



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:45 AM UTC

PDB ID : 4OP3 / pdb_00004op3
Title : Human GKRP bound to AMG-5112 and Sorbitol-6-phosphate
Authors : Jordan, S.R.; Chmait, S.
Deposited on : 2014-02-04
Resolution : 2.82 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

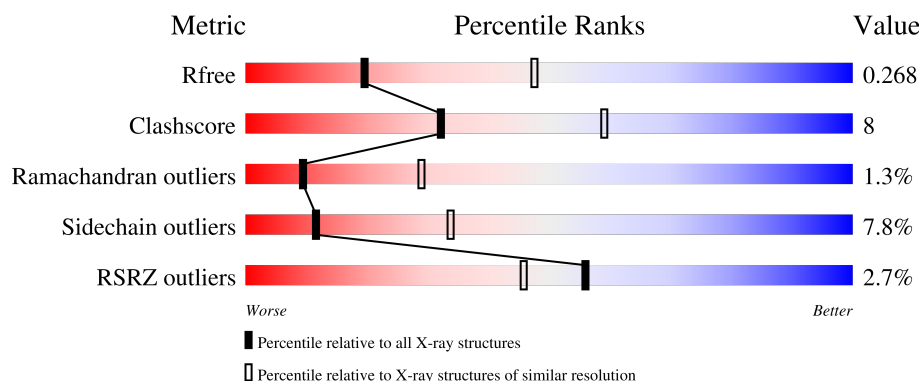
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

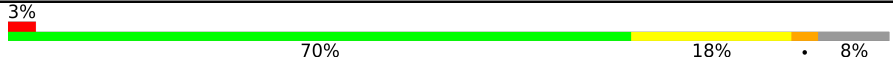
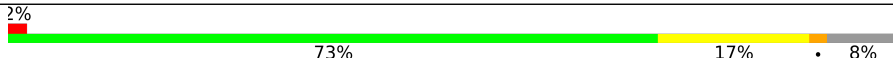
The reported resolution of this entry is 2.82 Å.

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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	638	
1	B	638	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9286 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

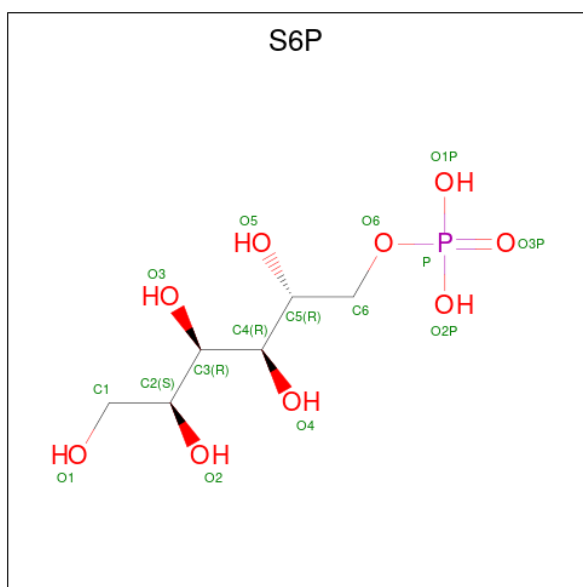
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Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	expression tag	UNP Q14397

-
- Chemical structure of 2UY (2-((4-(2-amino-5-sulfinylphenyl)-6-hydroxyphenyl)amino)pyridine) is shown. The structure features a central pyridine ring (N1, C2-C7) substituted with a hydroxyl group (O1) at C6 and a 4-(2-amino-5-sulfinylphenyl)amino group at C2. The 4-(2-amino-5-sulfinylphenyl)amino group consists of an aniline derivative (N4, C12-C16) with an amino group (NH2) at C4 and a sulfinyl group (S1, O3, O2) at C5, connected via an amine bridge (N2, C8, C9) to the central pyridine ring.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 36	C 24	F 3	N 5	O 3	S 1	0	0
2	B	1	Total 36	C 24	F 3	N 5	O 3	S 1	0	0

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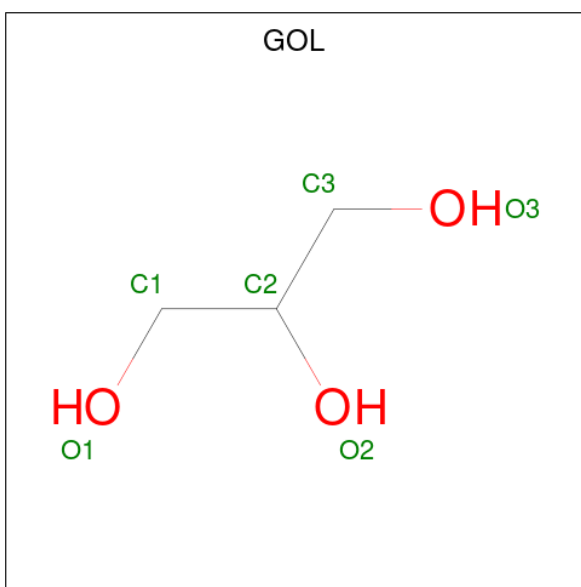


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- 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: C₃H₈O₃).



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

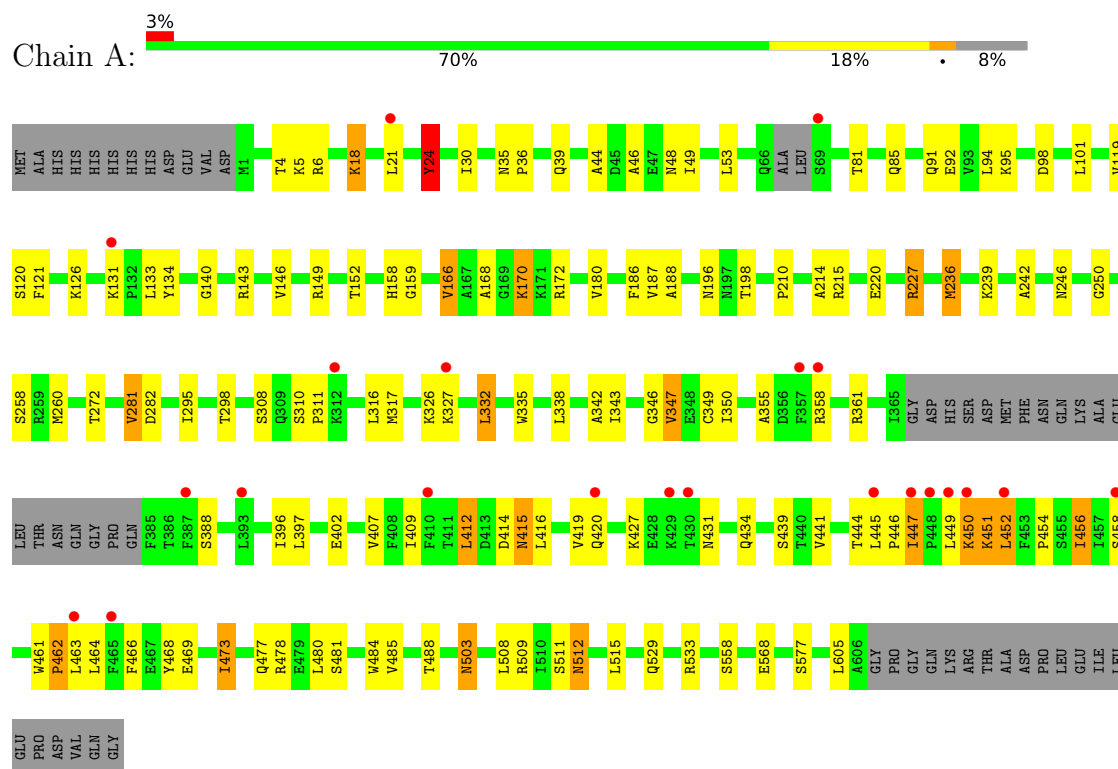
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	26	Total 26	O 26	0	0
7	B	34	Total 34	O 34	0	0

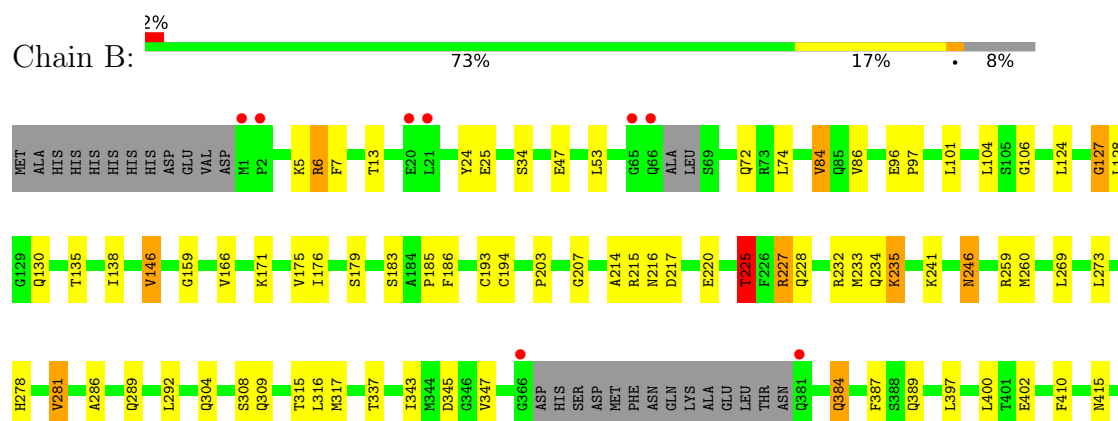
3 Residue-property plots [i](#)

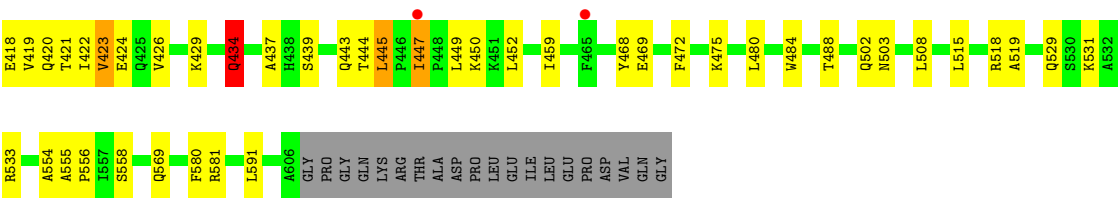
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 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	148.91Å 148.91Å 132.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 2.82 29.59 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.59-2.82) 99.5 (29.59-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.199 , 0.266 0.204 , 0.268	Depositor DCC
R_{free} test set	2007 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9286	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: SO4, IOD, S6P, 2UY, 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	0.86	0/4603	1.04	2/6228 (0.0%)
1	B	0.88	1/4637 (0.0%)	1.05	7/6274 (0.1%)
All	All	0.87	1/9240 (0.0%)	1.04	9/12502 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	ILE	CA-CB	6.00	1.57	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ILE	N-CA-CB	7.47	115.21	110.50
1	B	447	ILE	CB-CA-C	-7.14	106.78	114.35
1	A	24	TYR	N-CA-C	-6.93	103.72	111.28
1	B	434	GLN	N-CA-C	-6.92	98.21	108.79
1	B	234	GLN	N-CA-C	5.82	117.30	111.07
1	B	225	THR	N-CA-C	-5.36	101.22	109.52
1	B	475	LYS	N-CA-C	-5.35	105.34	111.07
1	A	434	GLN	N-CA-C	-5.30	101.65	109.18
1	B	443	GLN	N-CA-C	-5.17	100.61	109.24

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	73	0
1	B	4554	0	4647	67	0
2	A	36	0	20	6	0
2	B	36	0	20	4	0
3	A	16	0	13	0	0
3	B	16	0	13	1	0
4	A	12	0	0	5	0
4	B	13	0	0	2	0
5	B	12	0	16	0	0
6	B	10	0	0	0	0
7	A	26	0	0	0	0
7	B	34	0	0	1	0
All	All	9286	0	9347	148	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 (148) 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	1.69	0.92
1:A:447:ILE:HG22	1:A:449:LEU:C	2.14	0.73
1:B:389:GLN:OE1	1:B:421:THR:HG21	1.89	0.72
1:A:508:LEU:HD13	1:A:515:LEU:HD22	1.74	0.69
2:A:701:2UY:N2	2:A:701:2UY:H5	2.05	0.69
1:A:450:LYS:HA	1:A:452:LEU:HD12	1.78	0.65
1:A:140:GLY:H	1:A:158:HIS:HE1	1.42	0.64
2:A:701:2UY:F3	2:A:701:2UY:H15	1.87	0.64
1:A:503:ASN:HD22	1:A:503:ASN:C	2.05	0.63
2:B:701:2UY:N2	2:B:701:2UY:H5	2.14	0.63
1:B:86:VAL:HG12	1:B:273:LEU:HD21	1.81	0.61
1:A:414:ASP:O	1:A:415:ASN:CB	2.48	0.60
1:A:146:VAL:O	1:A:347:VAL:HG21	2.02	0.60
1:A:220:GLU:OE2	1:A:558:SER:OG	2.21	0.58
1:A:159:GLY:HA2	1:A:186:PHE:CE1	2.38	0.57
1:B:410:PHE:O	1:B:437:ALA:HA	2.03	0.57
1:A:412:LEU:HD23	1:A:412:LEU:N	2.19	0.57
1:A:480:LEU:HD21	1:A:484:TRP:CH2	2.40	0.57
2:A:701:2UY:N2	2:A:701:2UY:C22	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LEU:HA	1:B:400:LEU:HD12	1.85	0.57
1:B:220:GLU:OE2	1:B:558:SER:OG	2.17	0.56
1:A:140:GLY:N	1:A:158:HIS:HE1	2.04	0.55
1:B:384:GLN:HB3	1:B:387:PHE:CZ	2.42	0.55
1:B:246:ASN:HD22	1:B:246:ASN:N	2.03	0.55
1:B:215:ARG:HG2	1:B:217:ASP:OD1	2.07	0.55
1:A:18:LYS:O	1:A:18:LYS:CG	2.54	0.54
1:A:481:SER:O	1:A:485:VAL:HG23	2.07	0.54
1:A:512:ASN:C	1:A:512:ASN:HD22	2.15	0.54
1:A:140:GLY:H	1:A:158:HIS:CE1	2.25	0.54
1:A:180:VAL:HG11	1:A:258:SER:HB2	1.89	0.53
1:A:461:TRP:O	1:A:462:PRO:O	2.26	0.53
2:B:701:2UY:N1	2:B:701:2UY:N3	2.56	0.53
1:A:53:LEU:HD12	1:A:488:THR:HG23	1.91	0.53
1:B:419:VAL:O	1:B:423:VAL:HG12	2.07	0.53
1:B:146:VAL:O	1:B:347:VAL:HG21	2.09	0.53
1:B:84:VAL:HG23	1:B:292:LEU:HD11	1.89	0.52
1:A:146:VAL:O	1:A:146:VAL:HG12	2.08	0.52
1:B:469:GLU:HG2	7:B:801:HOH:O	2.10	0.52
1:B:124:LEU:HD12	1:B:472:PHE:CD2	2.44	0.52
1:B:480:LEU:HD21	1:B:484:TRP:CH2	2.44	0.52
1:A:196:ASN:OD1	4:A:712:IOD:I	2.98	0.52
1:B:259:ARG:NH2	1:B:345:ASP:OD1	2.43	0.52
1:A:449:LEU:HD12	1:A:449:LEU:O	2.09	0.52
1:B:53:LEU:HD12	1:B:488:THR:HG23	1.92	0.51
1:A:447:ILE:HG22	1:A:450:LYS:N	2.25	0.51
1:A:450:LYS:HA	1:A:452:LEU:CD1	2.39	0.51
1:B:232:ARG:HA	1:B:235:LYS:HD3	1.93	0.51
1:A:272:THR:HA	1:A:295:ILE:HG21	1.91	0.51
1:A:146:VAL:O	1:A:146:VAL:CG1	2.58	0.51
1:A:473:ILE:O	1:A:477:GLN:HG3	2.10	0.51
2:A:701:2UY:F3	2:A:701:2UY:C2	2.48	0.50
1:B:246:ASN:HD22	1:B:246:ASN:H	1.59	0.50
1:A:44:ALA:HB1	1:A:48:ASN:HB3	1.93	0.49
1:A:466:PHE:C	1:A:466:PHE:CD1	2.90	0.49
1:A:214:ALA:O	1:A:227:ARG:HD3	2.12	0.49
2:A:701:2UY:N1	2:A:701:2UY:N3	2.57	0.49
1:B:127:GLY:O	1:B:128:LEU:HD23	2.12	0.48
1:A:18:LYS:O	1:A:18:LYS:HG3	2.13	0.48
1:B:508:LEU:C	1:B:508:LEU:HD12	2.39	0.48
1:A:140:GLY:O	1:A:149:ARG:NH1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.60	0.48
1:B:215:ARG:HG3	2:B:701:2UY:C13	2.43	0.48
1:B:128:LEU:HD21	1:B:468:TYR:CD1	2.49	0.47
1:A:119:VAL:O	1:A:120:SER:C	2.58	0.47
1:B:207:GLY:O	1:B:246:ASN:HA	2.14	0.47
1:A:215:ARG:HG3	2:A:701:2UY:C14	2.45	0.47
1:B:555:ALA:HB1	1:B:556:PRO:HD2	1.96	0.47
1:B:315:THR:HG22	1:B:434:GLN:NE2	2.30	0.47
1:A:121:PHE:HB3	1:A:134:TYR:CE2	2.50	0.47
1:A:416:LEU:N	1:A:416:LEU:HD12	2.30	0.47
1:B:420:GLN:O	1:B:424:GLU:HB2	2.15	0.47
1:A:146:VAL:HG13	1:A:343:ILE:CG2	2.45	0.47
1:A:332:LEU:HB3	1:A:342:ALA:HB1	1.96	0.47
1:B:146:VAL:HG12	1:B:343:ILE:HG21	1.98	0.46
1:A:236:MET:HE2	1:A:242:ALA:HB2	1.98	0.46
2:B:701:2UY:N2	2:B:701:2UY:C22	2.79	0.46
1:B:74:LEU:CD1	1:B:269:LEU:HD13	2.45	0.46
1:A:420:GLN:NE2	1:A:447:ILE:HD11	2.30	0.46
1:A:332:LEU:HD12	1:A:407:VAL:HB	1.98	0.46
1:A:449:LEU:C	1:A:451:LYS:H	2.24	0.46
1:B:101:LEU:HD11	1:B:135:THR:CG2	2.46	0.46
1:A:414:ASP:O	1:A:415:ASN:HB3	2.16	0.46
1:A:447:ILE:HG23	1:A:449:LEU:HG	1.99	0.45
1:A:4:THR:HA	4:A:711:IOD:I	2.86	0.45
1:A:101:LEU:HD21	1:A:166:VAL:HG13	1.99	0.45
1:B:529:GLN:HE21	1:B:533:ARG:HE	1.63	0.45
1:B:96:GLU:N	1:B:97:PRO:HD3	2.32	0.45
1:B:106:GLY:O	1:B:138:ILE:HA	2.18	0.44
1:B:128:LEU:HD12	1:B:130:GLN:NE2	2.32	0.44
1:B:422:ILE:O	1:B:426:VAL:HG23	2.17	0.44
1:A:250:GLY:HA2	4:A:705:IOD:I	2.88	0.44
1:B:529:GLN:NE2	1:B:533:ARG:HE	2.15	0.44
1:B:175:VAL:HG21	1:B:194:CYS:SG	2.57	0.44
1:B:193:CYS:HA	4:B:714:IOD:I	2.88	0.44
1:B:445:LEU:HG	4:B:713:IOD:I	2.87	0.44
1:A:298:THR:OG1	4:A:707:IOD:I	3.03	0.44
1:B:225:THR:HG22	1:B:228:GLN:HG3	1.99	0.44
1:B:397:LEU:HD23	1:B:429:LYS:HE2	1.98	0.44
1:B:423:VAL:HG22	1:B:452:LEU:HD13	1.99	0.44
1:B:214:ALA:O	1:B:227:ARG:HD3	2.18	0.44
1:B:128:LEU:HD12	1:B:130:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD12	1:A:317:MET:HE1	1.99	0.43
1:A:447:ILE:O	1:A:450:LYS:N	2.48	0.43
1:B:508:LEU:HD13	1:B:515:LEU:HD22	1.99	0.43
1:A:509:ARG:NH2	1:A:568:GLU:OE2	2.51	0.43
1:B:203:PRO:HB2	1:B:233:MET:HE3	2.01	0.43
1:B:183:SER:O	1:B:185:PRO:HD3	2.19	0.43
1:B:179:SER:OG	3:B:702:S6P:O3P	2.20	0.43
1:A:310:SER:HB2	1:A:311:PRO:HD3	2.00	0.43
1:A:509:ARG:HG2	1:A:511:SER:OG	2.18	0.43
1:B:24:TYR:CD1	1:B:24:TYR:C	2.96	0.43
1:B:6:ARG:HD2	1:B:554:ALA:O	2.19	0.42
1:B:7:PHE:O	1:B:531:LYS:NZ	2.52	0.42
1:B:309:GLN:HG3	1:B:459:ILE:HD13	2.00	0.42
1:A:46:ALA:HA	1:A:317:MET:HE1	2.02	0.42
1:A:327:LYS:HG2	1:A:327:LYS:O	2.19	0.42
1:B:580:PHE:O	1:B:581:ARG:C	2.61	0.42
1:B:104:LEU:CD2	1:B:176:ILE:HD12	2.50	0.42
1:B:569:GLN:HG2	1:B:591:LEU:HD21	2.01	0.42
1:A:236:MET:HB2	1:A:242:ALA:HB3	2.01	0.42
1:A:350:ILE:HA	1:A:355:ALA:O	2.20	0.41
1:B:315:THR:HG22	1:B:434:GLN:HE22	1.85	0.41
1:A:36:PRO:O	1:A:39:GLN:HG2	2.21	0.41
1:A:46:ALA:HA	1:A:317:MET:CE	2.50	0.41
1:B:286:ALA:HA	1:B:289:GLN:NE2	2.35	0.41
1:A:95:LYS:HE3	1:A:281:VAL:HG12	2.03	0.41
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.56	0.41
1:A:24:TYR:CD1	1:A:24:TYR:C	2.98	0.41
1:B:415:ASN:C	1:B:415:ASN:HD22	2.26	0.41
1:B:518:ARG:O	1:B:519:ALA:C	2.62	0.41
1:A:81:THR:HG22	1:A:85:GLN:OE1	2.20	0.41
1:A:91:GLN:HG2	1:A:281:VAL:HG13	2.01	0.41
1:B:278:HIS:O	1:B:281:VAL:HG23	2.21	0.41
1:B:84:VAL:HG23	1:B:292:LEU:CD1	2.50	0.41
1:A:187:VAL:O	1:A:188:ALA:C	2.63	0.41
1:A:468:TYR:HB2	4:A:703:IOD:I	2.90	0.41
1:B:13:THR:OG1	1:B:529:GLN:O	2.33	0.41
1:A:30:ILE:HD12	1:A:210:PRO:HD3	2.03	0.41
1:A:101:LEU:HB2	1:A:170:LYS:HG2	2.03	0.41
1:A:335:TRP:CZ2	1:A:419:VAL:HG22	2.56	0.40
1:B:124:LEU:C	1:B:124:LEU:HD23	2.47	0.40
1:B:449:LEU:O	1:B:450:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HB3	1:A:409:ILE:HG22	2.03	0.40
1:A:346:GLY:O	1:A:349:CYS:HB2	2.21	0.40
1:A:91:GLN:O	1:A:92:GLU:C	2.63	0.40
1:A:94:LEU:HD23	1:A:133:LEU:HD12	2.03	0.40
1:B:316:LEU:O	1:B:317:MET:C	2.64	0.40
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.87	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%)	529 (91%)	39 (7%)	11 (2%)	6	20
1	B	584/638 (92%)	553 (95%)	27 (5%)	4 (1%)	18	45
All	All	1163/1276 (91%)	1082 (93%)	66 (6%)	15 (1%)	9	29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	SER
1	A	415	ASN
1	A	456	ILE
1	A	462	PRO
1	A	260	MET
1	B	127	GLY
1	B	418	GLU
1	A	168	ALA
1	A	402	GLU
1	B	502	GLN
1	A	326	LYS
1	A	454	PRO

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Mol	Chain	Res	Type
1	B	260	MET
1	A	446	PRO
1	A	447	ILE

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%)	448 (90%)	50 (10%)	7	23
1	B	501/542 (92%)	473 (94%)	28 (6%)	19	48
All	All	999/1084 (92%)	921 (92%)	78 (8%)	11	34

All (78) 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	21	LEU
1	A	24	TYR
1	A	35	ASN
1	A	98	ASP
1	A	126	LYS
1	A	131	LYS
1	A	143	ARG
1	A	152	THR
1	A	166	VAL
1	A	170	LYS
1	A	172	ARG
1	A	198	THR
1	A	227	ARG
1	A	236	MET
1	A	239	LYS
1	A	246	ASN
1	A	281	VAL

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Mol	Chain	Res	Type
1	A	282	ASP
1	A	308	SER
1	A	316	LEU
1	A	332	LEU
1	A	347	VAL
1	A	358	ARG
1	A	361	ARG
1	A	396	ILE
1	A	397	LEU
1	A	412	LEU
1	A	427	LYS
1	A	431	ASN
1	A	439	SER
1	A	441	VAL
1	A	444	THR
1	A	445	LEU
1	A	450	LYS
1	A	451	LYS
1	A	452	LEU
1	A	456	ILE
1	A	458	SER
1	A	463	LEU
1	A	464	LEU
1	A	469	GLU
1	A	473	ILE
1	A	478	ARG
1	A	503	ASN
1	A	512	ASN
1	A	577	SER
1	A	605	LEU
1	B	5	LYS
1	B	6	ARG
1	B	25	GLU
1	B	34	SER
1	B	47	GLU
1	B	72	GLN
1	B	84	VAL
1	B	146	VAL
1	B	166	VAL
1	B	171	LYS
1	B	225	THR
1	B	227	ARG

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Mol	Chain	Res	Type
1	B	235	LYS
1	B	241	LYS
1	B	246	ASN
1	B	281	VAL
1	B	304	GLN
1	B	308	SER
1	B	337	THR
1	B	384	GLN
1	B	402	GLU
1	B	423	VAL
1	B	434	GLN
1	B	439	SER
1	B	444	THR
1	B	445	LEU
1	B	447	ILE
1	B	503	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	91	GLN
1	A	123	GLN
1	A	158	HIS
1	A	190	GLN
1	A	196	ASN
1	A	246	ASN
1	A	289	GLN
1	A	309	GLN
1	A	471	ASN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN
1	B	9	HIS
1	B	130	GLN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	304	GLN
1	B	384	GLN
1	B	415	ASN
1	B	425	GLN

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Mol	Chain	Res	Type
1	B	434	GLN
1	B	471	ASN
1	B	503	ASN
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 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	$\# Z > 2$
5	GOL	B	716	-	5,5,5	0.49	0	5,5,5	0.56	0
3	S6P	B	702	-	15,15,15	1.25	3 (20%)	20,21,21	1.03	2 (10%)
6	SO4	B	719	-	4,4,4	0.37	0	6,6,6	0.44	0
2	2UY	A	701	-	38,39,39	1.66	6 (15%)	53,59,59	1.82	13 (24%)
6	SO4	B	718	-	4,4,4	0.52	0	6,6,6	0.43	0
3	S6P	A	702	-	15,15,15	1.39	1 (6%)	20,21,21	1.37	4 (20%)
2	2UY	B	701	-	38,39,39	1.53	5 (13%)	53,59,59	1.90	14 (26%)
5	GOL	B	717	-	5,5,5	0.37	0	5,5,5	1.17	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
5	GOL	B	716	-	-	2/4/4/4	-
3	S6P	B	702	-	-	1/20/20/20	-
2	2UY	A	701	-	-	4/35/35/35	0/4/4/4
3	S6P	A	702	-	-	2/20/20/20	-
2	2UY	B	701	-	-	5/35/35/35	0/4/4/4
5	GOL	B	717	-	-	1/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	2UY	O2-S1	5.01	1.53	1.44
2	A	701	2UY	C10-S1	-4.57	1.74	1.79
3	A	702	S6P	P-O3P	4.41	1.64	1.50
2	B	701	2UY	O2-S1	4.38	1.51	1.44
2	A	701	2UY	O3-S1	3.99	1.51	1.44
2	B	701	2UY	C10-S1	-3.93	1.74	1.79
2	B	701	2UY	O3-S1	3.66	1.50	1.44
3	B	702	S6P	P-O2P	2.98	1.65	1.54
2	B	701	2UY	C7-C4	-2.62	1.42	1.48
2	A	701	2UY	C7-C4	-2.46	1.42	1.48
2	A	701	2UY	C17-N3	-2.42	1.35	1.40
2	A	701	2UY	C12-S1	-2.39	1.73	1.77
3	B	702	S6P	P-O3P	2.11	1.57	1.50
3	B	702	S6P	P-O1P	-2.06	1.47	1.54
2	B	701	2UY	C24-C11	2.06	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2UY	C9-C10-N2	-4.88	120.38	125.42
2	A	701	2UY	O2-S1-C10	4.79	112.75	107.82
2	B	701	2UY	O3-S1-C10	4.46	112.42	107.82
2	B	701	2UY	O3-S1-O2	-4.22	110.72	119.25
2	A	701	2UY	S1-C10-N2	4.00	119.61	115.21
2	A	701	2UY	C5-N1-C4	3.93	123.04	117.93
2	A	701	2UY	C12-C13-N4	-3.90	118.44	123.19
3	A	702	S6P	O1-C1-C2	-3.86	103.05	111.16
2	A	701	2UY	F2-C24-C11	-3.77	107.07	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2UY	C9-C10-N2	-3.62	121.69	125.42
2	B	701	2UY	S1-C10-N2	3.56	119.13	115.21
2	B	701	2UY	C24-C11-C1	3.51	113.79	109.25
2	B	701	2UY	C5-N1-C4	3.51	122.50	117.93
2	B	701	2UY	F1-C24-C11	-3.39	107.60	112.40
2	A	701	2UY	C1-C5-N1	-3.30	120.28	123.38
2	B	701	2UY	O2-S1-C10	3.12	111.04	107.82
2	A	701	2UY	C7-C6-N2	-2.99	119.08	122.67
2	B	701	2UY	C1-C5-N1	-2.85	120.71	123.38
2	B	701	2UY	C7-C6-N2	-2.65	119.49	122.67
2	A	701	2UY	C3-C4-N1	-2.41	118.66	122.24
2	A	701	2UY	O3-S1-O2	-2.32	114.55	119.25
3	A	702	S6P	C5-C4-C3	-2.30	108.94	112.48
2	B	701	2UY	O2-S1-C12	2.26	110.73	107.96
2	B	701	2UY	C7-C4-N1	2.21	120.37	116.48
2	A	701	2UY	C23-C11-C24	2.21	111.96	109.04
3	A	702	S6P	O2P-P-O1P	2.19	116.01	107.80
3	B	702	S6P	O1-C1-C2	-2.18	106.58	111.16
2	B	701	2UY	C3-C4-N1	-2.14	119.05	122.24
2	B	701	2UY	C16-C12-S1	2.14	122.28	119.49
2	A	701	2UY	C7-C4-N1	2.13	120.24	116.48
3	B	702	S6P	O6-P-O3P	2.09	112.10	106.44
3	A	702	S6P	C2-C3-C4	-2.07	109.30	112.48
2	A	701	2UY	C8-C7-C6	2.01	118.88	117.46

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	2UY	C5-C1-C11-C24
2	B	701	2UY	C5-C1-C11-C24
3	A	702	S6P	O1-C1-C2-C3
3	A	702	S6P	O1-C1-C2-O2
5	B	716	GOL	O1-C1-C2-C3
5	B	716	GOL	O1-C1-C2-O2
5	B	717	GOL	O1-C1-C2-O2
2	A	701	2UY	C5-C1-C11-C23
2	A	701	2UY	C2-C1-C11-C23
2	B	701	2UY	C2-C1-C11-C23
2	A	701	2UY	C2-C1-C11-C24
2	B	701	2UY	C2-C1-C11-C24
3	B	702	S6P	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	701	2UY	C5-C1-C11-C23
2	B	701	2UY	N2-C6-N3-C17

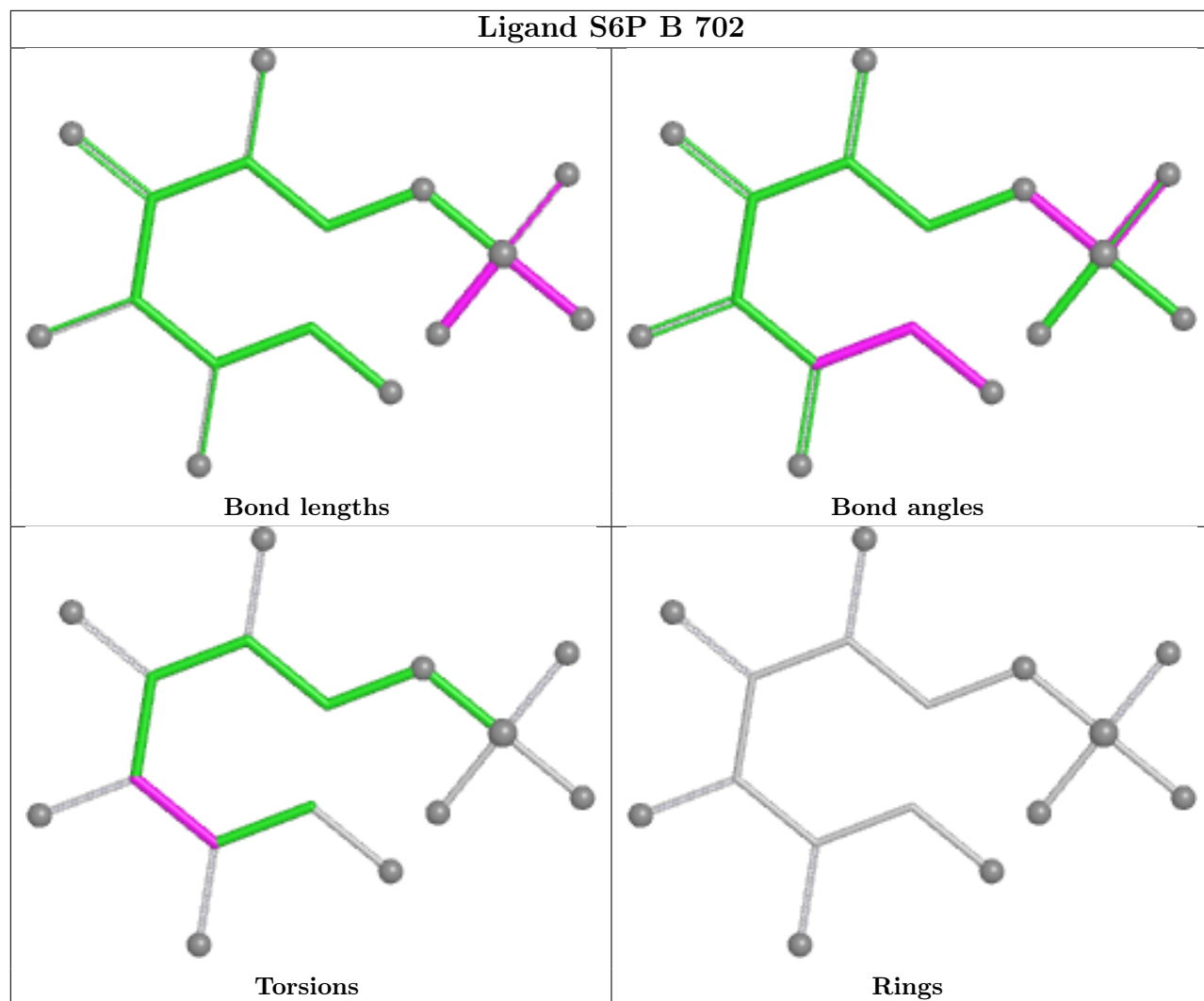
There are no ring outliers.

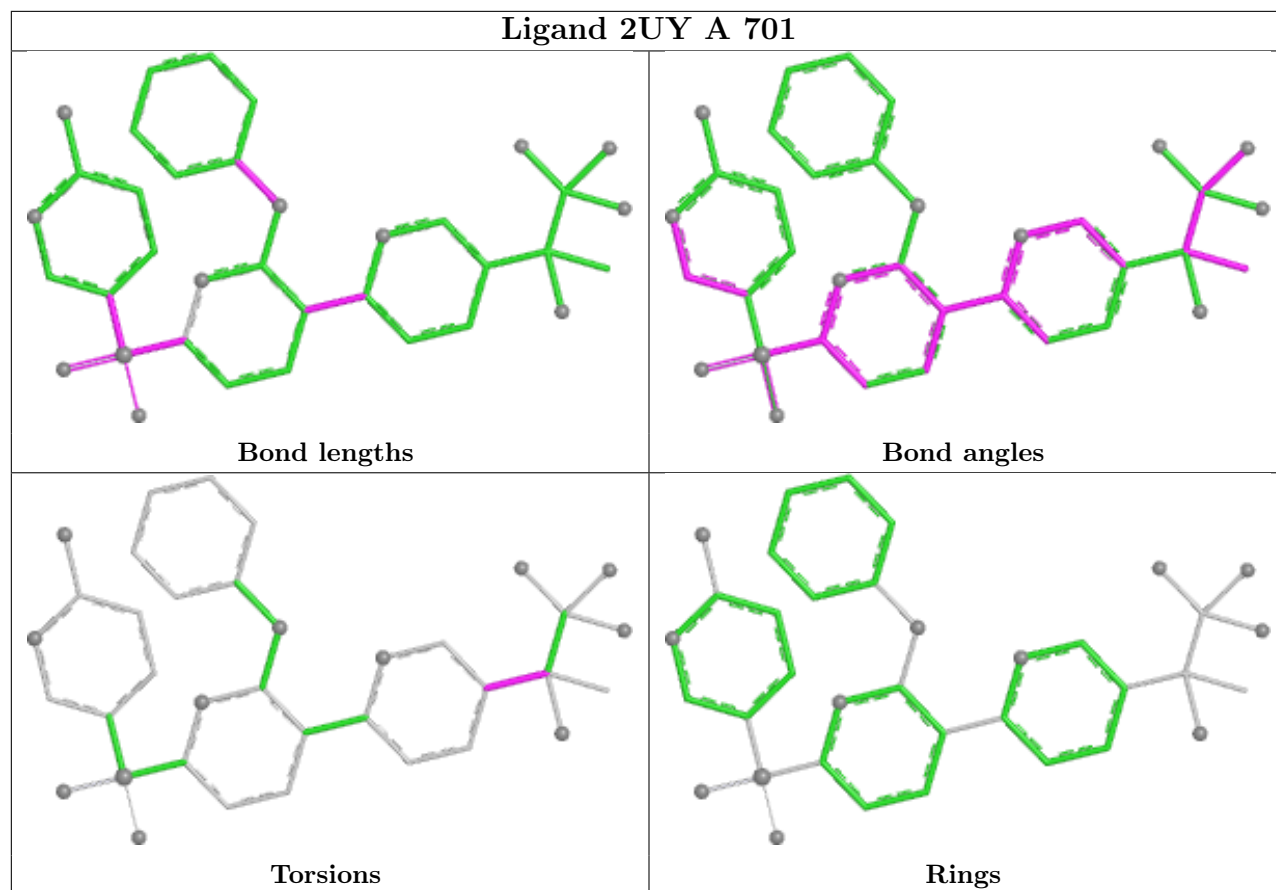
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	S6P	1	0
2	A	701	2UY	6	0
2	B	701	2UY	4	0

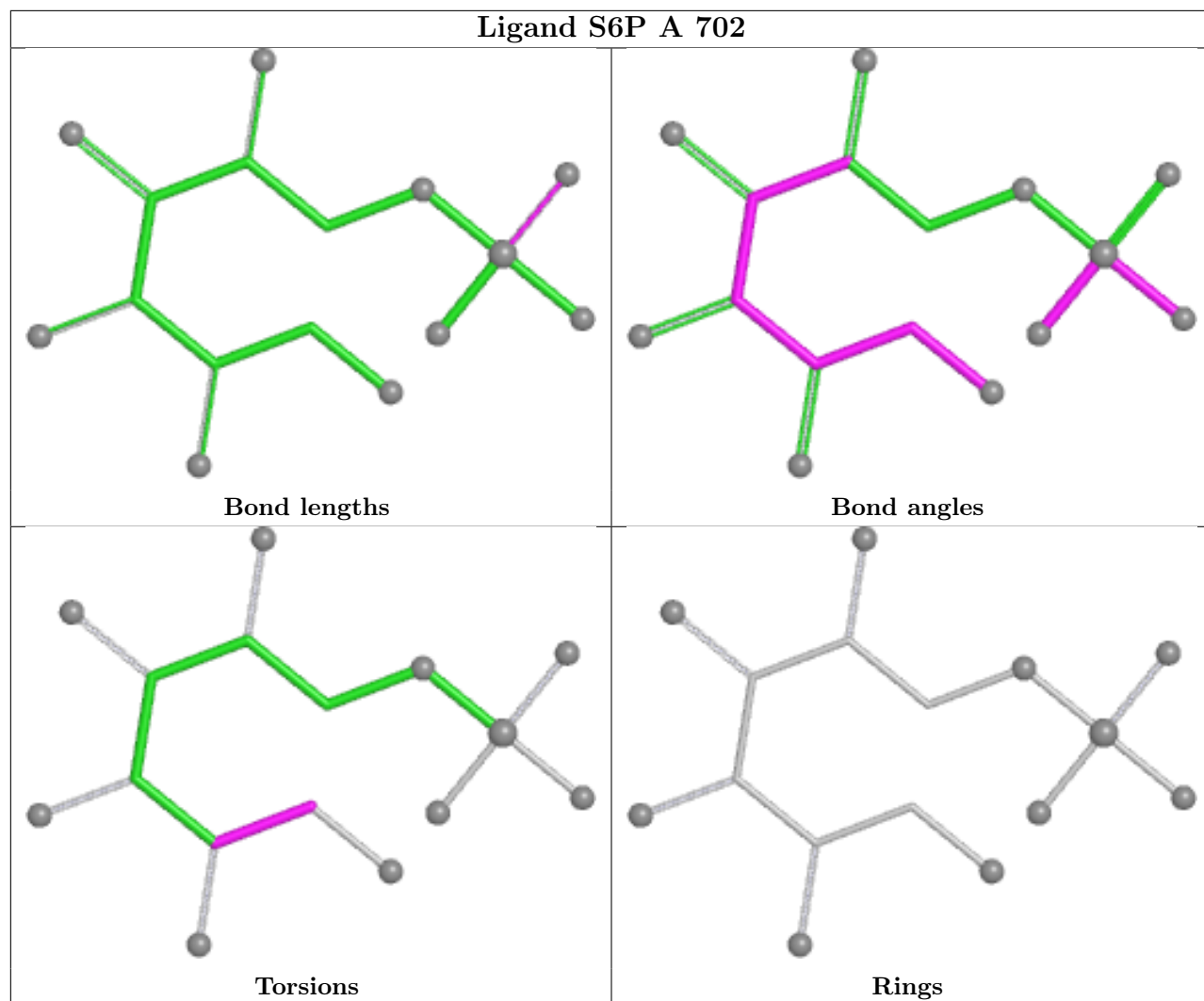
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

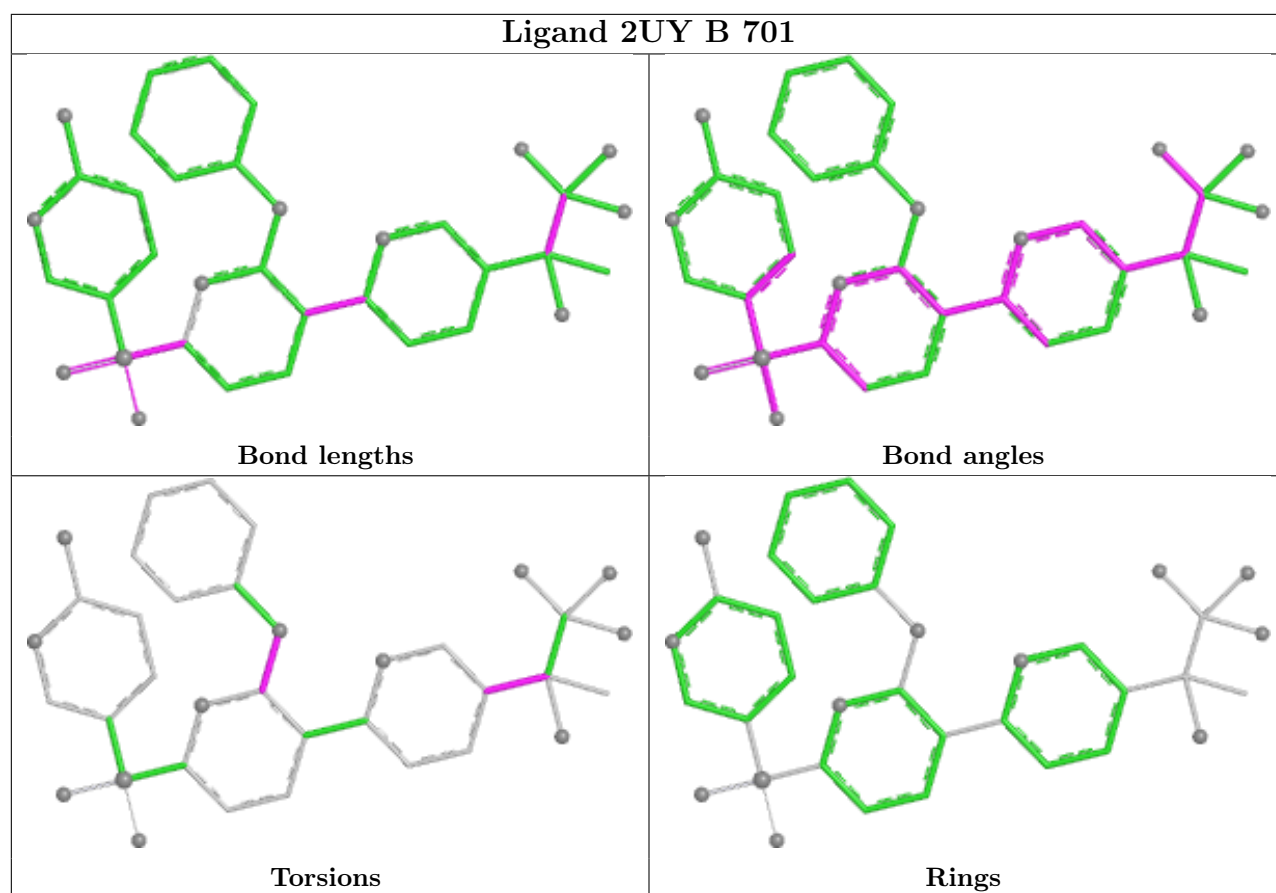
Ligand S6P B 702





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%)	0.08	22 (3%) 44 35	21, 41, 82, 117	0
1	B	590/638 (92%)	-0.19	10 (1%) 69 60	20, 36, 67, 110	0
All	All	1175/1276 (92%)	-0.05	32 (2%) 56 46	20, 39, 77, 117	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	LEU	4.9
1	A	465	PHE	4.5
1	A	449	LEU	4.2
1	B	65	GLY	4.2
1	A	387	PHE	3.9
1	B	447	ILE	3.7
1	A	458	SER	3.6
1	A	448	PRO	3.5
1	A	445	LEU	3.5
1	A	429	LYS	3.4
1	A	447	ILE	3.3
1	A	450	LYS	3.1
1	A	357	PHE	3.1
1	A	327	LYS	3.1
1	A	69	SER	3.0
1	A	452	LEU	2.9
1	B	66	GLN	2.8
1	A	21	LEU	2.8
1	A	131	LYS	2.6
1	B	20	GLU	2.6
1	A	430	THR	2.5
1	A	358	ARG	2.4
1	B	1	MET	2.3
1	A	410	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	463	LEU	2.2
1	A	393	LEU	2.2
1	A	312	LYS	2.2
1	A	420	GLN	2.2
1	B	366	GLY	2.1
1	B	381	GLN	2.1
1	B	2	PRO	2.1
1	B	465	PHE	2.1

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	718	5/5	0.81	0.12	69,76,86,87	0
4	IOD	B	712	1/1	0.87	0.21	109,109,109,109	1
4	IOD	A	711	1/1	0.87	0.12	133,133,133,133	1
4	IOD	B	713	1/1	0.91	0.09	63,63,63,63	1
5	GOL	B	716	6/6	0.91	0.12	46,51,57,60	0
2	2UY	A	701	36/36	0.91	0.12	39,50,64,66	0
2	2UY	B	701	36/36	0.93	0.11	46,51,60,61	0
5	GOL	B	717	6/6	0.93	0.11	30,31,33,33	0
4	IOD	B	710	1/1	0.93	0.13	100,100,100,100	1
4	IOD	A	709	1/1	0.94	0.10	81,81,81,81	1
4	IOD	A	712	1/1	0.94	0.06	54,54,54,54	1
4	IOD	A	714	1/1	0.94	0.07	59,59,59,59	1
4	IOD	B	715	1/1	0.96	0.06	87,87,87,87	1
4	IOD	B	714	1/1	0.96	0.05	52,52,52,52	1
4	IOD	A	708	1/1	0.97	0.10	83,83,83,83	1

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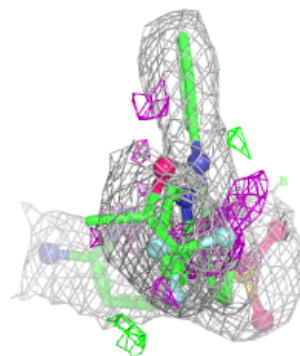
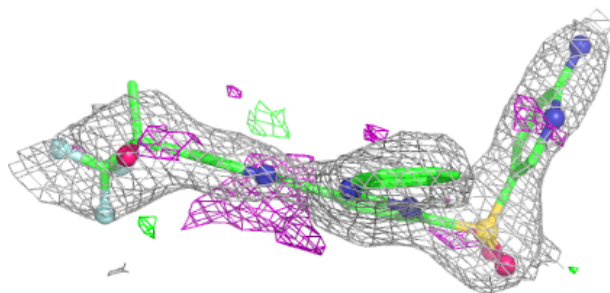
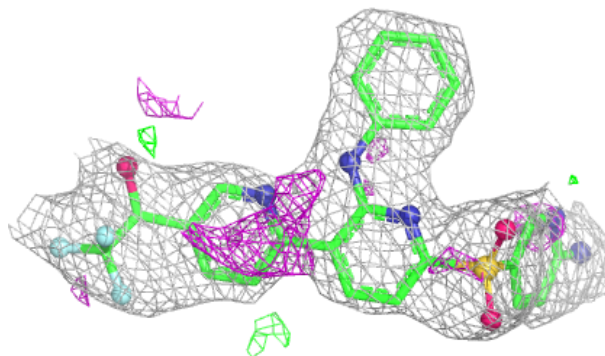
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IOD	A	713	1/1	0.97	0.06	47,47,47,47	1
4	IOD	A	703	1/1	0.97	0.04	60,60,60,60	0
4	IOD	B	703	1/1	0.97	0.03	45,45,45,45	0
4	IOD	B	707	1/1	0.97	0.05	62,62,62,62	0
4	IOD	B	709	1/1	0.97	0.06	60,60,60,60	1
4	IOD	A	706	1/1	0.97	0.05	73,73,73,73	0
4	IOD	B	708	1/1	0.98	0.08	51,51,51,51	1
4	IOD	A	707	1/1	0.98	0.03	53,53,53,53	1
3	S6P	A	702	16/16	0.98	0.06	19,24,30,32	0
4	IOD	B	706	1/1	0.98	0.03	44,44,44,44	0
3	S6P	B	702	16/16	0.98	0.06	17,18,20,20	0
6	SO4	B	719	5/5	0.98	0.07	18,18,19,19	5
4	IOD	A	710	1/1	0.99	0.03	32,32,32,32	1
4	IOD	B	711	1/1	0.99	0.05	30,30,30,30	1
4	IOD	A	704	1/1	0.99	0.03	54,54,54,54	0
4	IOD	A	705	1/1	0.99	0.04	44,44,44,44	1
4	IOD	B	705	1/1	0.99	0.04	50,50,50,50	0
4	IOD	B	704	1/1	1.00	0.02	45,45,45,45	0

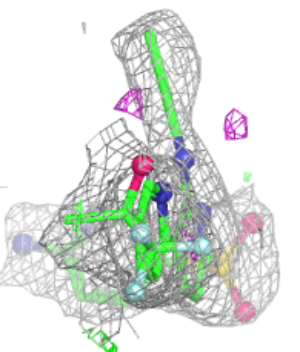
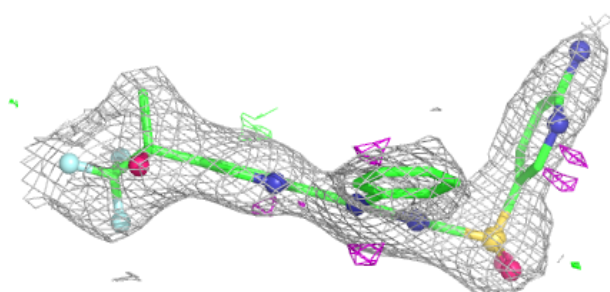
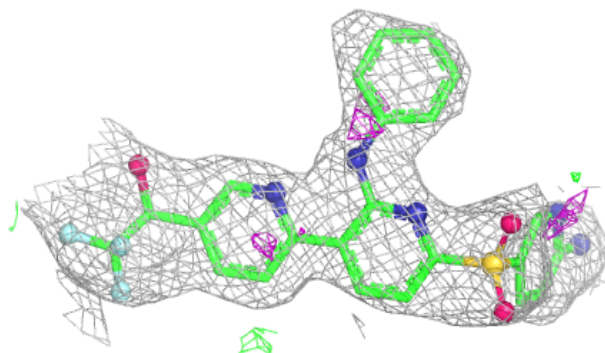
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2UY 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)

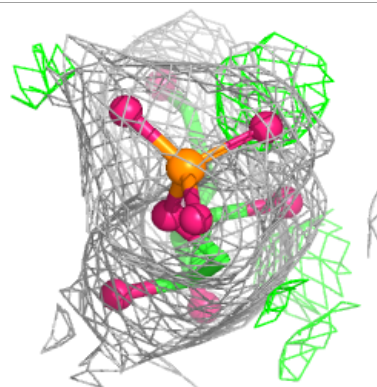
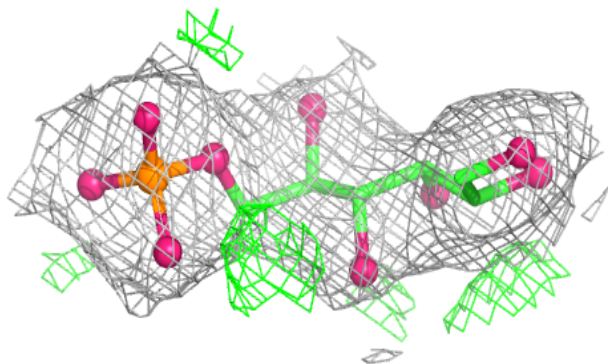
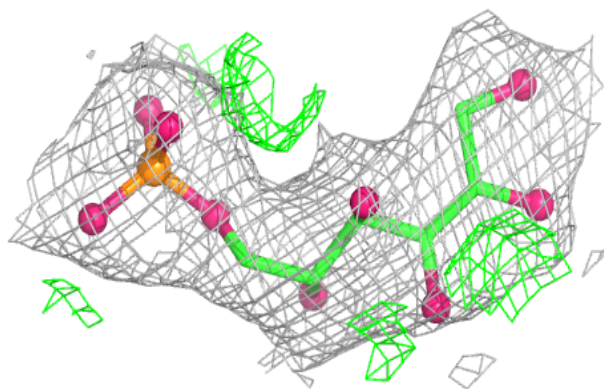
**Electron density around 2UY B 701:**

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

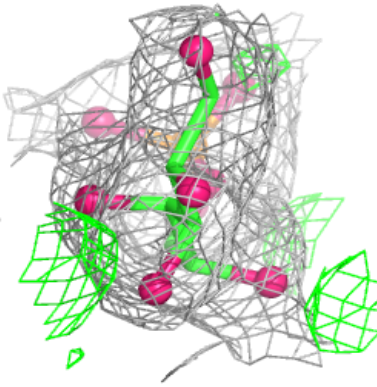
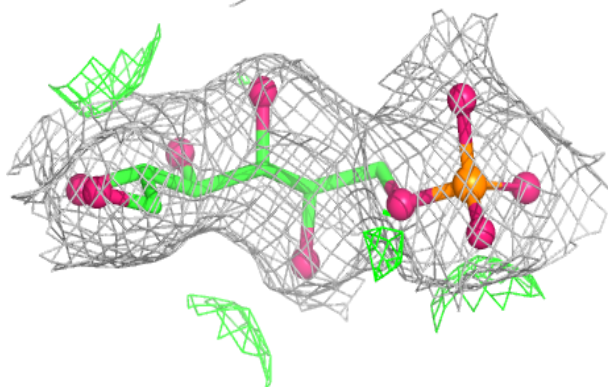
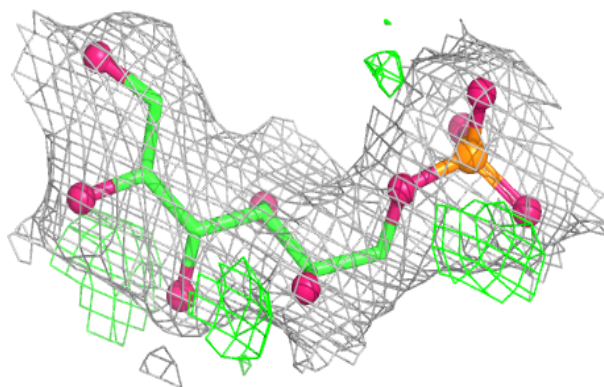


Electron density around S6P A 702:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.