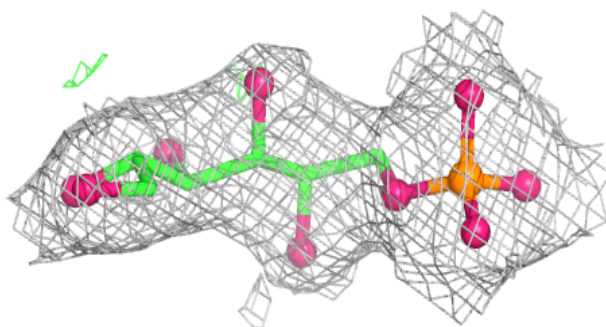
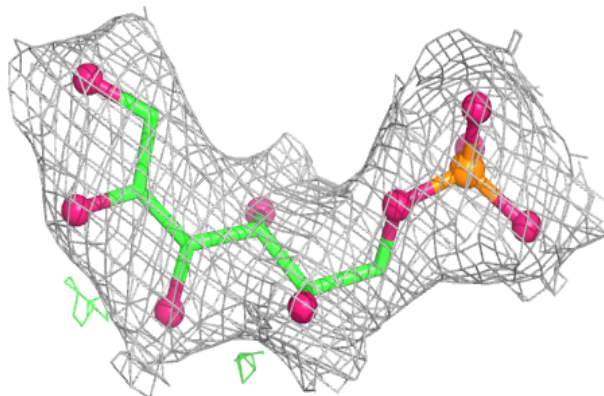


**Electron density around S6P B 702:**

$2mF_o-DF_c$  (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.