



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:48 AM UTC

PDB ID : 4OP1 / pdb_00004op1
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

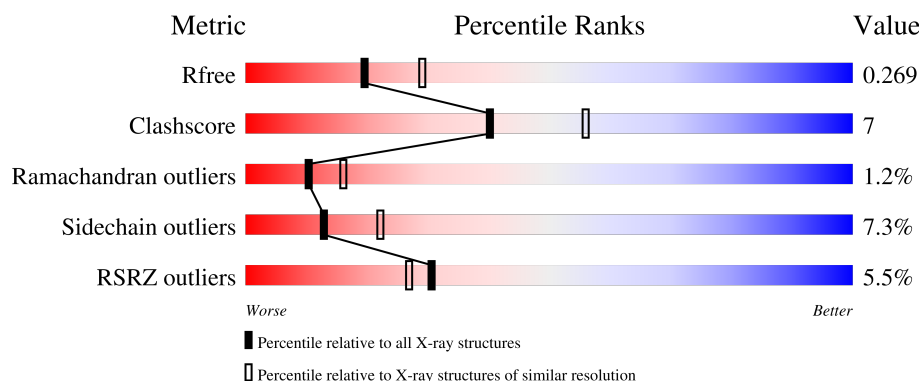
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	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	B	713	-	-	X	-

2 Entry composition [i](#)

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:

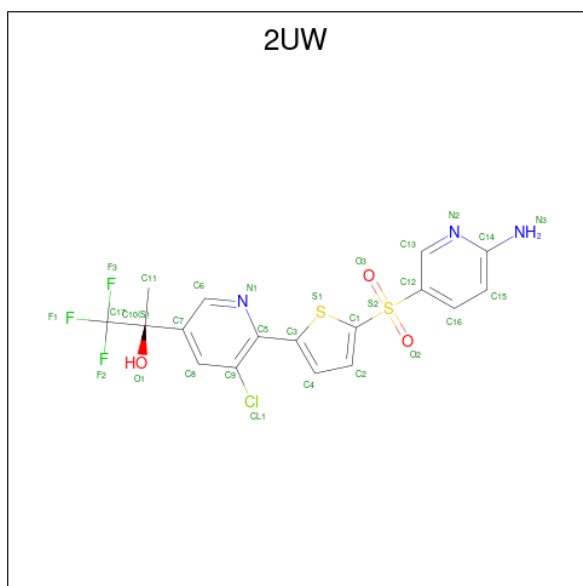
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q14397
A	-10	ALA	-	expression tag	UNP Q14397
A	-9	HIS	-	expression tag	UNP Q14397
A	-8	HIS	-	expression tag	UNP Q14397
A	-7	HIS	-	expression tag	UNP Q14397
A	-6	HIS	-	expression tag	UNP Q14397
A	-5	HIS	-	expression tag	UNP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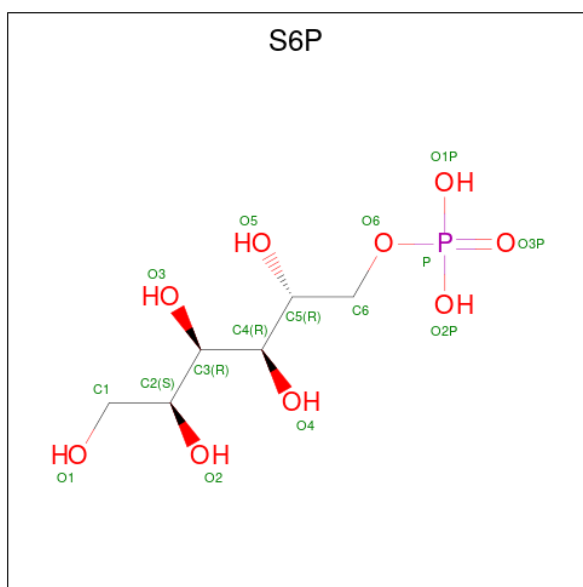
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	expression tag	UNP Q14397

- Molecule 2 is (2S)-2-(6-{5-[(6-aminopyridin-3-yl)sulfonyl]thiophen-2-yl}-5-chloropyridin-3-yl)-1,1,1-trifluoropropan-2-ol (CCD ID: 2UW) (formula: C₁₇H₁₃ClF₃N₃O₃S₂).



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

- Molecule 3 is D-SORBITOL-6-PHOSPHATE (CCD ID: S6P) (formula: C₆H₁₅O₉P).

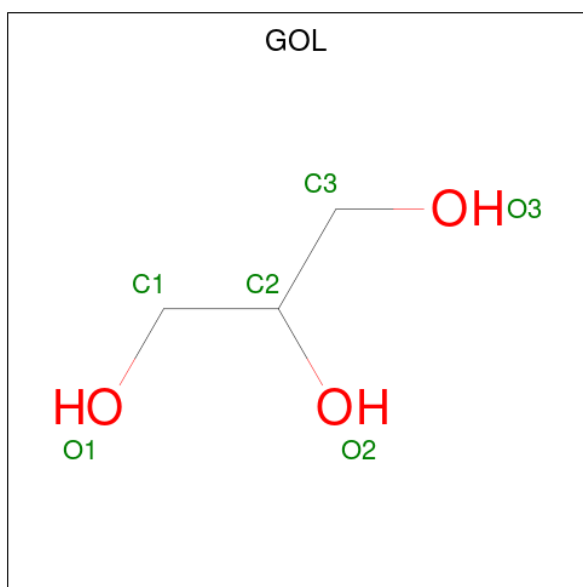


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

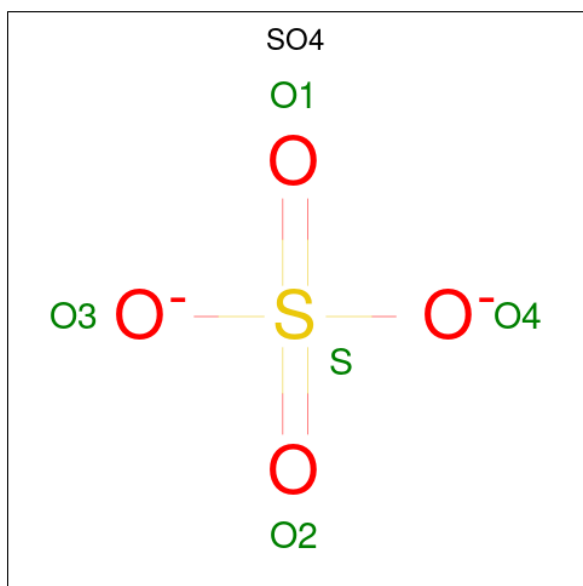
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	I	0	0
			13	13		
4	B	15	Total	I	0	0
			15	15		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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: O₄S).



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

- Molecule 1: Glucokinase Regulatory Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	149.18Å 149.18Å 132.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.39 50.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	86.9 (50.00-2.39) 87.0 (50.00-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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 ²)	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.*

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

5.1 Standard geometry

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

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	0.98	0/4603	1.09	7/6228 (0.1%)
1	B	1.02	0/4637	1.11	7/6274 (0.1%)
All	All	1.00	0/9240	1.10	14/12502 (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 (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	452	LEU	N-CA-C	-6.80	104.46	112.89
1	B	434	GLN	N-CA-C	-6.73	98.49	108.79
1	A	443	GLN	N-CA-C	-6.41	100.13	110.32
1	A	450	LYS	N-CA-C	-6.10	105.80	113.18
1	A	103	VAL	CB-CA-C	-5.95	102.75	110.84
1	B	495	VAL	CB-CA-C	-5.57	104.84	111.97
1	B	200	VAL	CB-CA-C	-5.53	105.19	111.55
1	A	71	TYR	N-CA-C	5.51	118.91	110.20
1	A	15	GLU	CA-C-N	-5.19	114.42	119.76
1	A	15	GLU	C-N-CA	-5.19	114.42	119.76
1	B	35	ASN	CA-C-N	-5.11	113.66	119.28
1	B	35	ASN	C-N-CA	-5.11	113.66	119.28
1	B	290	ARG	N-CA-C	-5.05	105.67	111.07
1	B	225	THR	N-CA-C	-5.04	102.33	110.14

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	73	0
1	B	4554	0	4647	47	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	2	0
4	B	15	0	0	6	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	122	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 7.

All (122) 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:S1	2:A:701:2UW:CL1	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:512:ASN:C	1:A:512:ASN:HD22	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:O	1:A:431:ASN:ND2	2.30	0.65
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: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: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:130:GLN:O	1:A:131:LYS:HB2	2.02	0.59
1:A:332:LEU:HB3	1:A:342:ALA:HB1	1.84	0.58
1:A:203:PRO:HB2	1:A:233:MET:HE3	1.86	0.57
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:CG1	1:A:146:VAL:O	2.53	0.57
1:A:35:ASN:C	1:A:35:ASN:HD22	2.13	0.56
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.53	0.56
1:A:125:MET:HE1	1:A:133:LEU:HG	1.88	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:49:ILE:HD12	1:A:317:MET:HE1	1.90	0.53
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:6:ARG:HD3	1:A:555:ALA:O	2.09	0.52
1:B:112:ARG:HD3	1:B:344:MET:HG2	1.91	0.52
1:A:450:LYS:C	1:A:452:LEU:H	2.17	0.52
1:A:146:VAL:O	1:A:146:VAL:HG12	2.10	0.51
1:B:508:LEU:C	1:B:508:LEU:HD12	2.36	0.51
1:A:117:MET:HE1	1:A:270:LEU:HD12	1.94	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:531:LYS:NZ	4:A:711:IOD:I	3.11	0.49
1:A:452:LEU:H	1:A:452:LEU:HD12	1.77	0.49
1:A:365:ILE:N	1:A:365:ILE:HD12	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: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:O	1:A:18:LYS:HD2	2.16	0.46
1:B:312:LYS:NZ	1:B:456:ILE:O	2.46	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: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:117:MET:HE1	1:A:270:LEU:CD1	2.45	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:HE1	1.98	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:A:158:HIS:O	1:A:159:GLY:C	2.61	0.44
1:A:447:ILE:HG22	1:A:449:LEU:C	2.43	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:A:512:ASN:C	1:A:512:ASN:ND2	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:LEU:O	1:B:446:PRO:C	2.62	0.42
1:A:30:ILE:HD12	1:A:210:PRO:HD3	2.01	0.42
1:A:267:LYS:O	1:A:268:ILE:C	2.62	0.42
1:A:427:LYS:O	1:A:427:LYS:HE2	2.19	0.42
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.80	0.42
1:A:450:LYS:C	1:A:452:LEU:N	2.77	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:B:35:ASN:O	1:B:36:PRO:C	2.60	0.42
1:A:461:TRP:O	1:A:462:PRO:C	2.63	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
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:A:461:TRP:C	1:A:462:PRO:O	2.63	0.41
1:B:24:TYR:CD1	1:B:24:TYR:C	2.99	0.41
1:B:74:LEU:HD21	1:B:296:LEU:HD22	2.03	0.41
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.93	0.41
1:A:473:ILE:O	1:A:473:ILE:HD13	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:49:ILE:CD1	1:A:317:MET:HE1	2.51	0.41
1:A:15:GLU:O	1:A:16:PRO:C	2.62	0.40
1:A:335:TRP:CZ2	1:A:419:VAL:HG22	2.56	0.40
1:A:591:LEU:HD12	1:A:591:LEU:HA	1.85	0.40
1:B:246:ASN:HD22	1:B:246:ASN:N	2.18	0.40
1:B:280:THR:O	1:B:281:VAL:C	2.62	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
1:B:344:MET:O	1:B:345:ASP:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	7	10
1	B	584/638 (92%)	561 (96%)	19 (3%)	4 (1%)	18	28
All	All	1163/1276 (91%)	1100 (95%)	49 (4%)	14 (1%)	10	16

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
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 ⓘ

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%)	451 (91%)	47 (9%)	8	13
1	B	501/542 (92%)	475 (95%)	26 (5%)	21	36
All	All	999/1084 (92%)	926 (93%)	73 (7%)	13	22

All (73) 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	25	GLU
1	A	35	ASN
1	A	98	ASP
1	A	143	ARG
1	A	166	VAL
1	A	170	LYS
1	A	198	THR
1	A	227	ARG
1	A	239	LYS
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	332	LEU
1	A	358	ARG
1	A	361	ARG
1	A	395	SER
1	A	397	LEU
1	A	399	SER
1	A	420	GLN
1	A	427	LYS
1	A	428	GLU
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	469	GLU
1	A	473	ILE
1	A	478	ARG
1	A	489	VAL

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Mol	Chain	Res	Type
1	A	500	ILE
1	A	503	ASN
1	A	512	ASN
1	A	605	LEU
1	B	6	ARG
1	B	21	LEU
1	B	47	GLU
1	B	69	SER
1	B	70	THR
1	B	72	GLN
1	B	84	VAL
1	B	126	LYS
1	B	143	ARG
1	B	166	VAL
1	B	171	LYS
1	B	225	THR
1	B	227	ARG
1	B	246	ASN
1	B	304	GLN
1	B	323	SER
1	B	337	THR
1	B	397	LEU
1	B	402	GLU
1	B	416	LEU
1	B	423	VAL
1	B	434	GLN
1	B	444	THR
1	B	445	LEU
1	B	456	ILE
1	B	503	ASN

Sometimes 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	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	289	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	9	HIS
1	B	39	GLN
1	B	48	ASN
1	B	55	GLN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	303	HIS
1	B	304	GLN
1	B	309	GLN
1	B	384	GLN
1	B	425	GLN
1	B	434	GLN
1	B	471	ASN
1	B	503	ASN
1	B	524	GLN
1	B	529	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
6	SO4	B	719	-	4,4,4	0.56	0	6,6,6	0.32	0
2	2UW	B	701	-	30,31,31	2.34	8 (26%)	43,49,49	3.76	21 (48%)
3	S6P	A	702	-	15,15,15	1.64	4 (26%)	20,21,21	1.19	2 (10%)
6	SO4	B	720	-	4,4,4	0.24	0	6,6,6	0.27	0
2	2UW	A	701	-	30,31,31	1.63	5 (16%)	43,49,49	2.37	14 (32%)
3	S6P	B	702	-	15,15,15	1.52	2 (13%)	20,21,21	0.87	0
5	GOL	B	718	-	5,5,5	0.61	0	5,5,5	0.67	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	2UW	B	701	-	-	15/31/31/31	0/3/3/3
3	S6P	A	702	-	-	1/20/20/20	-
2	2UW	A	701	-	-	8/31/31/31	0/3/3/3
3	S6P	B	702	-	-	0/20/20/20	-
5	GOL	B	718	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2UW	C17-C10	-6.11	1.44	1.52
2	B	701	2UW	C1-S1	-5.48	1.62	1.71
2	A	701	2UW	C5-C3	-5.12	1.40	1.46
3	B	702	S6P	P-O3P	4.60	1.64	1.50
2	B	701	2UW	O1-C10	-4.49	1.36	1.43
2	B	701	2UW	O3-S2	4.26	1.48	1.44
2	B	701	2UW	F2-C17	3.89	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2UW	C1-S2	-3.86	1.66	1.75
3	A	702	S6P	P-O3P	3.69	1.62	1.50
2	A	701	2UW	C1-S2	-3.50	1.67	1.75
2	B	701	2UW	C5-C3	-2.83	1.43	1.46
3	A	702	S6P	P-O2P	2.81	1.65	1.54
2	A	701	2UW	O3-S2	2.81	1.46	1.44
2	A	701	2UW	C17-C10	-2.65	1.49	1.52
2	A	701	2UW	C12-S2	-2.51	1.74	1.76
2	B	701	2UW	O2-S2	2.15	1.46	1.44
3	A	702	S6P	C6-C5	2.10	1.54	1.51
3	A	702	S6P	P-O1P	-2.07	1.47	1.54
3	B	702	S6P	P-O1P	-2.00	1.47	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2UW	F2-C17-C10	-13.17	93.77	112.40
2	B	701	2UW	C11-C10-C17	-8.90	97.23	109.04
2	A	701	2UW	O3-S2-C12	-7.09	100.57	108.03
2	B	701	2UW	F3-C17-F2	6.63	127.67	107.54
2	B	701	2UW	C1-S1-C3	6.17	95.88	90.41
2	B	701	2UW	O3-S2-C1	6.02	113.79	107.85
2	A	701	2UW	F2-C17-C10	-5.85	104.13	112.40
2	B	701	2UW	C4-C3-S1	-5.76	103.95	110.10
2	A	701	2UW	O3-S2-C1	5.53	113.31	107.85
2	A	701	2UW	F1-C17-C10	-5.53	104.59	112.40
2	B	701	2UW	O3-S2-O2	-5.51	113.41	118.73
2	B	701	2UW	C5-C3-S1	5.51	129.35	117.90
2	B	701	2UW	F3-C17-C10	-4.46	106.10	112.40
2	A	701	2UW	C17-C10-C7	3.92	114.32	109.25
2	B	701	2UW	C8-C7-C10	-3.92	115.73	120.52
2	B	701	2UW	F1-C17-F2	3.59	118.44	107.54
2	A	701	2UW	C11-C10-C17	-3.22	104.76	109.04
2	B	701	2UW	C17-C10-C7	3.21	113.40	109.25
2	B	701	2UW	O1-C10-C7	3.04	114.11	107.91
2	B	701	2UW	C6-N1-C5	3.02	123.12	117.92
2	A	701	2UW	C8-C9-C5	-2.81	119.03	121.88
2	B	701	2UW	C7-C6-N1	-2.74	120.81	123.38
2	B	701	2UW	C3-C5-N1	2.74	120.06	114.74
2	B	701	2UW	F1-C17-F3	-2.72	99.28	107.54
2	B	701	2UW	C2-C1-S1	-2.69	109.87	112.55
2	A	701	2UW	C5-C3-S1	2.68	123.47	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	S6P	O1-C1-C2	-2.45	106.01	111.16
2	B	701	2UW	C8-C9-CL1	-2.42	114.50	118.45
2	B	701	2UW	C6-C7-C10	2.36	125.78	121.52
2	A	701	2UW	C12-S2-C1	2.25	108.47	105.31
2	A	701	2UW	C12-C13-N2	-2.24	120.46	123.19
2	A	701	2UW	C15-C14-N3	-2.16	117.11	121.08
3	A	702	S6P	O6-P-O3P	2.14	112.23	106.44
2	A	701	2UW	C7-C6-N1	-2.12	121.39	123.38
2	A	701	2UW	F1-C17-F2	2.05	113.78	107.54
2	A	701	2UW	C6-N1-C5	2.05	121.45	117.92
2	B	701	2UW	O1-C10-C17	2.04	109.05	105.94

There are no chirality outliers.

All (26) torsion outliers are listed below:

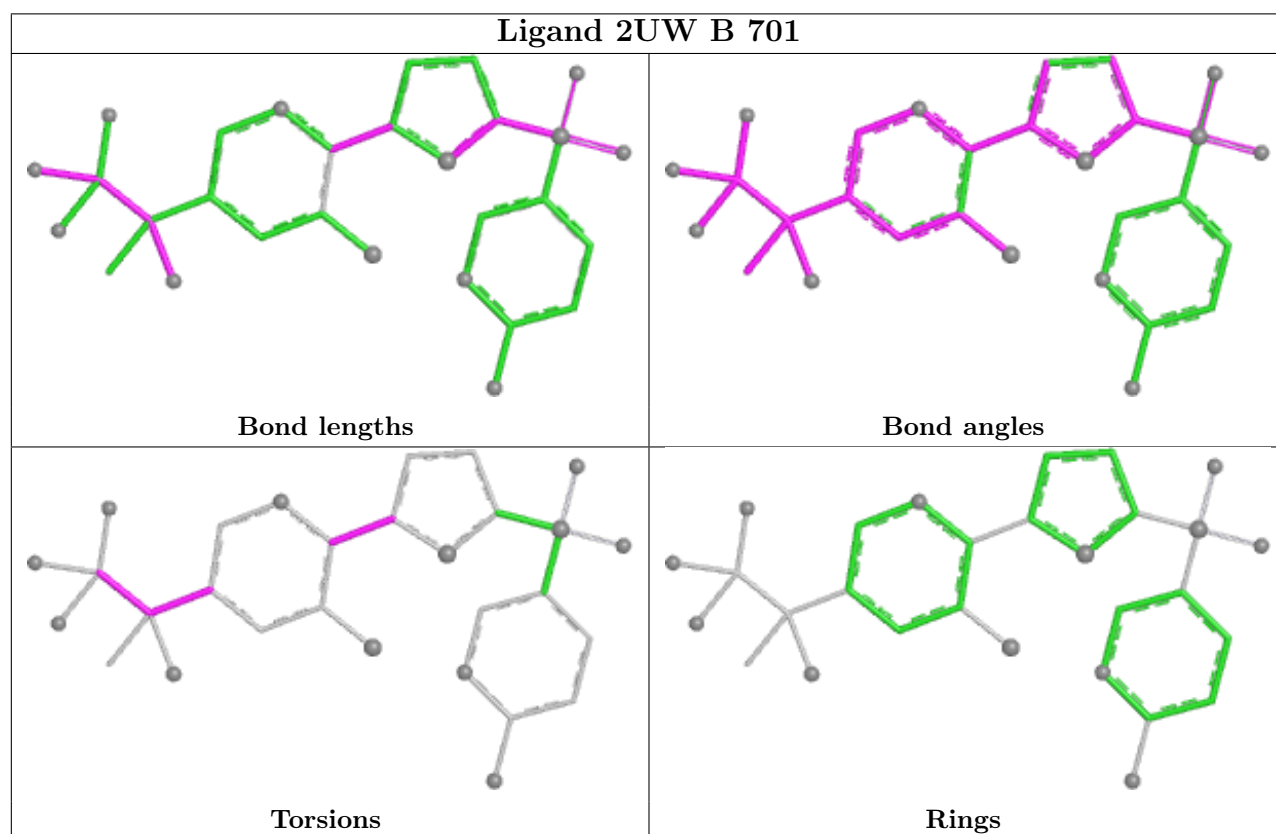
Mol	Chain	Res	Type	Atoms
2	A	701	2UW	C17-C10-C7-C8
2	B	701	2UW	C17-C10-C7-C8
2	B	701	2UW	C11-C10-C7-C6
2	B	701	2UW	C11-C10-C17-F2
2	B	701	2UW	C11-C10-C17-F1
2	B	701	2UW	O1-C10-C17-F2
2	B	701	2UW	O1-C10-C17-F1
5	B	718	GOL	O1-C1-C2-C3
5	B	718	GOL	O1-C1-C2-O2
2	B	701	2UW	O1-C10-C7-C8
2	B	701	2UW	C4-C3-C5-N1
2	A	701	2UW	C17-C10-C7-C6
2	B	701	2UW	O1-C10-C7-C6
2	B	701	2UW	C11-C10-C7-C8
2	A	701	2UW	S1-C3-C5-N1
2	B	701	2UW	S1-C3-C5-N1
2	B	701	2UW	C7-C10-C17-F1
2	A	701	2UW	C4-C3-C5-N1
3	A	702	S6P	C1-C2-C3-O3
2	A	701	2UW	C11-C10-C7-C6
2	A	701	2UW	C11-C10-C7-C8
2	A	701	2UW	S1-C3-C5-C9
2	B	701	2UW	S1-C3-C5-C9
2	A	701	2UW	C4-C3-C5-C9
2	B	701	2UW	C4-C3-C5-C9
2	B	701	2UW	C17-C10-C7-C6

There are no ring outliers.

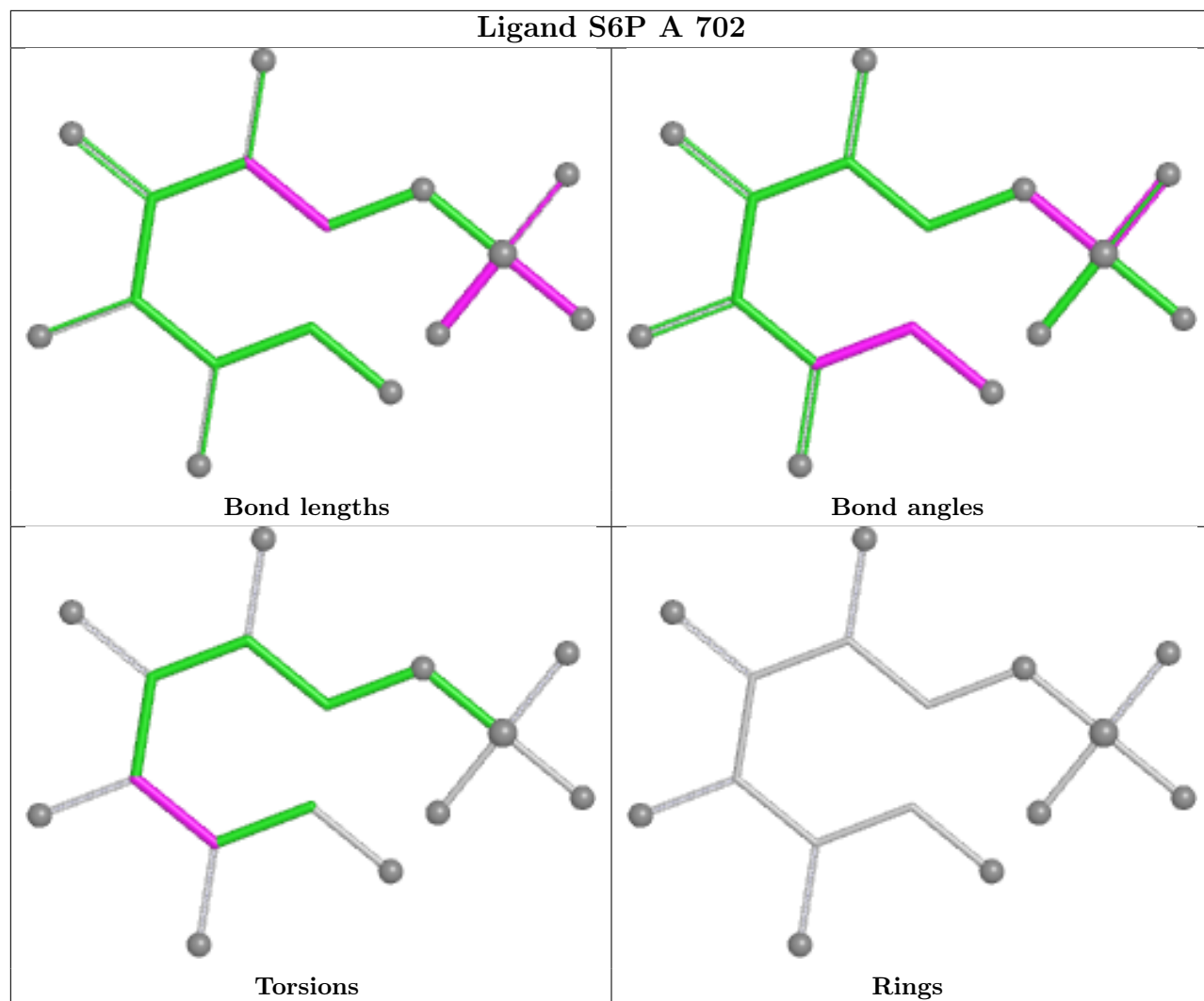
3 monomers are involved in 3 short contacts:

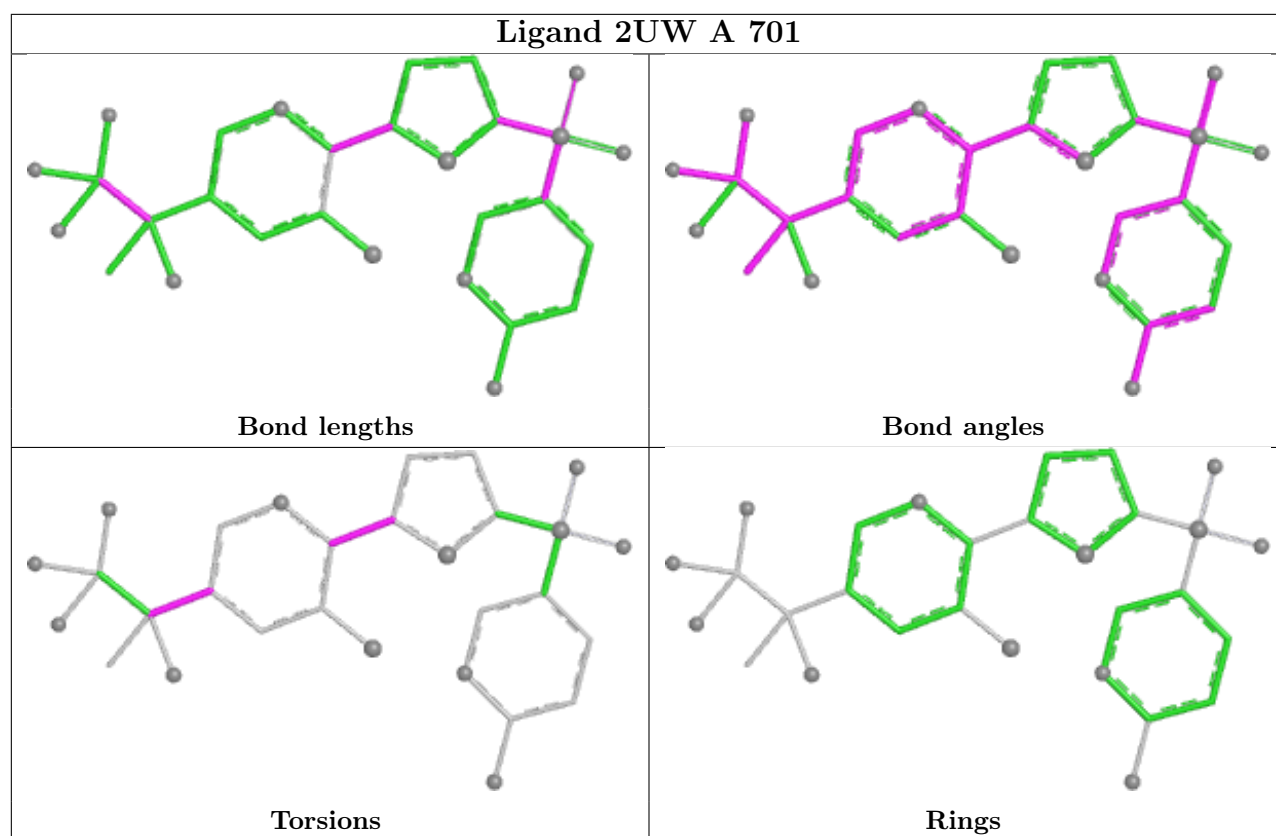
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	2UW	1	0
3	A	702	S6P	1	0
2	A	701	2UW	1	0

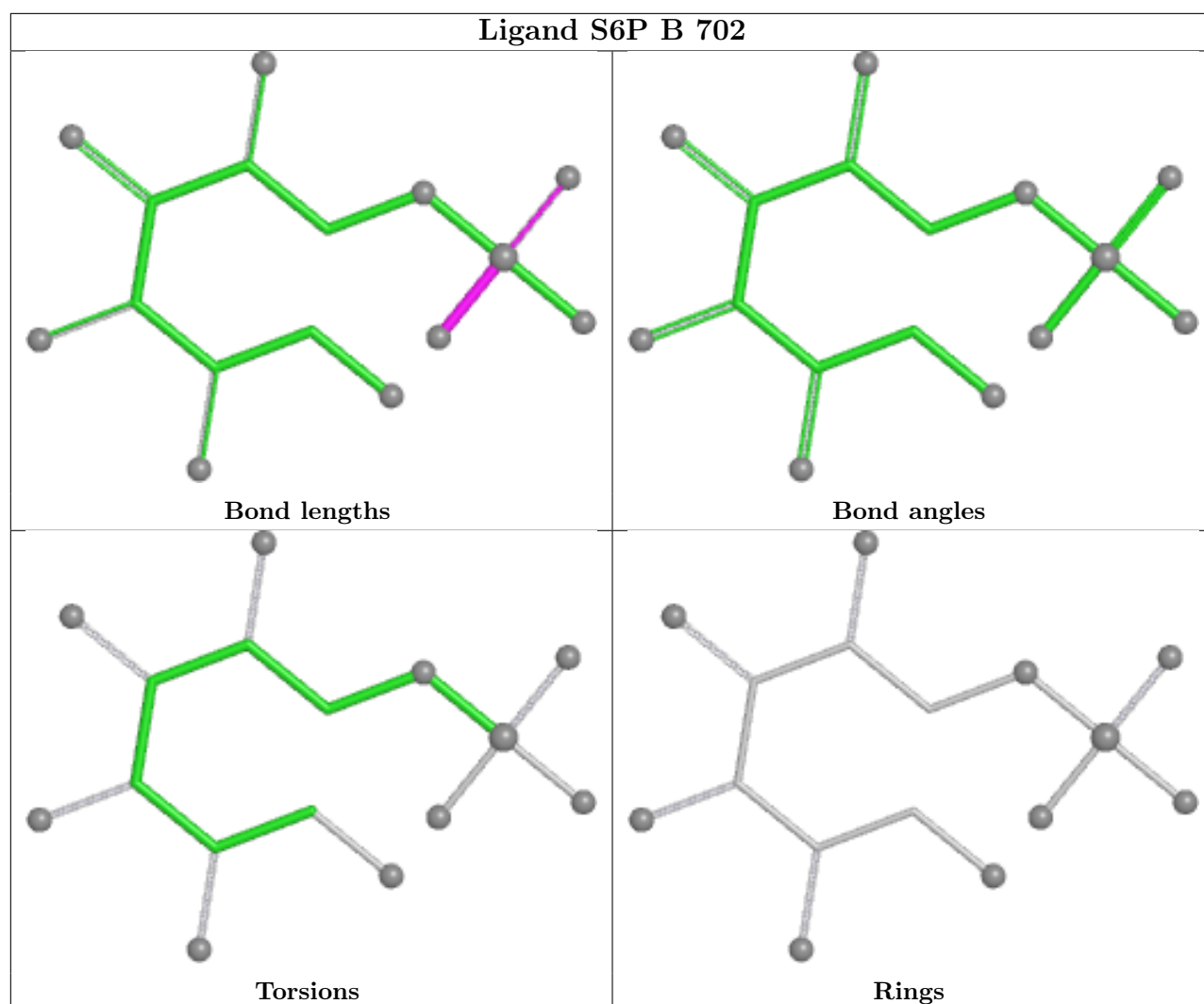
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 702







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	585/638 (91%)	0.52	45 (7%)	19 16	26, 46, 83, 127	0
1	B	590/638 (92%)	0.15	20 (3%)	48 44	23, 40, 69, 111	0
All	All	1175/1276 (92%)	0.33	65 (5%)	30 27	23, 43, 78, 127	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LEU	8.4
1	A	387	PHE	6.3
1	A	448	PRO	5.3
1	A	465	PHE	5.0
1	A	21	LEU	5.0
1	A	445	LEU	5.0
1	A	447	ILE	4.9
1	B	447	ILE	4.3
1	A	357	PHE	4.1
1	A	131	LYS	4.1
1	B	21	LEU	4.1
1	A	606	ALA	4.0
1	B	465	PHE	4.0
1	A	69	SER	3.8
1	A	429	LYS	3.8
1	A	397	LEU	3.6
1	A	403	ILE	3.6
1	A	358	ARG	3.5
1	B	381	GLN	3.4
1	B	66	GLN	3.4
1	A	463	LEU	3.3
1	A	454	PRO	3.3
1	B	1	MET	3.3
1	B	235	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	70	THR	3.2
1	A	410	PHE	3.2
1	A	469	GLU	3.2
1	A	430	THR	3.0
1	A	400	LEU	3.0
1	A	386	THR	2.9
1	A	464	LEU	2.9
1	A	452	LEU	2.8
1	B	366	GLY	2.8
1	B	131	LYS	2.8
1	A	392	PHE	2.7
1	A	456	ILE	2.7
1	B	5	LYS	2.6
1	B	18	LYS	2.6
1	A	1	MET	2.6
1	A	385	PHE	2.6
1	B	4	THR	2.6
1	A	363	PHE	2.5
1	A	453	PHE	2.5
1	A	365	ILE	2.5
1	A	450	LYS	2.5
1	B	454	PRO	2.5
1	B	65	GLY	2.5
1	A	18	LYS	2.4
1	A	420	GLN	2.4
1	A	282	ASP	2.3
1	A	451	LYS	2.3
1	A	441	VAL	2.3
1	A	466	PHE	2.3
1	A	393	LEU	2.3
1	A	331	TYR	2.3
1	B	463	LEU	2.2
1	A	390	GLU	2.2
1	A	460	THR	2.2
1	B	357	PHE	2.2
1	B	441	VAL	2.1
1	B	448	PRO	2.1
1	A	428	GLU	2.1
1	B	96	GLU	2.1
1	A	168	ALA	2.1
1	A	470	GLY	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, 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($\text{\AA}^2$)	Q<0.9
4	IOD	B	712	1/1	0.72	0.30	100,100,100,100	1
6	SO4	B	719	5/5	0.73	0.12	83,85,95,103	0
4	IOD	A	715	1/1	0.88	0.12	76,76,76,76	1
4	IOD	B	710	1/1	0.89	0.13	103,103,103,103	1
5	GOL	B	718	6/6	0.90	0.12	47,48,53,53	0
4	IOD	B	713	1/1	0.90	0.10	83,83,83,83	1
4	IOD	B	717	1/1	0.91	0.11	83,83,83,83	1
4	IOD	A	711	1/1	0.93	0.12	94,94,94,94	1
4	IOD	A	714	1/1	0.94	0.09	63,63,63,63	1
4	IOD	B	715	1/1	0.94	0.11	75,75,75,75	1
4	IOD	B	716	1/1	0.94	0.09	79,79,79,79	1
4	IOD	A	710	1/1	0.94	0.09	63,63,63,63	1
4	IOD	A	709	1/1	0.94	0.11	94,94,94,94	1
4	IOD	A	713	1/1	0.94	0.07	63,63,63,63	1
4	IOD	B	714	1/1	0.95	0.08	66,66,66,66	1
4	IOD	B	709	1/1	0.95	0.08	79,79,79,79	1
4	IOD	A	712	1/1	0.95	0.08	70,70,70,70	1
2	2UW	B	701	29/29	0.96	0.08	26,35,50,74	0
4	IOD	B	708	1/1	0.96	0.06	51,51,51,51	1
4	IOD	A	703	1/1	0.96	0.07	64,64,64,64	0
4	IOD	A	706	1/1	0.96	0.09	82,82,82,82	0
4	IOD	A	708	1/1	0.96	0.11	77,77,77,77	1
2	2UW	A	701	29/29	0.96	0.08	30,36,63,72	0
4	IOD	B	707	1/1	0.97	0.06	68,68,68,68	0
4	IOD	A	707	1/1	0.97	0.05	55,55,55,55	1
4	IOD	B	703	1/1	0.97	0.04	50,50,50,50	0
6	SO4	B	720	5/5	0.97	0.07	37,37,38,38	5

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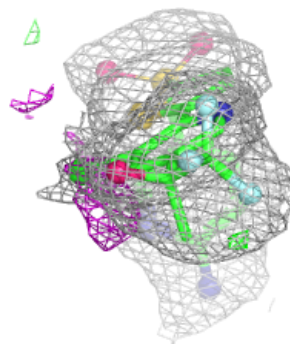
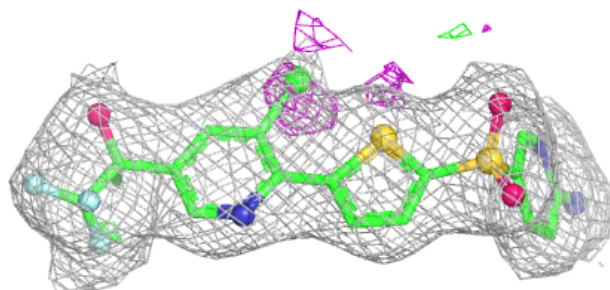
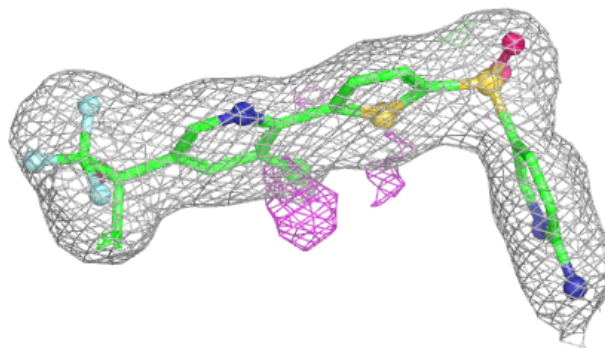
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IOD	A	705	1/1	0.98	0.04	46,46,46,46	1
3	S6P	B	702	16/16	0.98	0.04	20,22,24,24	0
3	S6P	A	702	16/16	0.98	0.05	24,29,33,37	0
4	IOD	A	704	1/1	0.98	0.05	60,60,60,60	0
4	IOD	B	711	1/1	0.98	0.07	66,66,66,66	1
4	IOD	B	705	1/1	0.98	0.03	46,46,46,46	1
4	IOD	B	706	1/1	0.98	0.04	45,45,45,45	1
4	IOD	B	704	1/1	0.99	0.03	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.

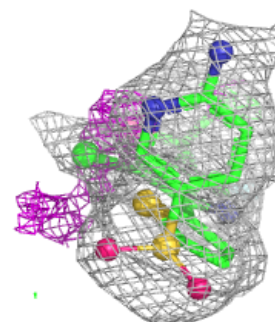
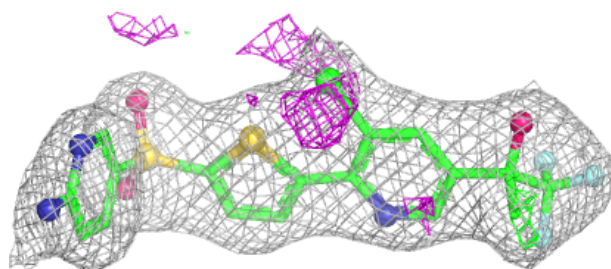
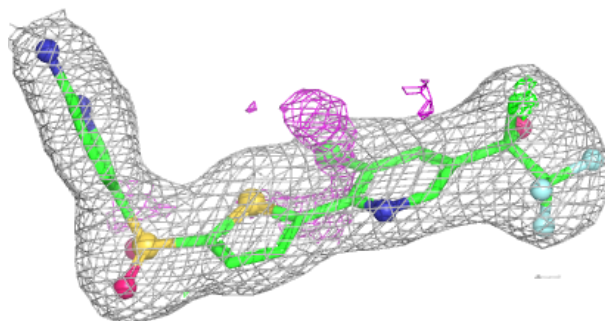
Electron density around 2UW B 701:

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

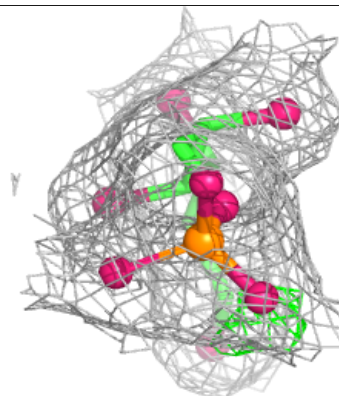
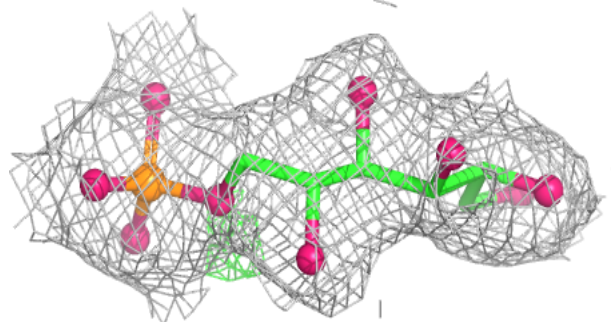
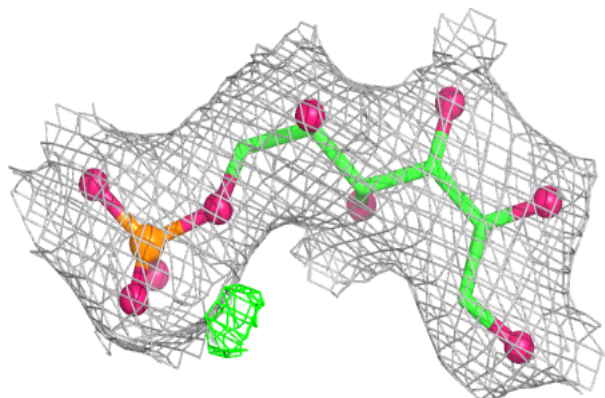


Electron density around 2UW A 701:

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

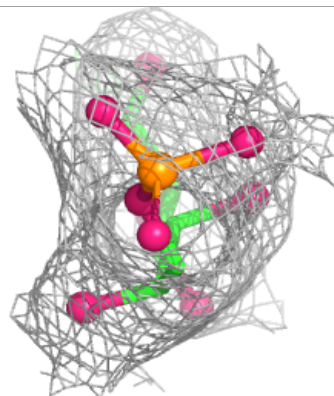
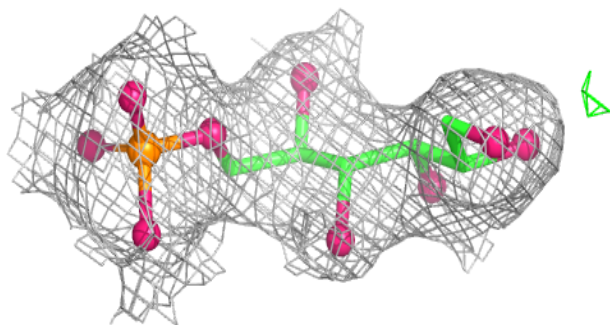
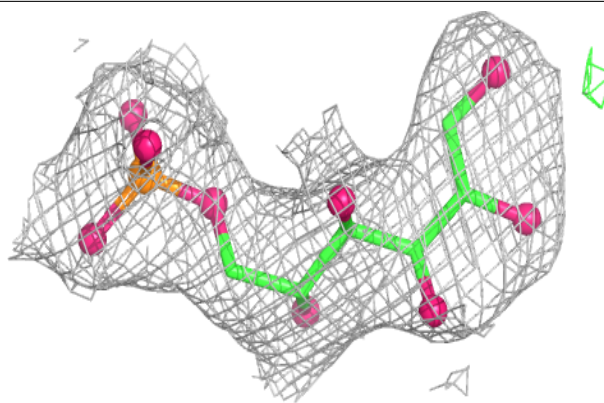
**Electron density around S6P B 702:**

$2mF_o-DF_c$ (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.