



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:06 PM UTC

PDB ID : 4PX3 / pdb_00004px3
Title : Human GKRP bound to AMG-3295 and Sorbitol-6-phosphate
Authors : Jordan, S.R.; Chmait, S.
Deposited on : 2014-03-21
Resolution : 2.43 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

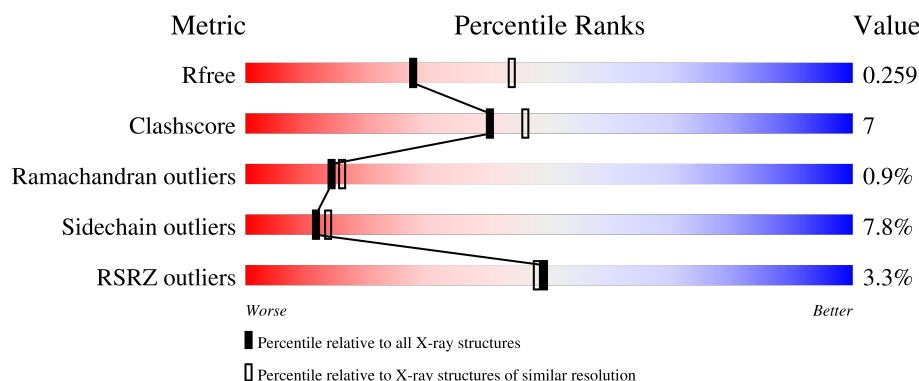
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	 4% 71% 17% • 8%
1	B	638	 2% 77% 13% • 8%

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	711	-	-	X	-
4	IOD	B	713	-	-	X	-
4	IOD	B	715	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9324 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:

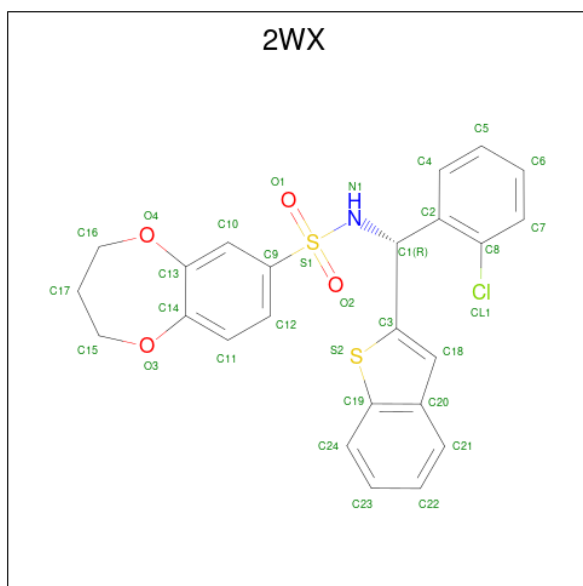
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q14397
A	-10	ALA	-	expression tag	UNP Q14397
A	-9	HIS	-	expression tag	UNP Q14397
A	-8	HIS	-	expression tag	UNP Q14397
A	-7	HIS	-	expression tag	UNP Q14397
A	-6	HIS	-	expression tag	UNP Q14397
A	-5	HIS	-	expression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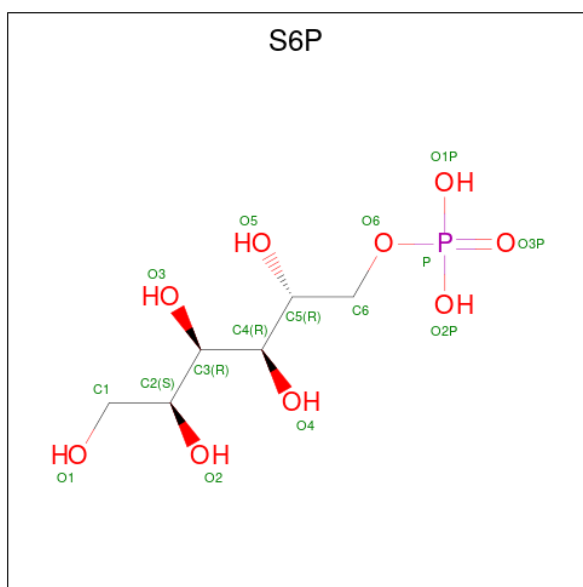
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	expression tag	UNP Q14397

- Molecule 2 is N-[(R)-1-benzothiophen-2-yl(2-chlorophenyl)methyl]-3,4-dihydro-2H-1,5-benzodioxepine-7-sulfonamide (CCD ID: 2WX) (formula: $C_{24}H_{20}ClNO_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			32	24	1	1	4	2		
2	B	1	Total	C	Cl	N	O	S	0	0
			32	24	1	1	4	2		

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

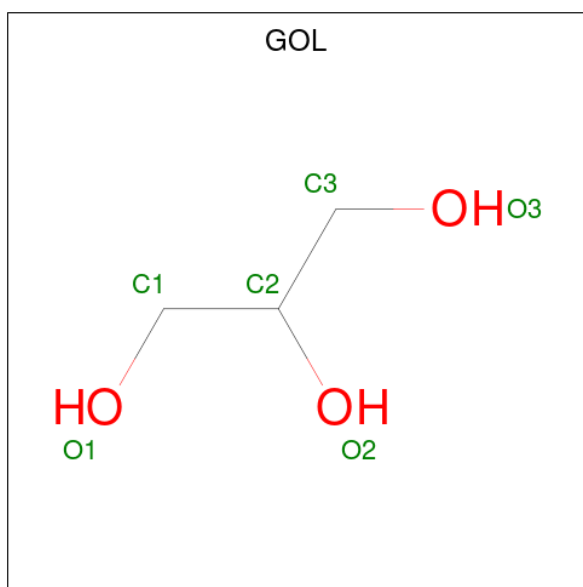


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

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

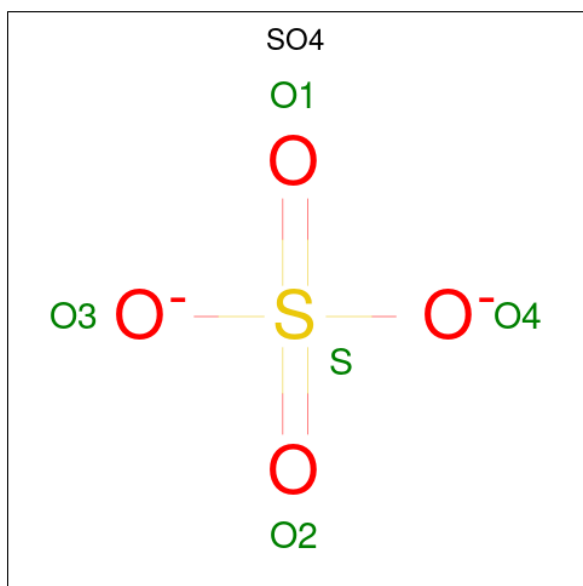
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	I	0	0
			13	13		
4	B	14	Total	I	0	0
			14	14		

- 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		
6	B	1	Total	O	S	0	0
			5	4	1		

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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		

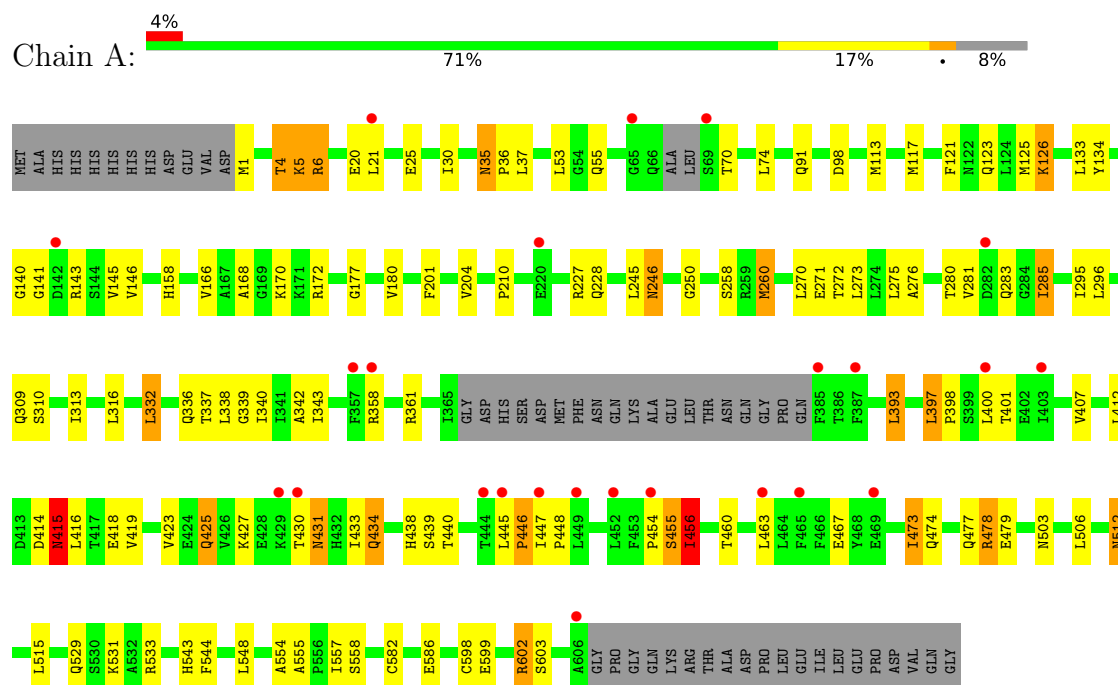
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	37	Total	O	0	0
			37	37		
7	B	58	Total	O	0	0
			58	58		

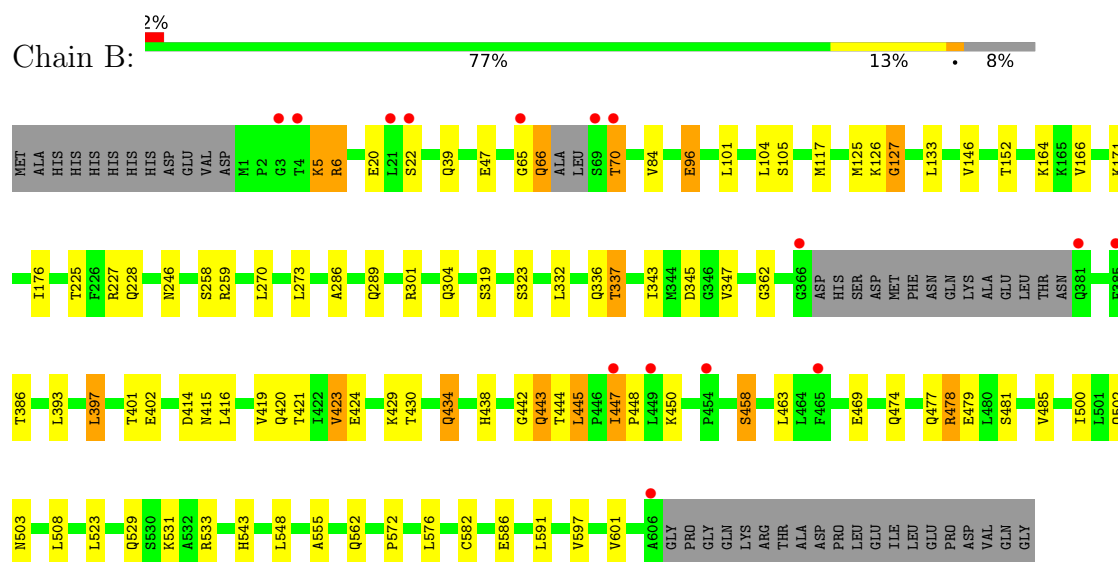
3 Residue-property plots

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

• Molecule 1: 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, α , β , γ	148.87Å 148.87Å 132.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.94 – 2.43 24.94 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.94-2.43) 99.8 (24.94-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.196 , 0.258 0.201 , 0.259	Depositor DCC
R_{free} test set	3152 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9324	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, IOD, GOL, 2WX, SO4

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	1.01	2/4603 (0.0%)	1.08	5/6228 (0.1%)
1	B	1.06	1/4637 (0.0%)	1.08	9/6274 (0.1%)
All	All	1.03	3/9240 (0.0%)	1.08	14/12502 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	GLY	C-O	-6.49	1.17	1.23
1	B	301	ARG	N-CA	5.70	1.53	1.46
1	A	204	VAL	N-CA	-5.01	1.40	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	SER	N-CA-C	6.19	119.58	109.24
1	B	434	GLN	N-CA-C	-6.17	99.69	109.07
1	A	70	THR	N-CA-C	6.13	117.46	108.14
1	B	336	GLN	CB-CA-C	-5.90	108.10	115.89
1	A	456	ILE	N-CA-C	5.56	120.90	109.34
1	B	152	THR	N-CA-C	5.47	119.57	113.01
1	A	434	GLN	N-CA-C	-5.32	100.83	108.60
1	B	319	SER	N-CA-C	-5.30	105.40	111.07
1	B	96	GLU	CA-C-N	5.21	125.66	120.04
1	B	96	GLU	C-N-CA	5.21	125.66	120.04
1	A	201	PHE	N-CA-C	5.06	118.06	109.76
1	B	543	HIS	N-CA-C	5.06	119.30	113.18
1	A	145	VAL	CB-CA-C	-5.02	105.46	112.04
1	B	301	ARG	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

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	76	0
1	B	4554	0	4647	49	0
2	A	32	0	20	0	0
2	B	32	0	20	0	0
3	A	16	0	13	0	0
3	B	16	0	13	1	0
4	A	13	0	0	5	0
4	B	14	0	0	7	0
5	B	6	0	8	1	0
6	B	25	0	0	0	0
7	A	37	0	0	0	0
7	B	58	0	0	0	0
All	All	9324	0	9339	123	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 (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.15	0.79
1:A:397:LEU:HD11	1:A:425:GLN:HB3	1.68	0.75
1:A:337:THR:HG21	1:A:479:GLU:OE2	1.86	0.74
1:B:458:SER:HB3	4:B:713:IOD:I	2.62	0.70
1:A:246:ASN:H	1:A:246:ASN:HD22	1.39	0.69
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.41	0.66
1:B:259:ARG:NH2	1:B:345:ASP:OD1	2.29	0.65
1:B:597:VAL:O	1:B:601:VAL:HG23	1.98	0.64
1:A:35:ASN:C	1:A:35:ASN:HD22	2.07	0.63
1:B:397:LEU:HD23	1:B:429:LYS:HE3	1.80	0.62
1:A:246:ASN:HD22	1:A:246:ASN:N	1.96	0.62
1:A:431:ASN:H	1:A:431:ASN:HD22	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ARG:HH11	1:A:602:ARG:HG3	1.66	0.61
1:A:433:ILE:O	1:A:434:GLN:HG2	2.01	0.61
1:B:146:VAL:HG12	1:B:146:VAL:O	2.01	0.60
1:B:393:LEU:HD23	1:B:397:LEU:HD12	1.83	0.60
1:A:439:SER:OG	1:A:460:THR:HG22	2.00	0.60
1:A:582:CYS:HB2	1:A:586:GLU:OE2	2.01	0.60
1:B:591:LEU:HD11	1:B:597:VAL:HG22	1.87	0.57
1:B:531:LYS:HE2	4:B:712:IOD:I	2.75	0.57
1:B:447:ILE:HG23	1:B:450:LYS:HE3	1.85	0.56
1:B:502:GLN:NE2	4:B:716:IOD:I	3.05	0.56
1:A:283:GLN:HB2	1:A:285:ILE:HG22	1.89	0.55
1:A:438:HIS:CG	1:A:478:ARG:HG2	2.41	0.55
1:B:419:VAL:O	1:B:423:VAL:HG12	2.07	0.55
1:B:164:LYS:HE2	5:B:717:GOL:H12	1.87	0.54
1:A:5:LYS:HB3	4:A:709:IOD:I	2.77	0.54
1:B:529:GLN:NE2	1:B:533:ARG:HE	2.05	0.54
1:B:337:THR:HG21	1:B:479:GLU:OE1	2.07	0.54
1:A:123:GLN:O	1:A:126:LYS:HG2	2.08	0.54
1:B:420:GLN:HA	1:B:423:VAL:HG13	1.88	0.54
1:B:445:LEU:HG	4:B:713:IOD:I	2.78	0.54
1:A:146:VAL:HG12	1:A:146:VAL:O	2.08	0.53
1:B:447:ILE:HG23	1:B:450:LYS:CE	2.38	0.53
1:A:415:ASN:HD22	1:A:418:GLU:H	1.57	0.53
1:A:419:VAL:O	1:A:423:VAL:HG23	2.08	0.53
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.74	0.52
1:B:125:MET:HE1	1:B:133:LEU:HD12	1.92	0.52
1:A:272:THR:HA	1:A:295:ILE:HG21	1.90	0.52
1:A:531:LYS:HE2	4:A:711:IOD:I	2.79	0.52
1:B:127:GLY:O	4:B:715:IOD:I	2.98	0.52
1:B:438:HIS:CG	1:B:478:ARG:HG2	2.46	0.51
1:B:6:ARG:HD2	1:B:555:ALA:O	2.11	0.51
1:A:309:GLN:HA	1:A:309:GLN:OE1	2.11	0.51
1:A:146:VAL:O	1:A:146:VAL:CG1	2.58	0.51
1:B:529:GLN:HE22	1:B:533:ARG:HH21	1.58	0.50
1:A:332:LEU:HB3	1:A:342:ALA:HB1	1.93	0.50
1:A:506:LEU:HD23	4:A:704:IOD:I	2.80	0.50
1:A:117:MET:HE1	1:A:270:LEU:CD1	2.42	0.50
1:A:1:MET:O	1:A:4:THR:OG1	2.23	0.50
1:A:180:VAL:HG11	1:A:258:SER:HB2	1.93	0.50
1:A:543:HIS:O	1:A:544:PHE:C	2.55	0.50
1:B:447:ILE:N	1:B:448:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:SER:HA	1:A:313:ILE:HD12	1.92	0.50
1:B:414:ASP:O	1:B:416:LEU:HD13	2.12	0.49
1:B:474:GLN:HA	1:B:477:GLN:OE1	2.12	0.49
1:A:339:GLY:O	1:A:342:ALA:HB3	2.12	0.49
1:A:20:GLU:HB3	1:A:21:LEU:HD22	1.95	0.49
1:B:332:LEU:O	1:B:362:GLY:HA2	2.13	0.48
1:B:258:SER:OG	3:B:702:S6P:H11	2.12	0.48
1:B:582:CYS:HB2	1:B:586:GLU:OE1	2.14	0.48
1:B:117:MET:HE1	1:B:270:LEU:HD12	1.95	0.48
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.79	0.47
1:A:30:ILE:HD12	1:A:210:PRO:HD3	1.96	0.47
1:A:91:GLN:HG2	1:A:281:VAL:HG13	1.95	0.47
1:B:225:THR:H	1:B:228:GLN:HE21	1.63	0.47
1:B:469:GLU:HG2	4:B:715:IOD:I	2.85	0.47
1:A:37:LEU:HD13	1:A:55:GLN:HG2	1.98	0.46
1:A:439:SER:HG	1:A:460:THR:HG22	1.78	0.46
1:A:283:GLN:HB2	1:A:285:ILE:CG2	2.46	0.46
1:A:439:SER:O	1:A:460:THR:HA	2.16	0.46
1:B:101:LEU:HD12	1:B:133:LEU:O	2.17	0.45
1:A:445:LEU:O	1:A:446:PRO:C	2.60	0.45
1:B:5:LYS:HB2	4:B:710:IOD:I	2.86	0.45
1:B:146:VAL:HG13	1:B:343:ILE:HG21	1.98	0.45
1:A:113:MET:HA	1:A:113:MET:HE2	1.99	0.45
1:A:271:GLU:O	1:A:272:THR:C	2.60	0.44
1:B:420:GLN:O	1:B:421:THR:C	2.60	0.44
1:B:481:SER:O	1:B:485:VAL:HG23	2.17	0.44
1:A:146:VAL:HG13	1:A:343:ILE:CG2	2.47	0.44
1:A:91:GLN:NE2	1:A:280:THR:OG1	2.50	0.44
1:A:430:THR:HG22	1:A:431:ASN:N	2.32	0.44
1:A:512:ASN:C	1:A:512:ASN:HD22	2.26	0.44
1:A:6:ARG:HD3	1:A:555:ALA:O	2.18	0.44
1:A:414:ASP:O	1:A:416:LEU:HD12	2.17	0.44
1:A:473:ILE:HD13	1:A:473:ILE:O	2.18	0.44
1:A:53:LEU:HD13	1:A:260:MET:HE1	1.99	0.44
1:A:121:PHE:HB3	1:A:134:TYR:CE2	2.53	0.44
1:A:332:LEU:HD12	1:A:407:VAL:HB	1.99	0.44
1:A:397:LEU:HB3	1:A:398:PRO:HD3	1.99	0.44
1:B:66:GLN:HE21	1:B:66:GLN:HB2	1.63	0.44
1:A:412:LEU:HD23	1:A:412:LEU:N	2.32	0.43
1:B:104:LEU:CD2	1:B:176:ILE:HD12	2.48	0.43
1:B:146:VAL:HG13	1:B:343:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD12	1:A:338:LEU:N	2.34	0.43
1:A:74:LEU:HD21	1:A:296:LEU:HD22	2.00	0.43
1:A:447:ILE:N	1:A:448:PRO:HD2	2.33	0.43
1:A:125:MET:HE1	1:A:133:LEU:HG	2.00	0.43
1:A:35:ASN:HD22	1:A:36:PRO:N	2.16	0.42
1:B:529:GLN:HE21	1:B:533:ARG:HE	1.67	0.42
1:A:113:MET:HE2	1:A:113:MET:N	2.35	0.42
1:B:523:LEU:HD23	1:B:523:LEU:HA	1.82	0.42
1:A:431:ASN:HD22	1:A:431:ASN:N	2.15	0.42
1:B:572:PRO:O	1:B:576:LEU:HG	2.19	0.42
1:A:283:GLN:CB	1:A:285:ILE:HG22	2.50	0.42
1:A:431:ASN:H	1:A:431:ASN:ND2	2.15	0.42
1:A:393:LEU:O	1:A:397:LEU:HB3	2.19	0.41
1:A:6:ARG:HD2	1:A:554:ALA:O	2.20	0.41
1:A:250:GLY:HA2	4:A:705:IOD:I	2.90	0.41
1:A:512:ASN:ND2	1:A:515:LEU:H	2.19	0.41
1:A:531:LYS:CE	4:A:711:IOD:I	3.38	0.41
1:A:140:GLY:H	1:A:158:HIS:HE1	1.68	0.41
1:A:397:LEU:O	1:A:400:LEU:HD13	2.21	0.41
1:B:65:GLY:O	1:B:70:THR:OG1	2.19	0.41
1:B:508:LEU:C	1:B:508:LEU:HD12	2.46	0.41
1:A:337:THR:HA	1:A:340:ILE:HD12	2.03	0.41
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.68	0.41
1:A:275:LEU:O	1:A:276:ALA:C	2.63	0.41
1:B:415:ASN:C	1:B:415:ASN:HD22	2.29	0.40
1:A:548:LEU:HA	1:A:548:LEU:HD23	1.84	0.40
1:A:228:GLN:HE22	1:B:228:GLN:NE2	2.12	0.40
1:A:455:SER:O	1:A:456:ILE:O	2.39	0.40
1:B:442:GLY:O	1:B:443:GLN:C	2.64	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%)	537 (93%)	35 (6%)	7 (1%)	10	10
1	B	584/638 (92%)	554 (95%)	27 (5%)	3 (0%)	24	29
All	All	1163/1276 (91%)	1091 (94%)	62 (5%)	10 (1%)	14	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ILE
1	B	443	GLN
1	A	141	GLY
1	A	168	ALA
1	A	415	ASN
1	B	548	LEU
1	A	454	PRO
1	B	127	GLY
1	A	260	MET
1	A	446	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%)	457 (92%)	41 (8%)	10	12
1	B	501/542 (92%)	464 (93%)	37 (7%)	13	15
All	All	999/1084 (92%)	921 (92%)	78 (8%)	11	13

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

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	LYS
1	A	6	ARG
1	A	25	GLU
1	A	35	ASN
1	A	98	ASP

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Mol	Chain	Res	Type
1	A	126	LYS
1	A	143	ARG
1	A	166	VAL
1	A	170	LYS
1	A	172	ARG
1	A	227	ARG
1	A	245	LEU
1	A	246	ASN
1	A	273	LEU
1	A	285	ILE
1	A	316	LEU
1	A	332	LEU
1	A	358	ARG
1	A	361	ARG
1	A	393	LEU
1	A	397	LEU
1	A	401	THR
1	A	415	ASN
1	A	425	GLN
1	A	427	LYS
1	A	431	ASN
1	A	440	THR
1	A	455	SER
1	A	463	LEU
1	A	467	GLU
1	A	473	ILE
1	A	478	ARG
1	A	503	ASN
1	A	512	ASN
1	A	557	ILE
1	A	558	SER
1	A	598	CYS
1	A	599	GLU
1	A	602	ARG
1	A	603	SER
1	B	5	LYS
1	B	6	ARG
1	B	20	GLU
1	B	22	SER
1	B	39	GLN
1	B	47	GLU
1	B	66	GLN

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Mol	Chain	Res	Type
1	B	70	THR
1	B	84	VAL
1	B	96	GLU
1	B	126	LYS
1	B	166	VAL
1	B	171	LYS
1	B	227	ARG
1	B	246	ASN
1	B	273	LEU
1	B	304	GLN
1	B	323	SER
1	B	337	THR
1	B	347	VAL
1	B	386	THR
1	B	397	LEU
1	B	401	THR
1	B	402	GLU
1	B	423	VAL
1	B	424	GLU
1	B	430	THR
1	B	434	GLN
1	B	444	THR
1	B	445	LEU
1	B	447	ILE
1	B	458	SER
1	B	463	LEU
1	B	478	ARG
1	B	500	ILE
1	B	503	ASN
1	B	562	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	91	GLN
1	A	158	HIS
1	A	190	GLN
1	A	196	ASN
1	A	216	ASN
1	A	246	ASN
1	A	289	GLN

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Mol	Chain	Res	Type
1	A	389	GLN
1	A	415	ASN
1	A	431	ASN
1	A	474	GLN
1	A	477	GLN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN
1	B	8	GLN
1	B	48	ASN
1	B	66	GLN
1	B	123	GLN
1	B	130	GLN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	415	ASN
1	B	431	ASN
1	B	503	ASN
1	B	504	HIS
1	B	529	GLN
1	B	590	HIS

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 [i](#)

Of 37 ligands modelled in this entry, 27 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	B	720	-	4,4,4	0.56	0	6,6,6	0.36	0
6	SO4	B	722	-	4,4,4	0.42	0	6,6,6	0.78	0
3	S6P	B	702	-	15,15,15	1.84	4 (26%)	20,21,21	1.52	4 (20%)
6	SO4	B	719	-	4,4,4	0.37	0	6,6,6	0.47	0
3	S6P	A	702	-	15,15,15	1.65	2 (13%)	20,21,21	1.90	6 (30%)
2	2WX	A	701	-	36,36,36	2.22	9 (25%)	48,52,52	2.35	20 (41%)
6	SO4	B	721	-	4,4,4	0.52	0	6,6,6	0.23	0
6	SO4	B	718	-	4,4,4	0.64	0	6,6,6	0.40	0
5	GOL	B	717	-	5,5,5	0.47	0	5,5,5	0.59	0
2	2WX	B	701	-	36,36,36	2.27	9 (25%)	48,52,52	2.80	21 (43%)

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
3	S6P	B	702	-	-	0/20/20/20	-
3	S6P	A	702	-	-	2/20/20/20	-
2	2WX	A	701	-	-	2/19/27/27	0/5/5/5
5	GOL	B	717	-	-	2/4/4/4	-
2	2WX	B	701	-	-	3/19/27/27	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2WX	O1-S1	7.57	1.52	1.43
2	A	701	2WX	O1-S1	7.15	1.51	1.43
2	B	701	2WX	C9-S1	7.04	1.87	1.76
2	A	701	2WX	O2-S1	5.08	1.49	1.43
3	A	702	S6P	P-O3P	4.59	1.64	1.50
3	B	702	S6P	C2-C3	-4.30	1.45	1.53
2	B	701	2WX	C1-C3	4.03	1.55	1.51
3	B	702	S6P	P-O3P	3.70	1.62	1.50
2	A	701	2WX	C20-C18	-3.46	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	2WX	C9-S1	3.37	1.81	1.76
2	A	701	2WX	C19-S2	-3.26	1.67	1.74
2	A	701	2WX	C4-C2	3.04	1.43	1.39
2	B	701	2WX	O2-S1	2.87	1.46	1.43
2	A	701	2WX	C12-C9	2.83	1.43	1.38
2	A	701	2WX	C1-C3	2.74	1.54	1.51
2	B	701	2WX	C17-C15	2.68	1.57	1.51
3	B	702	S6P	P-O1P	-2.49	1.45	1.54
3	B	702	S6P	C5-C4	-2.46	1.49	1.53
2	A	701	2WX	S1-N1	2.37	1.65	1.61
2	B	701	2WX	C20-C18	-2.30	1.36	1.44
2	B	701	2WX	C8-CL1	2.23	1.78	1.73
3	A	702	S6P	C4-C3	-2.08	1.49	1.53
2	B	701	2WX	C19-S2	-2.06	1.70	1.74
2	B	701	2WX	C4-C2	2.05	1.42	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2WX	C7-C8-C2	-7.18	115.20	121.98
2	B	701	2WX	O1-S1-C9	6.07	115.64	107.98
2	A	701	2WX	C7-C8-C2	-5.73	116.56	121.98
2	B	701	2WX	O3-C15-C17	5.66	124.67	112.80
2	A	701	2WX	C8-C2-C1	-5.36	115.31	121.96
2	B	701	2WX	O2-S1-O1	-5.25	113.15	119.52
3	A	702	S6P	C5-C4-C3	-4.97	104.85	112.48
2	B	701	2WX	C6-C5-C4	-4.53	114.65	120.24
2	B	701	2WX	C19-S2-C3	4.44	95.01	91.32
2	B	701	2WX	O4-C16-C17	4.41	122.06	112.80
2	B	701	2WX	O3-C14-C13	4.38	127.78	123.24
2	B	701	2WX	C4-C2-C8	4.38	121.21	116.82
2	A	701	2WX	C4-C2-C8	4.31	121.15	116.82
2	B	701	2WX	C11-C12-C9	4.21	123.54	119.44
2	A	701	2WX	O2-S1-O1	-4.01	114.64	119.52
2	A	701	2WX	O1-S1-C9	3.95	112.96	107.98
2	B	701	2WX	C12-C9-C10	-3.52	116.32	120.68
3	A	702	S6P	O2P-P-O6	3.46	115.69	106.67
2	A	701	2WX	C6-C5-C4	-3.40	116.04	120.24
2	A	701	2WX	C19-S2-C3	3.22	94.00	91.32
2	A	701	2WX	C22-C23-C24	3.20	124.18	120.24
2	B	701	2WX	C1-N1-S1	-3.17	114.97	121.56
2	A	701	2WX	C7-C8-CL1	3.06	124.46	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	S6P	C5-C4-C3	-3.05	107.79	112.48
3	B	702	S6P	O2P-P-O6	3.05	114.62	106.67
2	B	701	2WX	C18-C3-S2	-3.04	107.88	112.47
2	A	701	2WX	C18-C3-S2	-3.01	107.92	112.47
2	A	701	2WX	O4-C13-C14	2.96	126.30	123.24
2	B	701	2WX	C10-C9-S1	2.89	122.02	119.06
3	B	702	S6P	O5-C5-C4	-2.82	102.65	109.25
2	A	701	2WX	C16-O4-C13	-2.77	111.53	116.13
2	A	701	2WX	O1-S1-N1	-2.72	101.94	106.88
3	A	702	S6P	O1-C1-C2	-2.68	105.54	111.16
2	B	701	2WX	C8-C2-C1	-2.65	118.67	121.96
3	A	702	S6P	C2-C3-C4	2.63	116.51	112.48
2	A	701	2WX	O2-S1-C9	2.62	111.29	107.98
2	A	701	2WX	C21-C20-C18	-2.46	125.06	132.83
2	B	701	2WX	C7-C8-CL1	2.45	123.25	118.42
2	A	701	2WX	O4-C13-C10	-2.38	112.97	116.83
2	A	701	2WX	C23-C22-C21	-2.37	117.31	120.24
2	B	701	2WX	C20-C19-S2	-2.37	106.88	112.60
2	B	701	2WX	C6-C7-C8	2.33	122.92	119.42
3	A	702	S6P	O5-C5-C4	-2.29	103.88	109.25
2	B	701	2WX	O4-C13-C10	-2.29	113.12	116.83
3	A	702	S6P	O3-C3-C4	-2.21	104.30	109.46
2	A	701	2WX	C6-C7-C8	2.17	122.68	119.42
2	A	701	2WX	C12-C9-S1	2.11	122.08	119.76
2	B	701	2WX	C5-C4-C2	2.08	123.48	120.99
3	B	702	S6P	O2P-P-O1P	2.07	115.57	107.80
2	B	701	2WX	C10-C13-C14	2.03	122.44	119.83
2	A	701	2WX	C20-C19-S2	-2.03	107.70	112.60

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	717	GOL	C1-C2-C3-O3
5	B	717	GOL	O2-C2-C3-O3
3	A	702	S6P	C6-O6-P-O3P
3	A	702	S6P	C4-C5-C6-O6
2	A	701	2WX	C2-C1-C3-C18
2	B	701	2WX	C2-C1-C3-C18
2	A	701	2WX	N1-C1-C3-S2
2	B	701	2WX	N1-C1-C3-S2
2	B	701	2WX	C3-C1-C2-C8

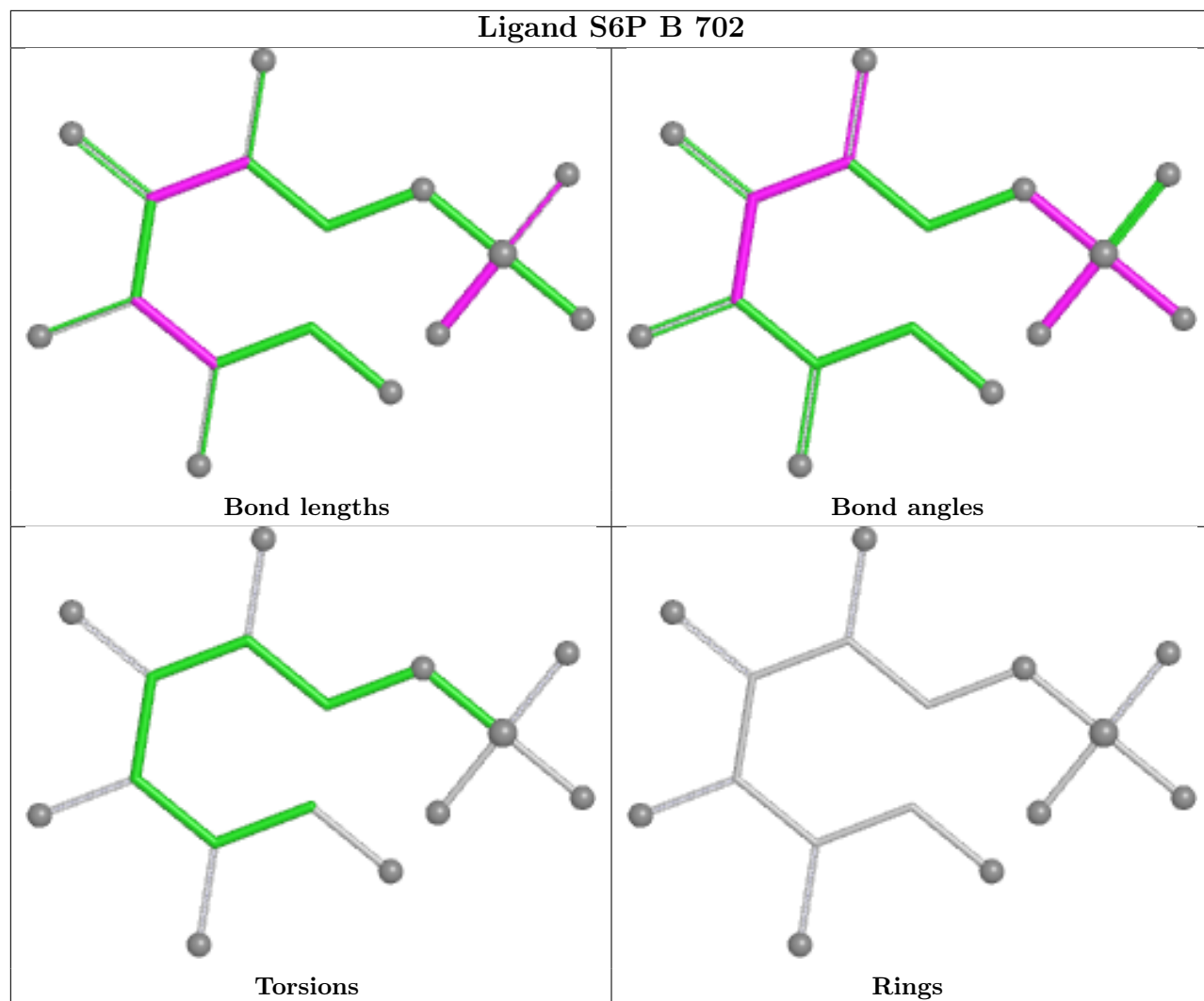
There are no ring outliers.

2 monomers are involved in 2 short contacts:

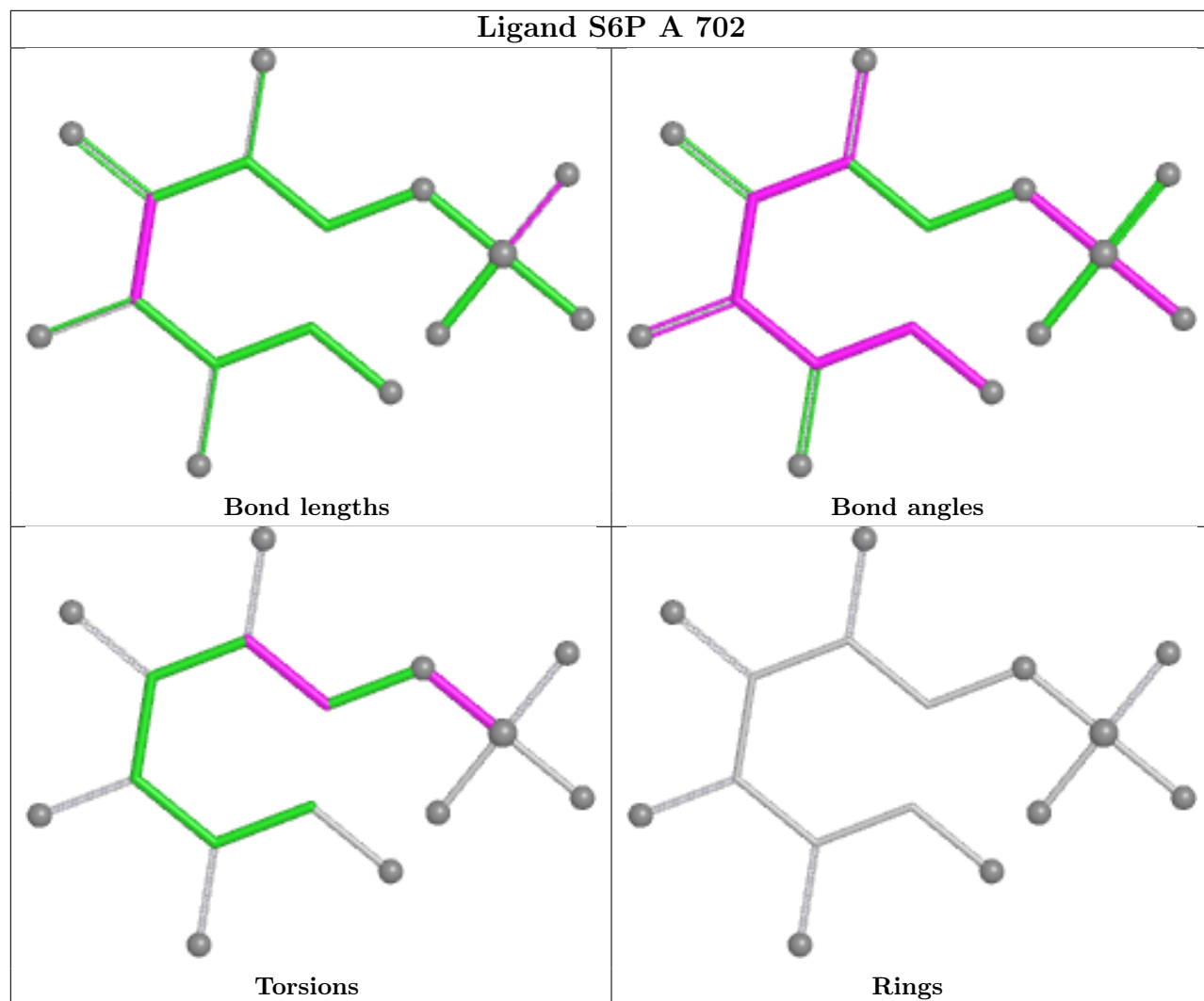
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	S6P	1	0
5	B	717	GOL	1	0

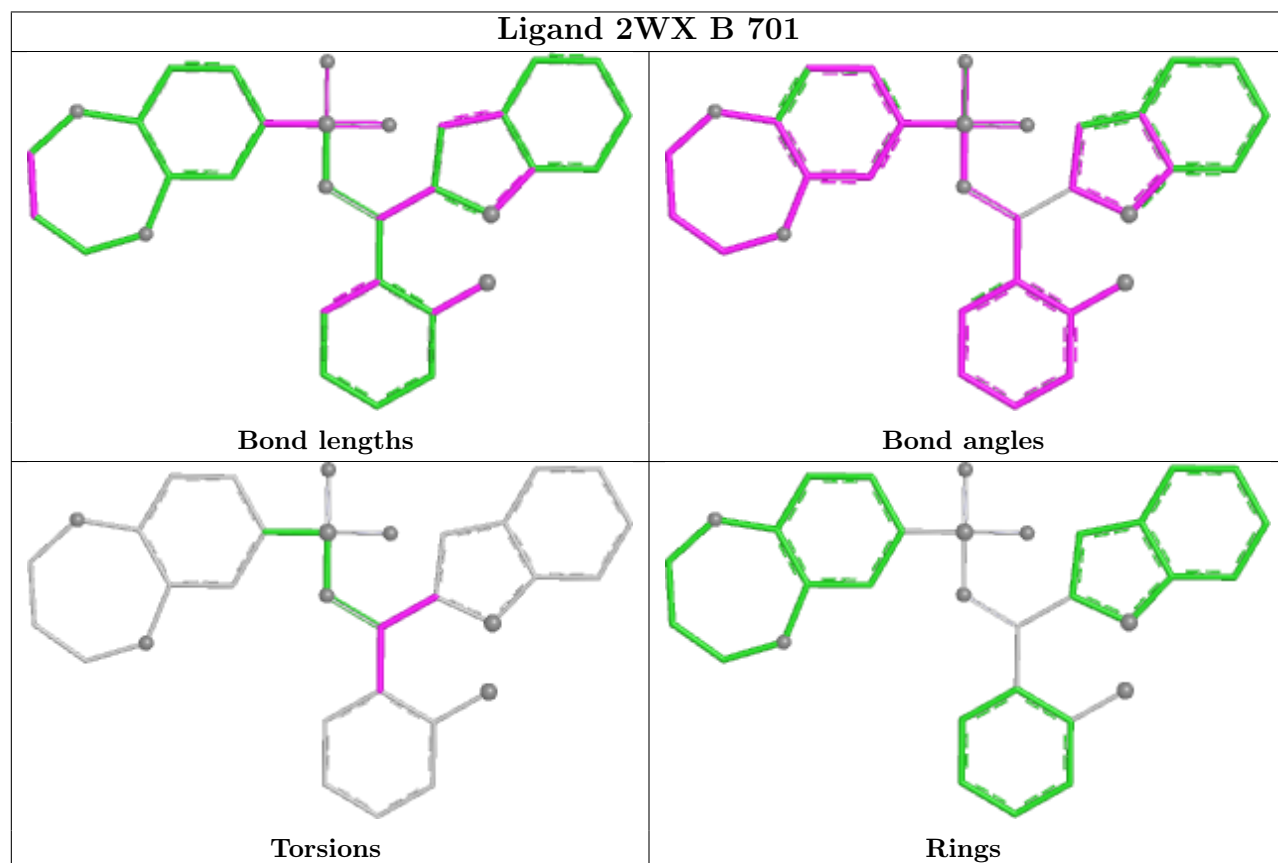
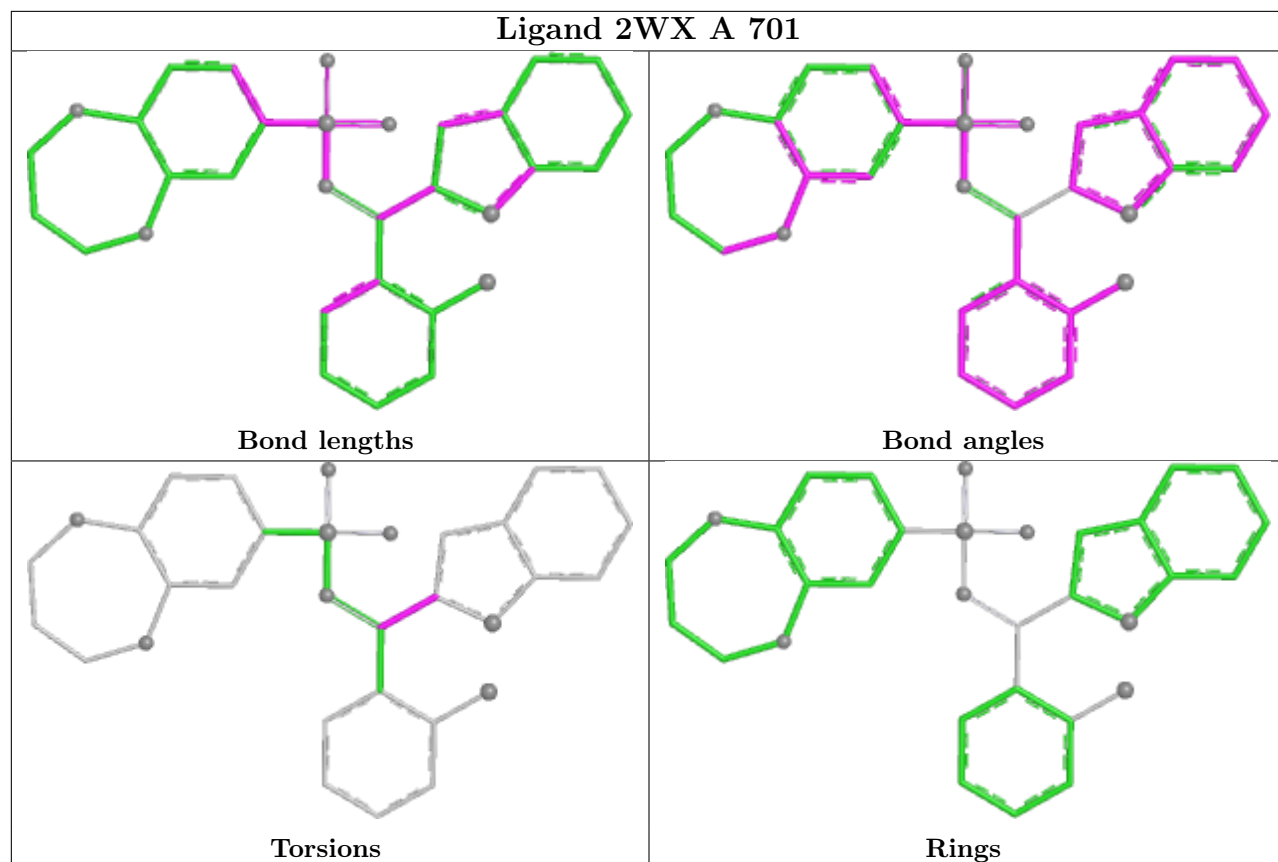
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





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%)	0.21	24 (4%)	41 39	29, 56, 95, 141	0
1	B	590/638 (92%)	-0.06	15 (2%)	58 59	27, 50, 83, 126	0
All	All	1175/1276 (92%)	0.07	39 (3%)	49 48	27, 53, 90, 141	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	PHE	5.8
1	A	387	PHE	4.3
1	A	447	ILE	4.0
1	B	22	SER	3.9
1	B	366	GLY	3.4
1	B	21	LEU	3.1
1	A	403	ILE	3.1
1	A	454	PRO	2.9
1	B	381	GLN	2.9
1	A	430	THR	2.9
1	A	449	LEU	2.8
1	A	220	GLU	2.8
1	B	65	GLY	2.7
1	A	21	LEU	2.7
1	B	606	ALA	2.7
1	A	452	LEU	2.7
1	A	142	ASP	2.6
1	A	445	LEU	2.6
1	B	449	LEU	2.6
1	B	447	ILE	2.5
1	A	358	ARG	2.5
1	A	606	ALA	2.5
1	A	357	PHE	2.4
1	A	400	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	4	THR	2.4
1	A	463	LEU	2.4
1	B	3	GLY	2.3
1	A	65	GLY	2.3
1	A	385	PHE	2.2
1	A	282	ASP	2.2
1	B	70	THR	2.2
1	A	69	SER	2.1
1	A	429	LYS	2.1
1	B	69	SER	2.1
1	B	465	PHE	2.1
1	A	469	GLU	2.1
1	B	385	PHE	2.0
1	A	444	THR	2.0
1	B	454	PRO	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(Å ²)	Q<0.9
6	SO4	B	720	5/5	0.73	0.14	84,98,109,114	0
6	SO4	B	721	5/5	0.83	0.15	74,79,94,96	5
6	SO4	B	722	5/5	0.84	0.16	44,45,49,50	5
5	GOL	B	717	6/6	0.86	0.13	51,53,60,73	0
4	IOD	A	711	1/1	0.86	0.13	88,88,88,88	1
4	IOD	B	712	1/1	0.87	0.10	90,90,90,90	1
4	IOD	A	715	1/1	0.89	0.11	97,97,97,97	1
6	SO4	B	718	5/5	0.90	0.10	84,87,96,105	0

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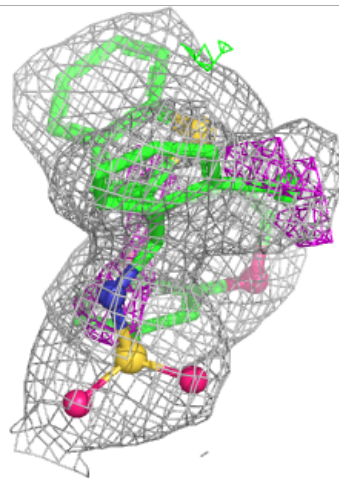
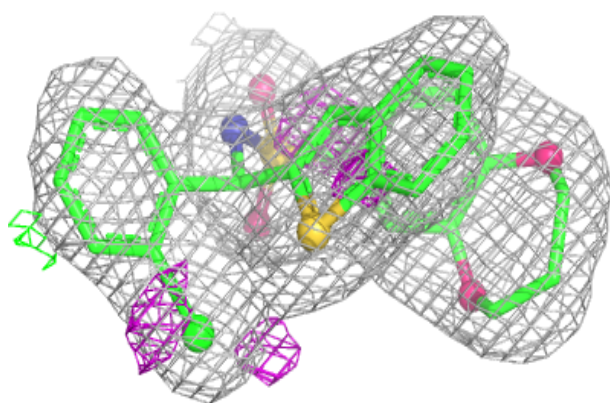
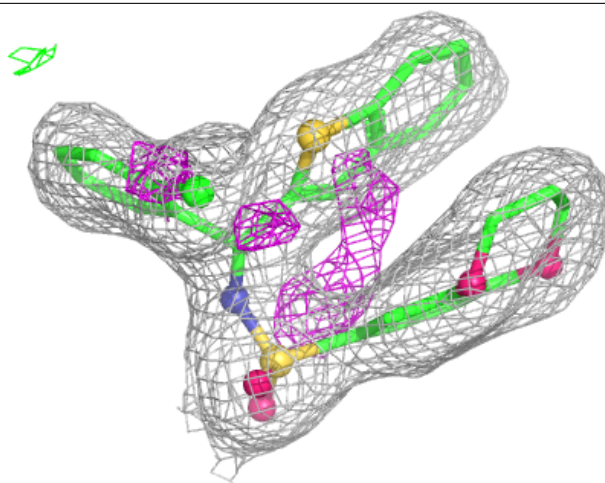
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IOD	B	713	1/1	0.91	0.10	93,93,93,93	1
4	IOD	A	706	1/1	0.91	0.12	97,97,97,97	0
4	IOD	B	708	1/1	0.92	0.11	69,69,69,69	1
4	IOD	A	713	1/1	0.94	0.07	75,75,75,75	1
4	IOD	A	708	1/1	0.94	0.15	93,93,93,93	1
4	IOD	B	707	1/1	0.94	0.10	83,83,83,83	0
2	2WX	B	701	32/32	0.94	0.09	42,50,56,57	0
4	IOD	B	710	1/1	0.94	0.11	97,97,97,97	1
4	IOD	A	712	1/1	0.94	0.07	80,80,80,80	1
4	IOD	B	716	1/1	0.95	0.06	95,95,95,95	1
4	IOD	B	709	1/1	0.95	0.08	84,84,84,84	1
4	IOD	A	709	1/1	0.95	0.10	98,98,98,98	1
6	SO4	B	719	5/5	0.95	0.07	49,50,52,56	5
2	2WX	A	701	32/32	0.95	0.08	41,47,52,59	0
4	IOD	A	714	1/1	0.95	0.07	77,77,77,77	1
4	IOD	B	715	1/1	0.95	0.07	87,87,87,87	1
4	IOD	A	710	1/1	0.96	0.10	74,74,74,74	1
4	IOD	A	703	1/1	0.96	0.08	74,74,74,74	0
4	IOD	B	703	1/1	0.96	0.05	58,58,58,58	0
4	IOD	B	714	1/1	0.96	0.06	79,79,79,79	1
4	IOD	B	711	1/1	0.97	0.11	88,88,88,88	1
4	IOD	A	707	1/1	0.97	0.05	67,67,67,67	1
3	S6P	B	702	16/16	0.98	0.05	28,31,34,34	0
4	IOD	B	706	1/1	0.98	0.04	58,58,58,58	1
4	IOD	A	704	1/1	0.98	0.09	77,77,77,77	0
3	S6P	A	702	16/16	0.99	0.04	28,35,40,42	0
4	IOD	B	704	1/1	0.99	0.09	67,67,67,67	0
4	IOD	B	705	1/1	0.99	0.05	55,55,55,55	1
4	IOD	A	705	1/1	0.99	0.03	50,50,50,50	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.

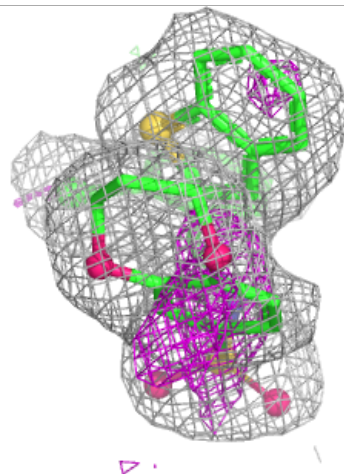
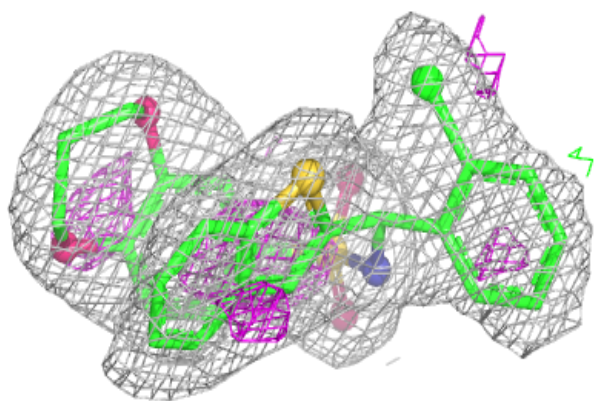
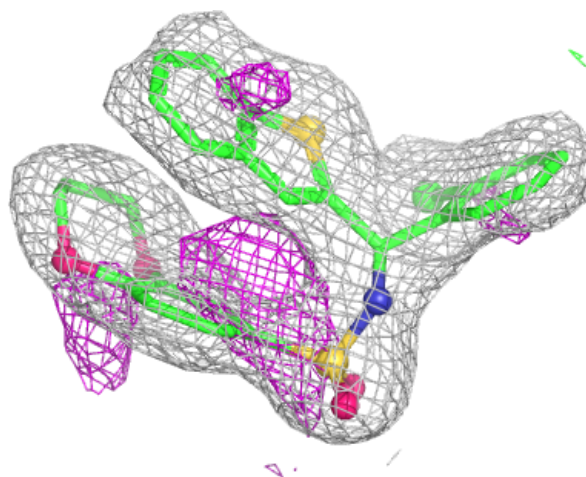
Electron density around 2WX B 701:

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



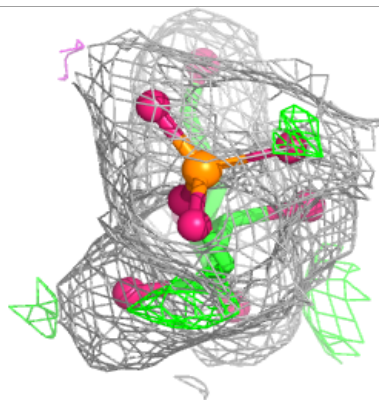
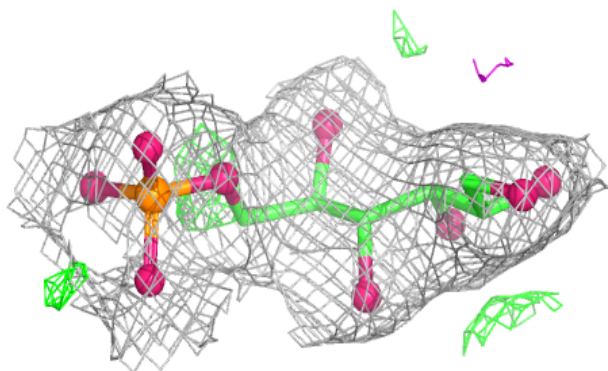
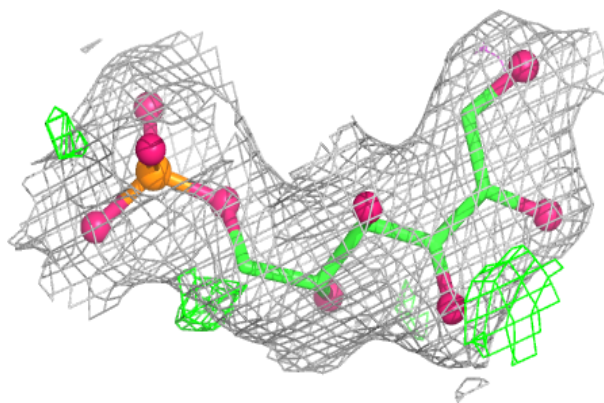
Electron density around 2WX A 701:

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

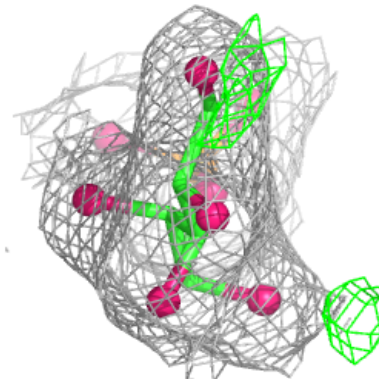
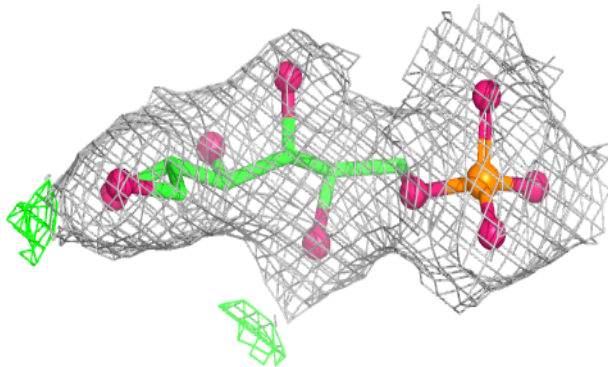
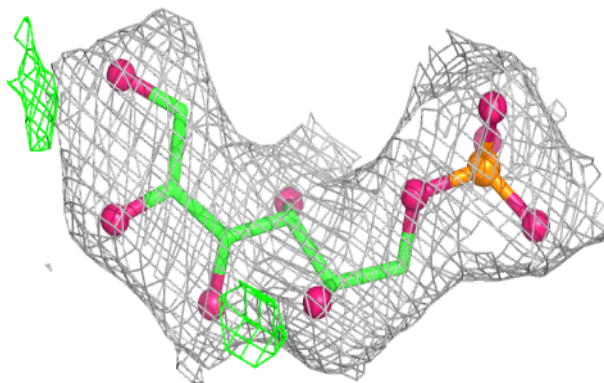


Electron density around S6P B 702:

$2mF_o-DF_c$ (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.