



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:31 AM UTC

PDB ID : 4PX2 / pdb_00004px2
Title : Human GKRP bound to AMG2882 and Sorbitol-6-Phosphate
Authors : Jordan, S.R.; Chmait, S.
Deposited on : 2014-03-21
Resolution : 2.15 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

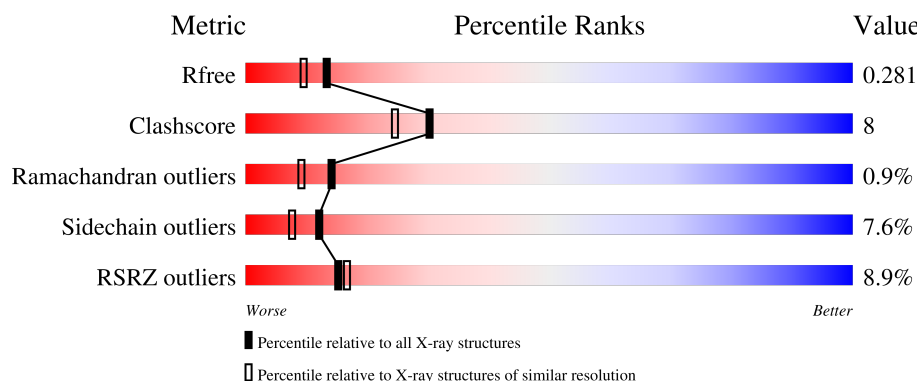
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	A	711	-	-	X	-
4	IOD	B	712	-	-	X	-
4	IOD	B	713	-	-	X	-
4	IOD	B	716	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9386 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:

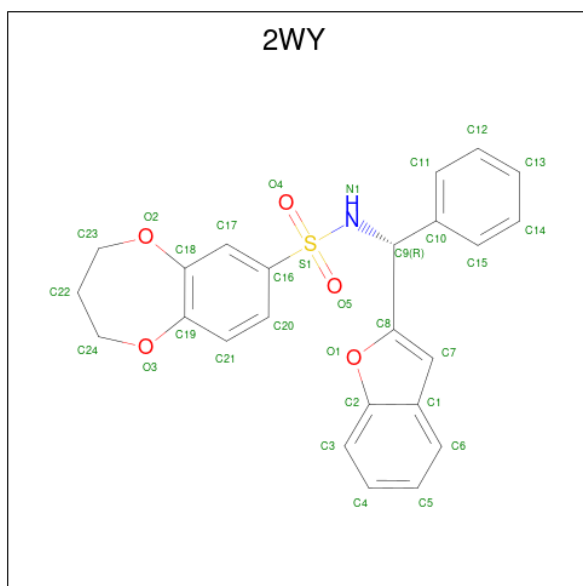
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q14397
A	-10	ALA	-	expression tag	UNP Q14397
A	-9	HIS	-	expression tag	UNP Q14397
A	-8	HIS	-	expression tag	UNP Q14397
A	-7	HIS	-	expression tag	UNP Q14397
A	-6	HIS	-	expression tag	UNP Q14397
A	-5	HIS	-	expression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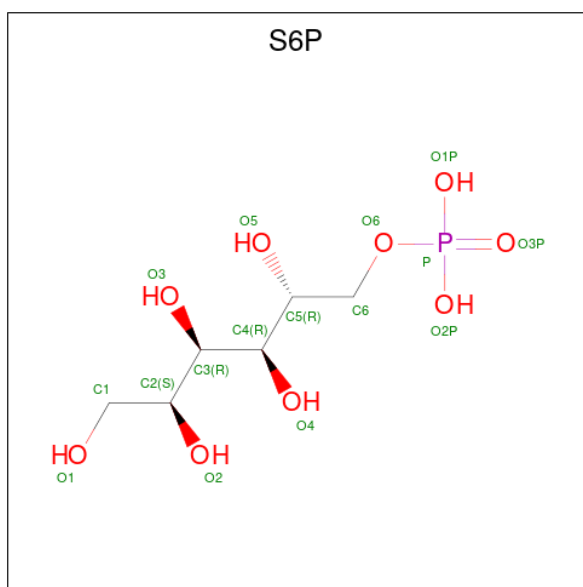
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	expression tag	UNP Q14397

- Molecule 2 is N-[(R)-1-benzofuran-2-yl(phenyl)methyl]-3,4-dihydro-2H-1,5-benzodioxepine-7-sulfonamide (CCD ID: 2WY) (formula: $C_{24}H_{21}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	24	1	5	1		
2	B	1	Total	C	N	O	S	0	0
			31	24	1	5	1		

- 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).

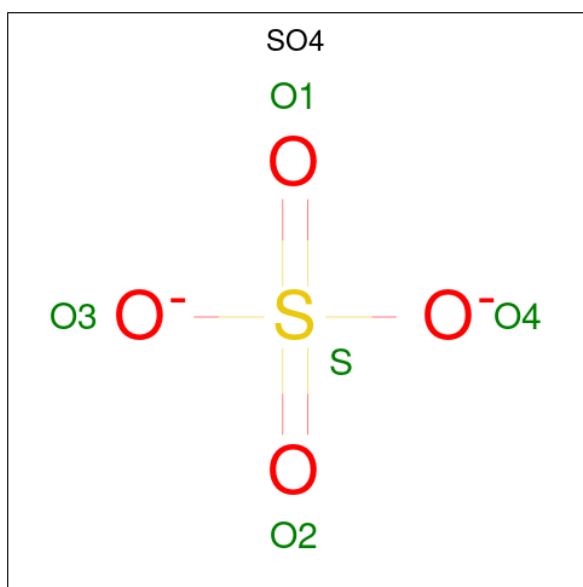
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	I	0	0
			13	13		
4	B	15	Total	I	0	0
			15	15		

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



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

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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		
6	B	1	Total	O	S	0	0
			5	4	1		

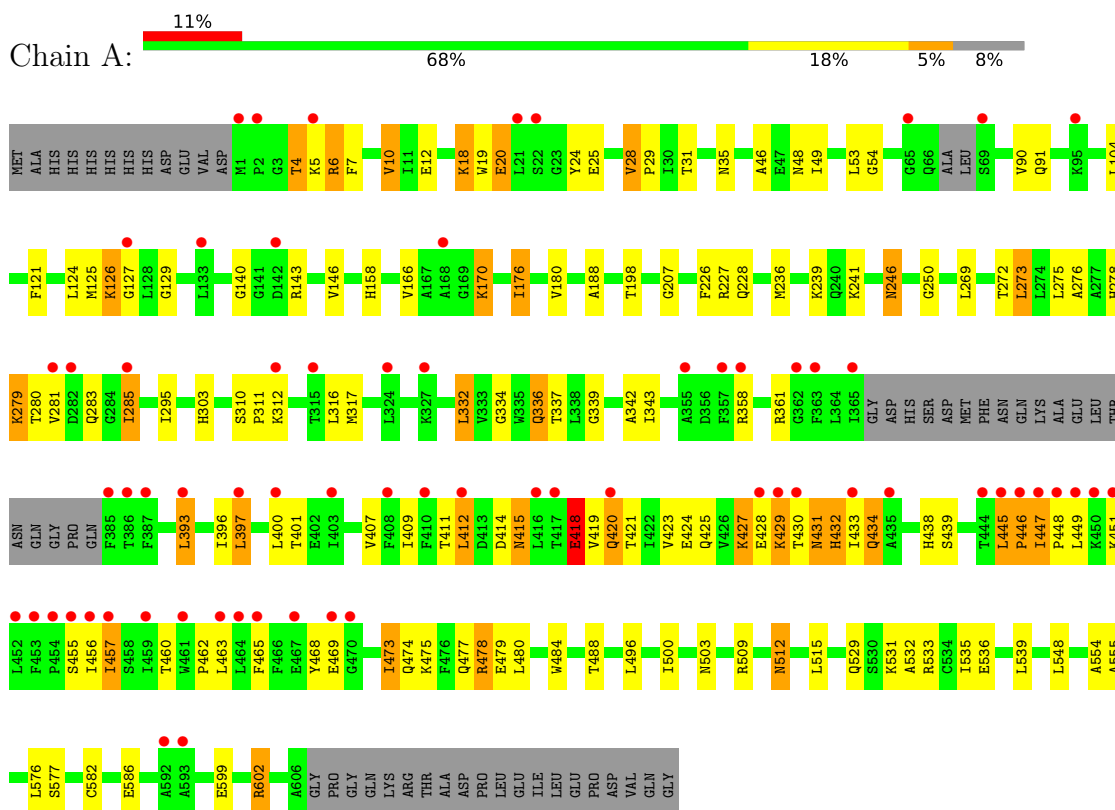
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	98	Total	O	0	0
			98	98		

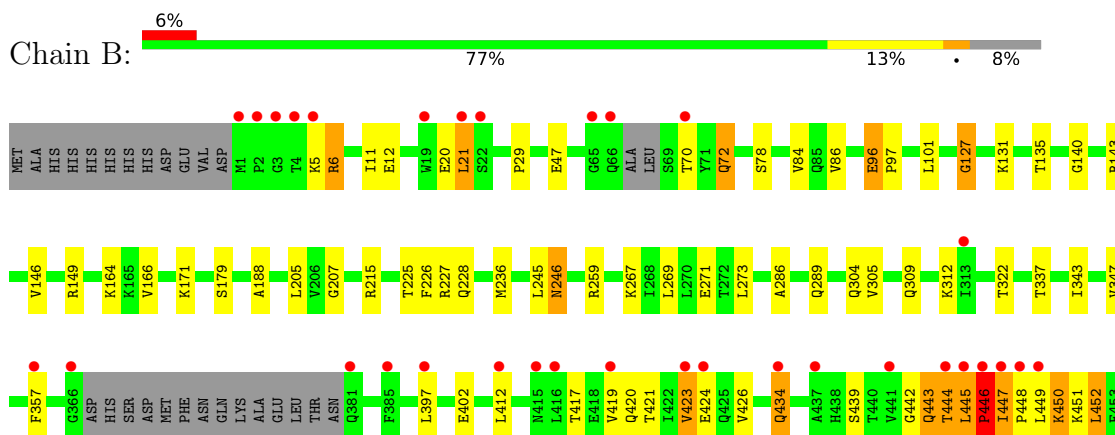
3 Residue-property plots

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	148.16Å 148.16Å 131.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.00 – 2.15 27.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (27.00-2.15) 98.3 (27.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.227 , 0.279 0.234 , 0.281	Depositor DCC
R_{free} test set	4370 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.3	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	0.95	EDS
Total number of atoms	9386	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, 2WY, GOL, 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	1.11	4/4603 (0.1%)	1.14	10/6228 (0.2%)
1	B	1.13	3/4637 (0.1%)	1.13	12/6274 (0.2%)
All	All	1.12	7/9240 (0.1%)	1.14	22/12502 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	VAL	C-O	-5.85	1.17	1.24
1	A	269	LEU	C-O	5.72	1.30	1.24
1	A	176	ILE	N-CA	-5.39	1.39	1.46
1	A	31	THR	C-O	-5.38	1.17	1.24
1	B	478	ARG	C-O	-5.36	1.17	1.24
1	B	179	SER	CA-C	-5.25	1.46	1.52
1	B	205	LEU	CA-C	-5.09	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH2	-8.95	111.14	119.20
1	B	96	GLU	CA-C-N	6.48	126.11	119.56
1	B	96	GLU	C-N-CA	6.48	126.11	119.56
1	A	90	VAL	N-CA-C	-6.24	104.43	110.42
1	B	259	ARG	NE-CZ-NH1	6.24	127.74	121.50
1	A	180	VAL	N-CA-C	6.08	116.74	110.36
1	A	434	GLN	N-CA-C	-5.86	99.61	108.52
1	A	28	VAL	CA-C-N	-5.72	113.87	119.76
1	A	28	VAL	C-N-CA	-5.72	113.87	119.76
1	A	457	ILE	CB-CA-C	-5.71	106.17	112.68
1	B	417	THR	N-CA-C	-5.64	104.77	111.03
1	A	468	TYR	N-CA-C	5.58	119.19	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	ILE	N-CA-C	-5.48	98.57	107.28
1	B	552	ILE	N-CA-C	-5.43	105.43	110.53
1	B	452	LEU	N-CA-C	5.26	117.02	111.28
1	B	305	VAL	N-CA-C	-5.25	105.38	110.42
1	B	426	VAL	CB-CA-C	-5.24	105.17	112.04
1	B	357	PHE	N-CA-C	5.19	118.40	111.75
1	A	418	GLU	N-CA-C	-5.10	105.63	111.14
1	A	48	ASN	N-CA-C	5.09	116.83	111.28
1	B	434	GLN	N-CA-C	-5.06	101.38	109.07
1	A	24	TYR	N-CA-C	-5.05	105.66	111.07

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	92	0
1	B	4554	0	4647	66	0
2	A	31	0	21	2	0
2	B	31	0	21	2	0
3	A	16	0	13	0	0
3	B	16	0	13	0	0
4	A	13	0	0	4	0
4	B	15	0	0	10	0
5	A	6	0	8	0	0
5	B	12	0	16	1	0
6	B	20	0	0	1	0
7	A	53	0	0	4	0
7	B	98	0	0	1	1
All	All	9386	0	9357	156	1

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 (156) 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:429:LYS:NZ	7:A:849:HOH:O	1.61	1.28
1:B:458:SER:HB3	4:B:713:IOD:I	2.37	0.94
1:A:337:THR:HG21	1:A:479:GLU:OE2	1.67	0.94
1:A:400:LEU:O	1:A:401:THR:OG1	1.92	0.87
1:B:20:GLU:HG2	1:B:21:LEU:HD22	1.64	0.80
1:A:6:ARG:HD3	1:A:555:ALA:O	1.82	0.78
1:A:4:THR:O	4:A:711:IOD:I	2.76	0.72
1:A:602:ARG:HH11	1:A:602:ARG:HG3	1.58	0.69
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.37	0.69
1:B:469:GLU:HG2	4:B:716:IOD:I	2.63	0.69
1:A:439:SER:OG	1:A:460:THR:HG22	1.91	0.69
1:A:393:LEU:O	1:A:397:LEU:HB3	1.93	0.68
1:B:140:GLY:O	1:B:149:ARG:NH2	2.27	0.68
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.58	0.67
1:A:532:ALA:O	1:A:536:GLU:HG3	1.94	0.67
1:B:72:GLN:CD	1:B:78:SER:HG	2.02	0.66
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.29	0.66
1:A:140:GLY:H	1:A:158:HIS:HE1	1.42	0.65
1:A:433:ILE:O	1:A:434:GLN:HG2	1.98	0.63
1:A:474:GLN:O	1:A:478:ARG:HD3	1.98	0.62
1:B:502:GLN:NE2	4:B:717:IOD:I	3.01	0.62
1:A:415:ASN:HD22	1:A:418:GLU:H	1.46	0.62
1:B:445:LEU:HG	4:B:713:IOD:I	2.70	0.61
1:A:283:GLN:HB2	1:A:285:ILE:HG22	1.84	0.60
1:B:448:PRO:O	1:B:451:LYS:HB2	2.01	0.60
1:B:6:ARG:HD2	1:B:554:ALA:O	2.02	0.59
1:A:146:VAL:HG12	1:A:146:VAL:O	2.03	0.59
1:B:146:VAL:HG12	1:B:146:VAL:O	2.01	0.59
1:A:582:CYS:HB2	1:A:586:GLU:OE2	2.02	0.58
1:A:339:GLY:O	1:A:342:ALA:HB3	2.04	0.58
1:A:246:ASN:H	1:A:246:ASN:HD22	1.50	0.58
1:A:19:TRP:O	1:A:20:GLU:CB	2.52	0.58
1:A:480:LEU:HD21	1:A:484:TRP:CH2	2.39	0.57
1:A:246:ASN:HD22	1:A:246:ASN:N	2.03	0.56
1:B:286:ALA:HA	1:B:289:GLN:HE21	1.70	0.56
1:A:317:MET:CE	1:A:496:LEU:HD11	2.36	0.56
1:B:6:ARG:HD3	1:B:555:ALA:O	2.05	0.56
1:A:312:LYS:HB3	1:A:457:ILE:HG12	1.88	0.55
1:A:529:GLN:HE22	1:A:533:ARG:HH21	1.54	0.55
1:B:127:GLY:O	4:B:716:IOD:I	2.94	0.55
1:B:419:VAL:O	1:B:423:VAL:HG12	2.05	0.55
1:B:531:LYS:HE2	4:B:712:IOD:I	2.76	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HB2	4:B:710:IOD:I	2.77	0.55
1:B:529:GLN:HE21	1:B:533:ARG:HE	1.53	0.55
1:B:503:ASN:HD22	1:B:503:ASN:H	1.56	0.54
1:A:512:ASN:ND2	1:A:515:LEU:H	2.03	0.54
1:A:420:GLN:HB3	1:A:449:LEU:HG	1.90	0.54
1:B:225:THR:H	1:B:228:GLN:HE21	1.54	0.54
1:B:164:LYS:HE2	5:B:719:GOL:H12	1.89	0.54
1:A:228:GLN:HE22	1:B:228:GLN:NE2	2.04	0.54
1:B:146:VAL:HG13	1:B:343:ILE:CG2	2.38	0.53
1:B:442:GLY:O	1:B:443:GLN:O	2.26	0.53
1:B:146:VAL:HG13	1:B:343:ILE:HG21	1.91	0.53
1:A:431:ASN:H	1:A:431:ASN:HD22	1.56	0.52
1:A:317:MET:HE2	1:A:496:LEU:HD11	1.91	0.52
1:A:6:ARG:HD2	1:A:554:ALA:O	2.10	0.52
1:A:602:ARG:HH11	1:A:602:ARG:CG	2.21	0.51
1:A:46:ALA:HA	1:A:317:MET:CE	2.39	0.51
1:A:447:ILE:N	1:A:448:PRO:HD2	2.25	0.51
1:B:420:GLN:HA	1:B:423:VAL:HG13	1.92	0.51
1:A:104:LEU:HD23	1:A:176:ILE:HB	1.93	0.51
1:A:53:LEU:HD12	1:A:488:THR:HG23	1.93	0.50
1:A:419:VAL:O	1:A:423:VAL:HG23	2.11	0.50
1:B:309:GLN:NE2	1:B:458:SER:O	2.45	0.50
1:A:146:VAL:HG13	1:A:343:ILE:CG2	2.40	0.50
1:A:473:ILE:HD13	1:A:473:ILE:O	2.12	0.50
1:A:29:PRO:HG2	2:A:701:2WY:C11	2.42	0.50
1:A:397:LEU:O	1:A:400:LEU:HD13	2.12	0.50
1:A:397:LEU:O	1:A:397:LEU:HD22	2.12	0.50
1:A:280:THR:HB	1:A:285:ILE:O	2.12	0.50
1:A:512:ASN:C	1:A:512:ASN:HD22	2.19	0.50
1:A:4:THR:HA	4:A:711:IOD:I	2.82	0.50
1:B:447:ILE:HG22	1:B:450:LYS:CE	2.41	0.50
1:A:124:LEU:C	1:A:124:LEU:HD23	2.37	0.49
1:A:236:MET:CE	1:A:241:LYS:HB3	2.42	0.49
1:B:246:ASN:HD22	1:B:246:ASN:N	2.09	0.49
1:A:91:GLN:HG2	1:A:281:VAL:HG13	1.95	0.49
1:B:458:SER:CB	4:B:713:IOD:I	3.23	0.49
1:B:444:THR:O	1:B:446:PRO:HD3	2.13	0.49
1:A:7:PHE:HB2	4:A:711:IOD:I	2.83	0.49
1:B:529:GLN:HE22	1:B:533:ARG:HH21	1.60	0.49
1:B:412:LEU:CD1	1:B:439:SER:HB3	2.43	0.48
1:A:121:PHE:O	1:A:125:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD12	1:A:407:VAL:HB	1.94	0.48
1:A:400:LEU:C	1:A:401:THR:HG1	2.08	0.48
1:B:236:MET:HG2	6:B:722:SO4:O3	2.13	0.48
1:A:207:GLY:O	1:A:246:ASN:HA	2.14	0.48
1:B:421:THR:O	1:B:424:GLU:HB2	2.13	0.48
1:A:18:LYS:HE2	7:A:850:HOH:O	2.14	0.47
1:A:46:ALA:HA	1:A:317:MET:HE2	1.95	0.47
1:A:475:LYS:HE2	1:A:479:GLU:OE2	2.14	0.47
1:A:126:LYS:O	1:A:129:GLY:N	2.38	0.47
1:A:198:THR:HG21	1:A:236:MET:HE1	1.97	0.47
1:B:207:GLY:O	1:B:246:ASN:HA	2.15	0.47
1:A:54:GLY:O	1:A:303:HIS:NE2	2.48	0.47
1:A:170:LYS:N	1:A:170:LYS:HD2	2.30	0.47
1:A:334:GLY:HA2	1:A:409:ILE:O	2.14	0.47
1:B:309:GLN:HG3	1:B:459:ILE:HD13	1.96	0.47
1:A:18:LYS:CE	7:A:850:HOH:O	2.63	0.46
1:B:571:ILE:HB	1:B:572:PRO:HD3	1.97	0.46
1:A:412:LEU:HD23	1:A:412:LEU:N	2.30	0.46
1:B:246:ASN:HD22	1:B:246:ASN:H	1.64	0.46
1:B:267:LYS:NZ	1:B:271:GLU:OE1	2.49	0.46
1:A:91:GLN:HG2	1:A:281:VAL:CG1	2.46	0.46
1:B:582:CYS:HB2	1:B:586:GLU:OE1	2.16	0.45
1:A:400:LEU:C	1:A:401:THR:OG1	2.57	0.45
1:A:535:ILE:O	1:A:539:LEU:HG	2.17	0.44
1:A:427:LYS:O	1:A:427:LYS:HE2	2.17	0.44
1:A:49:ILE:HD12	1:A:317:MET:HE1	1.99	0.44
1:A:509:ARG:NH1	7:A:841:HOH:O	2.43	0.44
1:A:273:LEU:C	1:A:273:LEU:HD23	2.43	0.44
1:A:275:LEU:O	1:A:276:ALA:C	2.60	0.44
1:B:529:GLN:NE2	1:B:533:ARG:HE	2.15	0.44
1:A:430:THR:HG22	1:A:432:HIS:H	1.81	0.44
1:B:245:LEU:HG	1:B:269:LEU:HD21	1.98	0.44
1:A:278:HIS:O	1:A:279:LYS:C	2.61	0.44
1:A:283:GLN:CB	1:A:285:ILE:HG22	2.48	0.44
1:B:11:ILE:HG22	1:B:12:GLU:N	2.33	0.44
1:A:10:VAL:HB	1:A:531:LYS:HE3	2.00	0.44
1:A:317:MET:HE3	1:A:496:LEU:CD1	2.48	0.44
1:B:72:GLN:CG	1:B:78:SER:OG	2.66	0.44
1:B:503:ASN:HD22	1:B:503:ASN:N	2.14	0.44
1:B:503:ASN:H	1:B:503:ASN:ND2	2.16	0.44
1:B:449:LEU:HA	1:B:452:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HB2	1:A:226:PHE:CD2	2.53	0.43
1:A:250:GLY:HA2	4:A:705:IOD:I	2.88	0.43
1:A:445:LEU:O	1:A:446:PRO:C	2.61	0.43
1:B:86:VAL:HG12	1:B:273:LEU:HD21	2.00	0.43
1:B:445:LEU:O	1:B:446:PRO:C	2.61	0.43
1:B:215:ARG:HG3	2:B:701:2WY:C11	2.48	0.43
1:A:146:VAL:HG13	1:A:343:ILE:HG21	1.99	0.43
1:A:576:LEU:O	1:A:577:SER:C	2.62	0.43
1:B:503:ASN:ND2	1:B:503:ASN:N	2.66	0.43
1:B:447:ILE:N	1:B:448:PRO:HD2	2.34	0.42
1:B:464:LEU:O	1:B:465:PHE:C	2.61	0.42
1:A:272:THR:HA	1:A:295:ILE:HG21	2.00	0.42
1:A:310:SER:HB2	1:A:311:PRO:HD3	2.01	0.42
1:B:412:LEU:HD12	1:B:443:GLN:HB3	2.01	0.42
1:B:101:LEU:HD11	1:B:135:THR:HG22	2.02	0.42
1:B:447:ILE:HG22	1:B:450:LYS:HE3	2.02	0.42
1:B:531:LYS:CE	4:B:712:IOD:I	3.38	0.42
1:A:28:VAL:HG22	2:A:701:2WY:C4	2.49	0.42
1:A:146:VAL:O	1:A:146:VAL:CG1	2.66	0.42
1:B:312:LYS:HB3	1:B:457:ILE:HG12	2.01	0.42
1:B:572:PRO:O	1:B:576:LEU:HG	2.20	0.41
1:B:188:ALA:HB2	1:B:226:PHE:CD2	2.55	0.41
1:B:96:GLU:N	1:B:97:PRO:HD3	2.35	0.41
1:A:430:THR:HG22	1:A:432:HIS:N	2.35	0.41
1:B:29:PRO:HG2	2:B:701:2WY:C11	2.51	0.41
1:B:601:VAL:HG21	4:B:704:IOD:I	2.91	0.41
1:A:400:LEU:HD12	1:A:400:LEU:N	2.35	0.41
1:B:322:THR:HB	7:B:826:HOH:O	2.20	0.41
1:A:421:THR:O	1:A:424:GLU:HB2	2.21	0.40
1:A:438:HIS:CG	1:A:478:ARG:HG2	2.56	0.40
1:A:548:LEU:HA	1:A:548:LEU:HD23	1.89	0.40
1:B:286:ALA:HA	1:B:289:GLN:NE2	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:891:HOH:O	7:B:895:HOH:O[6_554]	1.55	0.65

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%)	540 (93%)	31 (5%)	8 (1%)	9	4
1	B	584/638 (92%)	554 (95%)	27 (5%)	3 (0%)	24	20
All	All	1163/1276 (91%)	1094 (94%)	58 (5%)	11 (1%)	14	9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	B	443	GLN
1	A	456	ILE
1	B	127	GLY
1	A	127	GLY
1	A	336	GLN
1	A	469	GLU
1	A	446	PRO
1	A	432	HIS
1	A	462	PRO
1	B	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%)	451 (91%)	47 (9%)	8	4
1	B	501/542 (92%)	472 (94%)	29 (6%)	18	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	999/1084 (92%)	923 (92%)	76 (8%)	12 8

All (76) 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	12	GLU
1	A	18	LYS
1	A	25	GLU
1	A	35	ASN
1	A	126	LYS
1	A	143	ARG
1	A	166	VAL
1	A	170	LYS
1	A	227	ARG
1	A	239	LYS
1	A	246	ASN
1	A	273	LEU
1	A	279	LYS
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	396	ILE
1	A	397	LEU
1	A	411	THR
1	A	412	LEU
1	A	415	ASN
1	A	418	GLU
1	A	420	GLN
1	A	425	GLN
1	A	427	LYS
1	A	428	GLU
1	A	429	LYS
1	A	431	ASN
1	A	445	LEU
1	A	447	ILE
1	A	451	LYS

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Mol	Chain	Res	Type
1	A	455	SER
1	A	463	LEU
1	A	465	PHE
1	A	473	ILE
1	A	478	ARG
1	A	500	ILE
1	A	503	ASN
1	A	512	ASN
1	A	599	GLU
1	A	602	ARG
1	B	6	ARG
1	B	21	LEU
1	B	47	GLU
1	B	70	THR
1	B	72	GLN
1	B	84	VAL
1	B	131	LYS
1	B	143	ARG
1	B	166	VAL
1	B	171	LYS
1	B	227	ARG
1	B	246	ASN
1	B	304	GLN
1	B	337	THR
1	B	347	VAL
1	B	397	LEU
1	B	402	GLU
1	B	423	VAL
1	B	434	GLN
1	B	444	THR
1	B	445	LEU
1	B	446	PRO
1	B	447	ILE
1	B	450	LYS
1	B	458	SER
1	B	463	LEU
1	B	467	GLU
1	B	503	ASN
1	B	562	GLN

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

Mol	Chain	Res	Type
1	A	35	ASN
1	A	72	GLN
1	A	123	GLN
1	A	158	HIS
1	A	190	GLN
1	A	196	ASN
1	A	240	GLN
1	A	246	ASN
1	A	289	GLN
1	A	415	ASN
1	A	420	GLN
1	A	431	ASN
1	A	471	ASN
1	A	477	GLN
1	A	503	ASN
1	A	512	ASN
1	A	529	GLN
1	B	8	GLN
1	B	9	HIS
1	B	39	GLN
1	B	48	ASN
1	B	55	GLN
1	B	130	GLN
1	B	196	ASN
1	B	197	ASN
1	B	228	GLN
1	B	246	ASN
1	B	283	GLN
1	B	289	GLN
1	B	384	GLN
1	B	389	GLN
1	B	415	ASN
1	B	431	ASN
1	B	434	GLN
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 [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 39 ligands modelled in this entry, 28 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	S6P	B	702	-	15,15,15	2.20	5 (33%)	20,21,21	1.15	1 (5%)
6	SO4	B	721	-	4,4,4	0.38	0	6,6,6	0.56	0
6	SO4	B	723	-	4,4,4	0.52	0	6,6,6	0.33	0
2	2WY	B	701	-	35,35,35	2.47	11 (31%)	47,50,50	2.77	21 (44%)
5	GOL	B	719	-	5,5,5	0.50	0	5,5,5	0.23	0
3	S6P	A	702	-	15,15,15	1.22	1 (6%)	20,21,21	2.06	3 (15%)
2	2WY	A	701	-	35,35,35	2.46	14 (40%)	47,50,50	2.57	22 (46%)
5	GOL	B	718	-	5,5,5	0.71	0	5,5,5	0.96	0
5	GOL	A	716	-	5,5,5	0.41	0	5,5,5	1.85	2 (40%)
6	SO4	B	722	-	4,4,4	0.69	0	6,6,6	0.61	0
6	SO4	B	720	-	4,4,4	0.61	0	6,6,6	0.47	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
3	S6P	B	702	-	-	0/20/20/20	-
2	2WY	B	701	-	-	0/19/27/27	0/5/5/5
5	GOL	B	719	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	S6P	A	702	-	-	0/20/20/20	-
2	2WY	A	701	-	-	1/19/27/27	0/5/5/5
5	GOL	B	718	-	-	2/4/4/4	-
5	GOL	A	716	-	-	2/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2WY	C16-S1	7.62	1.88	1.76
2	A	701	2WY	O4-S1	6.35	1.50	1.43
2	B	701	2WY	O5-S1	6.10	1.50	1.43
2	A	701	2WY	S1-N1	5.70	1.71	1.61
2	B	701	2WY	C9-C8	5.55	1.55	1.50
2	B	701	2WY	O4-S1	5.06	1.49	1.43
2	A	701	2WY	O5-S1	5.00	1.49	1.43
3	B	702	S6P	P-O3P	4.75	1.65	1.50
3	B	702	S6P	C2-C3	-4.11	1.46	1.53
2	A	701	2WY	C9-C8	3.94	1.53	1.50
3	A	702	S6P	C2-C3	-3.45	1.47	1.53
2	A	701	2WY	C16-S1	3.27	1.81	1.76
2	A	701	2WY	C11-C10	3.21	1.44	1.39
2	A	701	2WY	C1-C7	-3.20	1.34	1.44
2	B	701	2WY	C1-C7	-3.09	1.34	1.44
3	B	702	S6P	C6-C5	2.97	1.55	1.51
2	B	701	2WY	S1-N1	2.63	1.66	1.61
2	A	701	2WY	C20-C16	2.61	1.43	1.38
2	A	701	2WY	C9-N1	2.53	1.52	1.47
2	A	701	2WY	C22-C23	2.53	1.57	1.51
2	A	701	2WY	C22-C24	2.52	1.57	1.51
2	B	701	2WY	C22-C23	2.46	1.57	1.51
3	B	702	S6P	P-O1P	-2.39	1.45	1.54
2	B	701	2WY	C22-C24	2.34	1.56	1.51
2	B	701	2WY	C9-N1	2.31	1.51	1.47
3	B	702	S6P	C5-C4	-2.30	1.49	1.53
2	A	701	2WY	C7-C8	-2.29	1.32	1.34
2	A	701	2WY	O3-C24	2.23	1.49	1.44
2	A	701	2WY	C4-C5	2.12	1.42	1.38
2	B	701	2WY	C1-C2	2.06	1.42	1.39
2	B	701	2WY	O2-C23	2.02	1.49	1.44

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2WY	O5-S1-O4	-7.53	110.37	119.52
2	B	701	2WY	O5-S1-O4	-7.16	110.83	119.52
2	B	701	2WY	O5-S1-C16	6.97	116.77	107.98
2	A	701	2WY	O4-S1-C16	6.46	116.12	107.98
3	A	702	S6P	C5-C4-C3	-5.79	103.59	112.48
2	B	701	2WY	O2-C23-C22	5.50	124.34	112.80
2	B	701	2WY	O3-C19-C18	5.32	128.75	123.24
2	A	701	2WY	C13-C12-C11	-4.54	114.63	120.24
2	B	701	2WY	O3-C24-C22	4.52	122.29	112.80
2	B	701	2WY	C21-C20-C16	4.48	123.80	119.44
3	A	702	S6P	O6-P-O3P	4.42	118.37	106.44
2	B	701	2WY	C13-C12-C11	-4.38	114.83	120.24
3	A	702	S6P	O1-C1-C2	-4.10	102.54	111.16
2	A	701	2WY	O2-C18-C19	4.04	127.42	123.24
2	B	701	2WY	C17-C16-S1	3.95	123.11	119.06
2	A	701	2WY	C5-C4-C3	3.83	124.96	120.24
2	B	701	2WY	C14-C15-C10	-3.80	116.09	120.65
2	A	701	2WY	O2-C23-C22	3.50	120.15	112.80
2	B	701	2WY	C20-C16-C17	-3.42	116.44	120.68
2	A	701	2WY	C6-C1-C2	3.22	122.75	118.59
2	A	701	2WY	C24-O3-C19	-3.12	110.95	116.13
2	A	701	2WY	O2-C18-C17	-3.00	111.96	116.83
2	A	701	2WY	C12-C11-C10	2.94	124.17	120.65
2	A	701	2WY	C10-C9-N1	-2.93	105.13	111.36
2	A	701	2WY	C9-C8-C7	-2.87	123.32	133.30
2	B	701	2WY	C2-C1-C7	2.77	108.50	105.64
2	A	701	2WY	C5-C6-C1	-2.70	116.86	120.95
2	B	701	2WY	O1-C2-C3	2.67	132.11	126.49
5	A	716	GOL	O2-C2-C1	-2.67	98.13	109.18
2	A	701	2WY	C14-C15-C10	-2.66	117.46	120.65
2	A	701	2WY	O3-C19-C18	2.64	125.97	123.24
5	A	716	GOL	O2-C2-C3	2.62	120.05	109.18
2	A	701	2WY	C13-C14-C15	2.55	123.38	120.24
2	B	701	2WY	C9-C8-C7	-2.52	124.56	133.30
2	B	701	2WY	C14-C13-C12	2.50	123.29	119.87
2	A	701	2WY	O1-C2-C1	-2.49	107.01	110.12
2	B	701	2WY	C15-C10-C11	2.48	121.38	118.30
2	A	701	2WY	C1-C7-C8	2.46	108.79	107.01
2	B	701	2WY	O1-C2-C1	-2.39	107.12	110.12
2	A	701	2WY	C4-C3-C2	-2.34	115.34	119.60
3	B	702	S6P	O2P-P-O6	2.34	112.76	106.67
2	B	701	2WY	O3-C19-C21	-2.27	112.39	117.31
2	A	701	2WY	C9-N1-S1	2.22	126.17	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2WY	O2-C18-C17	-2.22	113.22	116.83
2	A	701	2WY	O1-C2-C3	2.21	131.13	126.49
2	A	701	2WY	C2-C1-C7	2.19	107.89	105.64
2	B	701	2WY	O2-C18-C19	2.12	125.43	123.24
2	B	701	2WY	C3-C2-C1	-2.03	120.76	123.81
2	B	701	2WY	C9-N1-S1	-2.03	117.34	121.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	716	GOL	O1-C1-C2-C3
5	B	718	GOL	O1-C1-C2-O2
5	B	718	GOL	O1-C1-C2-C3
2	A	701	2WY	C9-N1-S1-O4
5	A	716	GOL	O1-C1-C2-O2

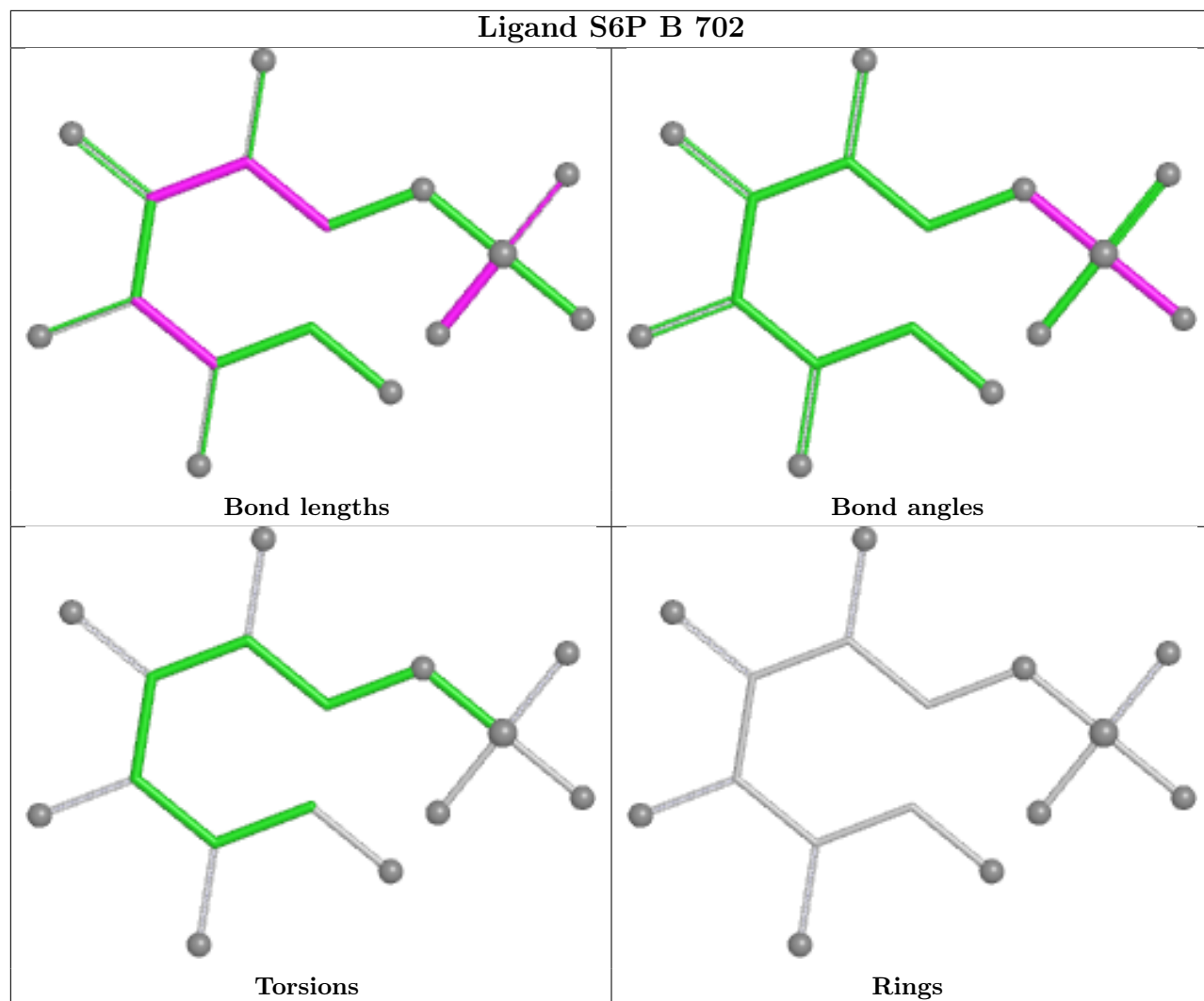
There are no ring outliers.

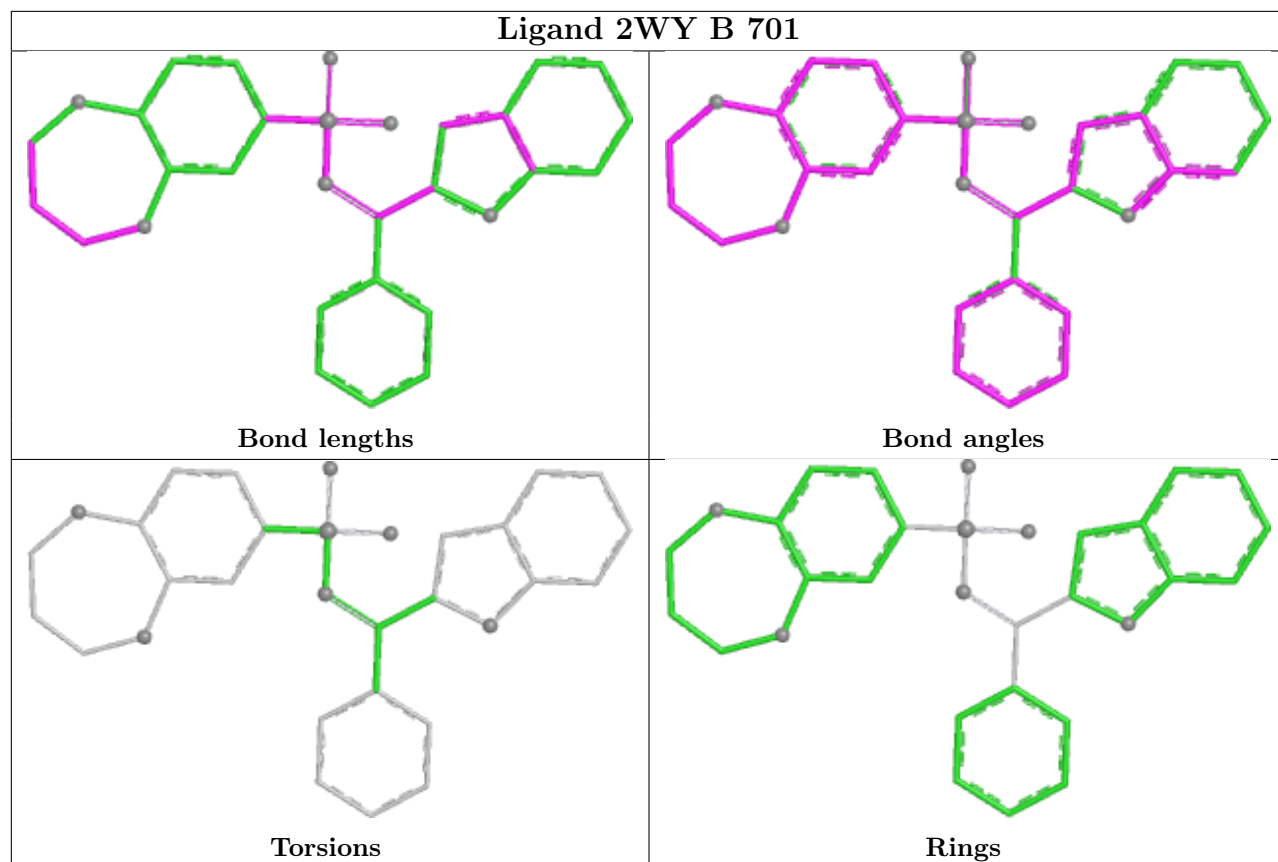
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	2WY	2	0
5	B	719	GOL	1	0
2	A	701	2WY	2	0
6	B	722	SO4	1	0

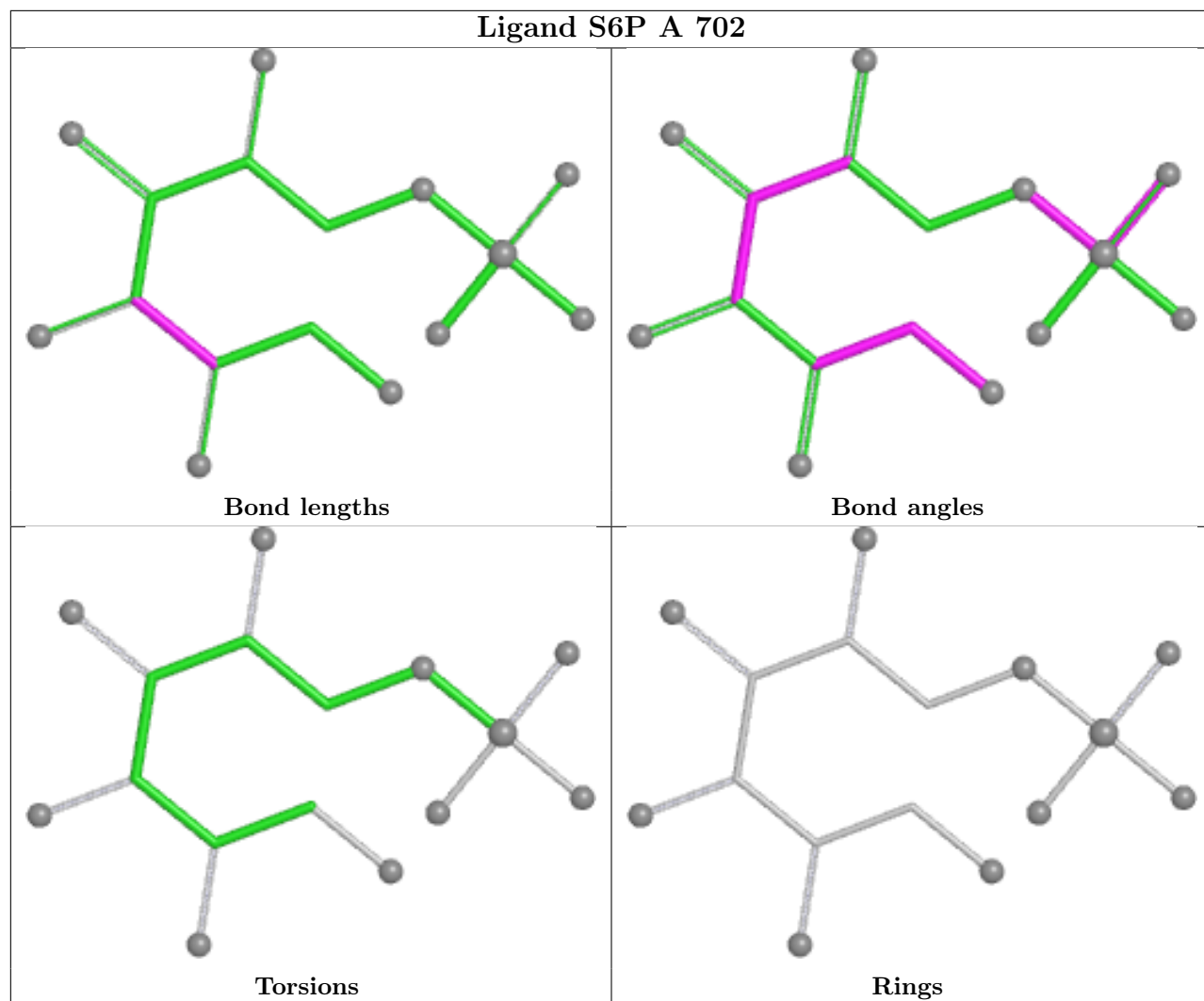
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

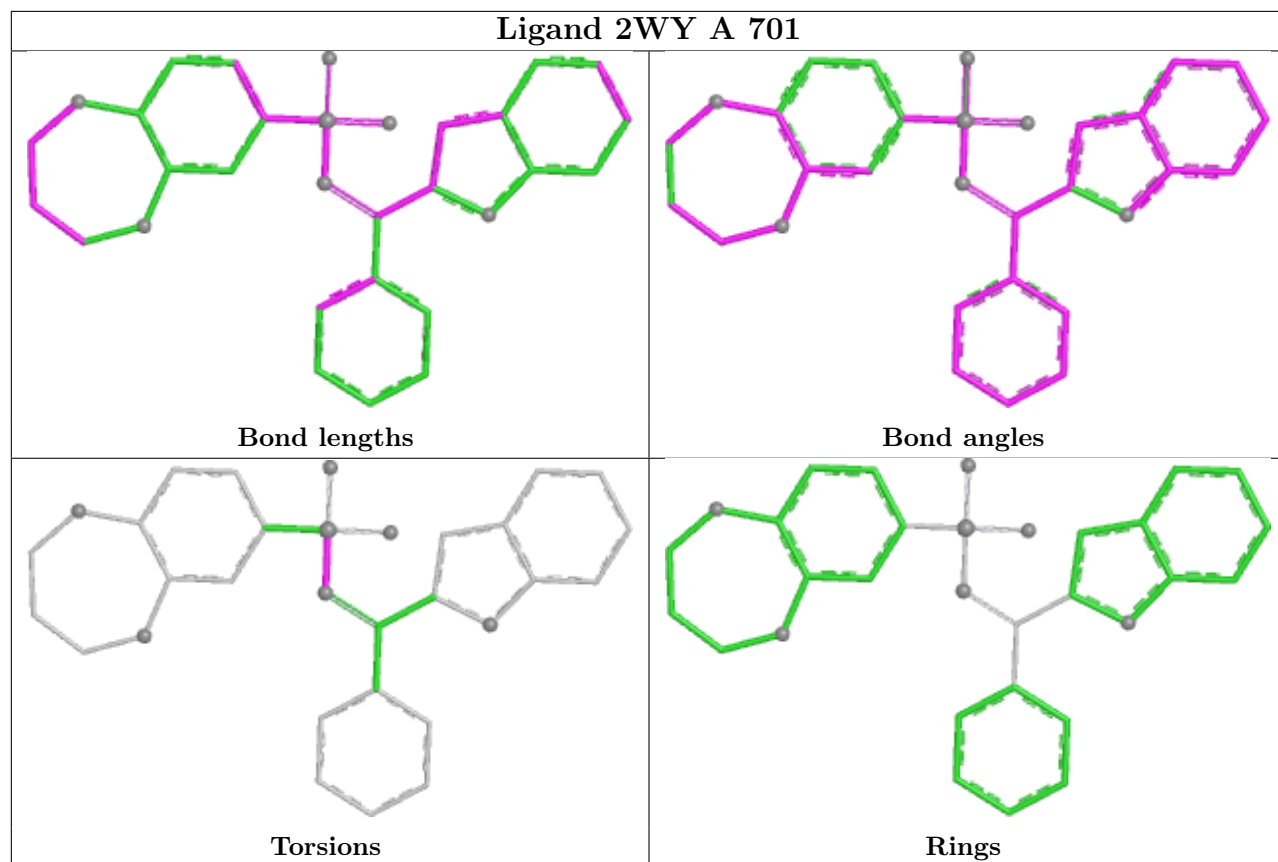
Ligand S6P B 702





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%)	0.75	67 (11%) 9 10	26, 48, 81, 109	0
1	B	590/638 (92%)	0.49	37 (6%) 26 29	25, 45, 74, 109	0
All	All	1175/1276 (92%)	0.62	104 (8%) 15 17	25, 46, 79, 109	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	PHE	5.8
1	A	465	PHE	5.8
1	A	357	PHE	5.1
1	A	447	ILE	5.1
1	B	447	ILE	5.0
1	B	2	PRO	4.9
1	B	465	PHE	4.8
1	A	445	LEU	4.7
1	A	449	LEU	4.7
1	B	449	LEU	4.3
1	A	21	LEU	4.2
1	A	358	ARG	4.1
1	A	452	LEU	4.1
1	A	430	THR	4.1
1	B	366	GLY	4.0
1	A	69	SER	3.9
1	B	3	GLY	3.9
1	B	454	PRO	3.8
1	A	454	PRO	3.8
1	B	22	SER	3.7
1	A	412	LEU	3.6
1	A	403	ILE	3.6
1	B	4	THR	3.6
1	A	5	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	5	LYS	3.4
1	A	397	LEU	3.3
1	A	469	GLU	3.3
1	A	400	LEU	3.3
1	A	463	LEU	3.3
1	B	357	PHE	3.3
1	A	451	LYS	3.2
1	A	365	ILE	3.2
1	A	464	LEU	3.1
1	A	355	ALA	3.1
1	A	1	MET	3.0
1	B	419	VAL	2.9
1	A	410	PHE	2.9
1	B	21	LEU	2.9
1	A	457	ILE	2.9
1	B	385	PHE	2.8
1	B	448	PRO	2.8
1	A	408	PHE	2.8
1	A	393	LEU	2.8
1	B	446	PRO	2.8
1	A	385	PHE	2.7
1	A	429	LYS	2.7
1	A	435	ALA	2.7
1	A	433	ILE	2.7
1	A	142	ASP	2.7
1	B	445	LEU	2.6
1	A	448	PRO	2.6
1	A	416	LEU	2.6
1	A	453	PHE	2.6
1	B	65	GLY	2.6
1	B	1	MET	2.6
1	A	444	THR	2.6
1	A	446	PRO	2.6
1	B	381	GLN	2.5
1	B	441	VAL	2.5
1	B	70	THR	2.5
1	A	315	THR	2.5
1	A	324	LEU	2.4
1	A	363	PHE	2.4
1	A	127	GLY	2.3
1	A	282	ASP	2.3
1	A	456	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	2	PRO	2.3
1	A	592	ALA	2.3
1	B	412	LEU	2.3
1	A	327	LYS	2.3
1	B	397	LEU	2.3
1	B	19	TRP	2.3
1	B	461	TRP	2.3
1	A	428	GLU	2.2
1	B	415	ASN	2.2
1	A	95	LYS	2.2
1	A	467	GLU	2.2
1	A	312	LYS	2.2
1	B	460	THR	2.2
1	B	424	GLU	2.2
1	A	285	ILE	2.2
1	A	459	ILE	2.2
1	B	444	THR	2.2
1	A	281	VAL	2.2
1	B	455	SER	2.2
1	A	593	ALA	2.1
1	B	437	ALA	2.1
1	A	22	SER	2.1
1	A	455	SER	2.1
1	A	65	GLY	2.1
1	A	133	LEU	2.1
1	B	416	LEU	2.1
1	A	386	THR	2.1
1	B	66	GLN	2.1
1	B	434	GLN	2.1
1	B	313	ILE	2.1
1	A	362	GLY	2.1
1	B	423	VAL	2.1
1	A	461	TRP	2.1
1	A	168	ALA	2.1
1	A	450	LYS	2.0
1	A	470	GLY	2.0
1	A	420	GLN	2.0
1	A	417	THR	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	723	5/5	0.70	0.13	76,80,90,91	0
4	IOD	B	712	1/1	0.77	0.15	89,89,89,89	1
5	GOL	A	716	6/6	0.81	0.17	38,50,55,62	0
6	SO4	B	722	5/5	0.84	0.12	53,69,75,87	0
4	IOD	B	713	1/1	0.85	0.15	80,80,80,80	1
5	GOL	B	718	6/6	0.86	0.13	40,55,60,64	0
5	GOL	B	719	6/6	0.86	0.15	41,43,50,58	0
4	IOD	B	715	1/1	0.87	0.11	90,90,90,90	1
4	IOD	A	711	1/1	0.88	0.12	90,90,90,90	1
6	SO4	B	720	5/5	0.88	0.07	65,67,73,90	0
2	2WY	A	701	31/31	0.88	0.13	37,48,54,57	0
2	2WY	B	701	31/31	0.88	0.14	42,56,65,65	0
4	IOD	A	715	1/1	0.89	0.15	85,85,85,85	1
4	IOD	B	716	1/1	0.89	0.11	92,92,92,92	1
4	IOD	B	717	1/1	0.92	0.07	86,86,86,86	1
4	IOD	B	710	1/1	0.93	0.16	91,91,91,91	1
4	IOD	A	709	1/1	0.93	0.14	87,87,87,87	1
4	IOD	A	703	1/1	0.93	0.09	61,61,61,61	0
4	IOD	A	712	1/1	0.93	0.09	66,66,66,66	1
4	IOD	A	713	1/1	0.93	0.08	62,62,62,62	1
4	IOD	A	708	1/1	0.93	0.15	73,73,73,73	1
4	IOD	A	714	1/1	0.94	0.09	65,65,65,65	1
4	IOD	A	706	1/1	0.94	0.10	77,77,77,77	0
4	IOD	B	703	1/1	0.94	0.08	53,53,53,53	0
4	IOD	B	707	1/1	0.94	0.08	72,72,72,72	0
4	IOD	B	708	1/1	0.94	0.10	57,57,57,57	1
4	IOD	B	709	1/1	0.94	0.09	74,74,74,74	1
6	SO4	B	721	5/5	0.95	0.08	40,44,46,52	5
4	IOD	B	714	1/1	0.95	0.07	61,61,61,61	1
4	IOD	A	707	1/1	0.95	0.06	51,51,51,51	1
4	IOD	B	706	1/1	0.97	0.04	48,48,48,48	1
4	IOD	A	704	1/1	0.97	0.06	60,60,60,60	0

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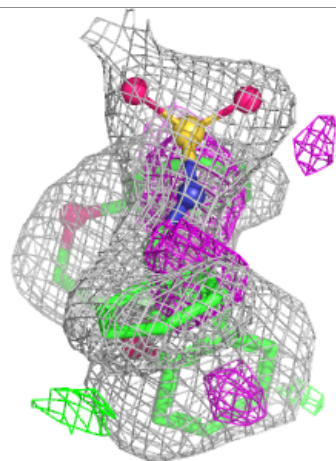
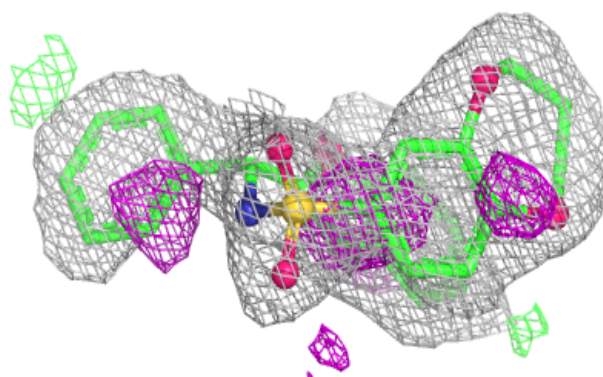
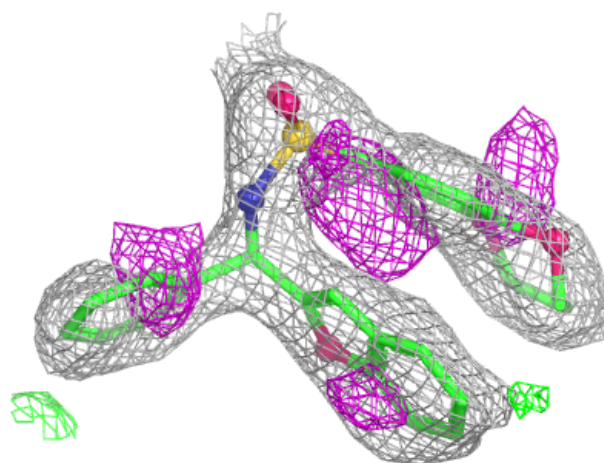
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	S6P	B	702	16/16	0.98	0.05	25,28,33,33	0
4	IOD	A	710	1/1	0.98	0.06	53,53,53,53	1
4	IOD	B	705	1/1	0.98	0.04	48,48,48,48	1
3	S6P	A	702	16/16	0.99	0.04	25,28,31,33	0
4	IOD	B	704	1/1	0.99	0.04	53,53,53,53	0
4	IOD	B	711	1/1	0.99	0.08	62,62,62,62	1
4	IOD	A	705	1/1	0.99	0.03	42,42,42,42	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.

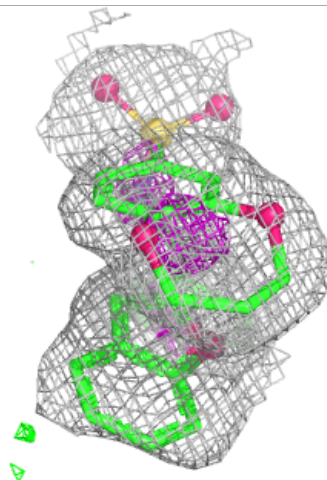
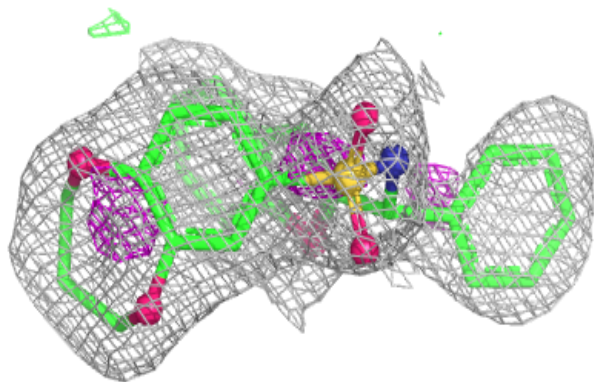
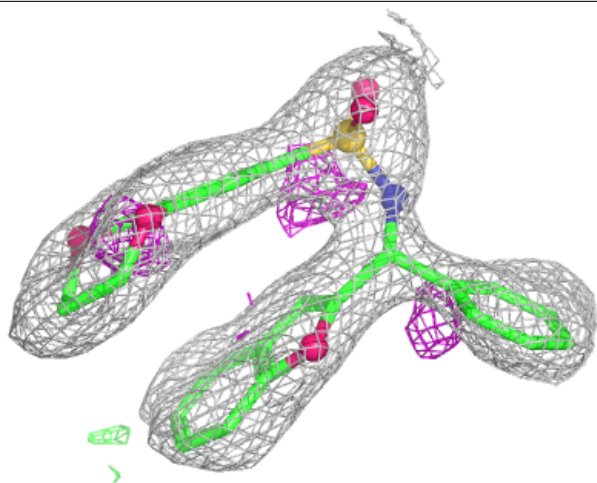
Electron density around 2WY A 701:

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



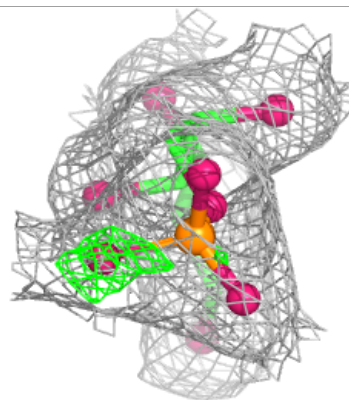
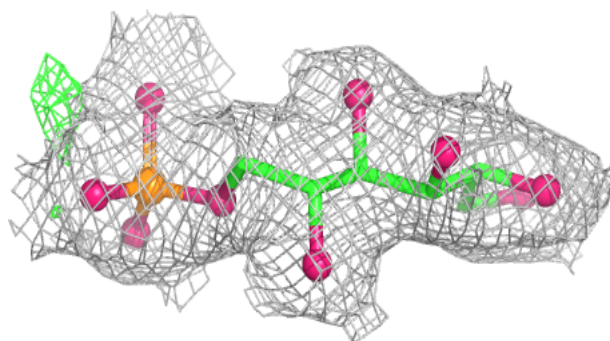
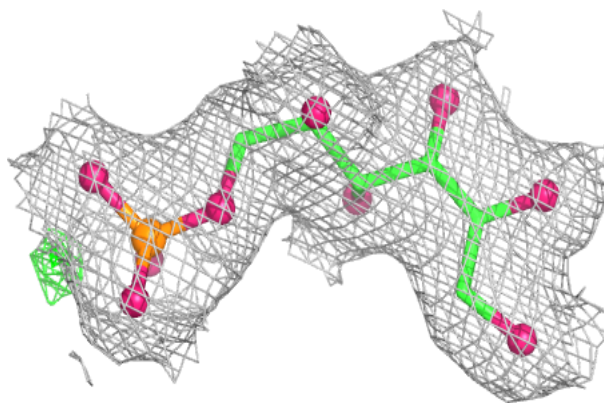
Electron density around 2WY B 701:

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

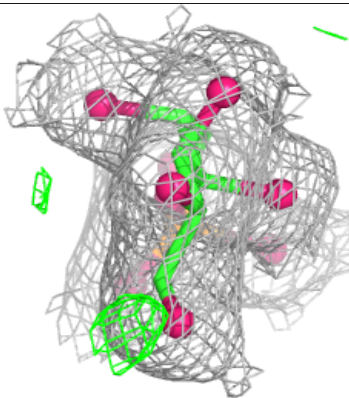
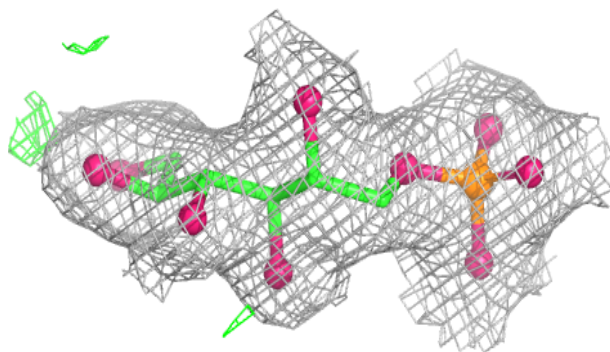
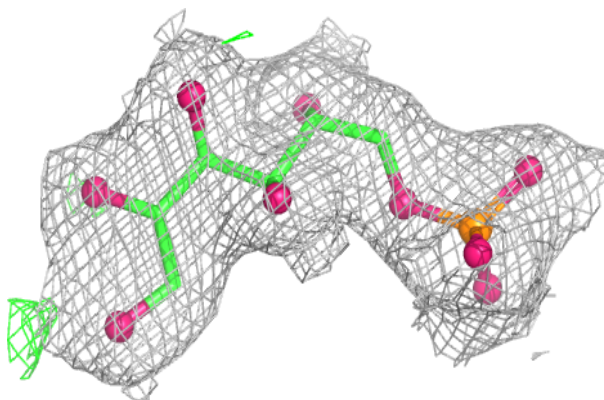


Electron density around S6P B 702:

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

**Electron density around S6P A 702:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.