



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:14 AM UTC

PDB ID : 4PX5 / pdb_00004px5
Title : Human GKRP bound to AMG-0696 and Sorbitol-6-phosphate
Authors : Jordan, S.R.; Chmait, S.
Deposited on : 2014-03-21
Resolution : 2.20 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

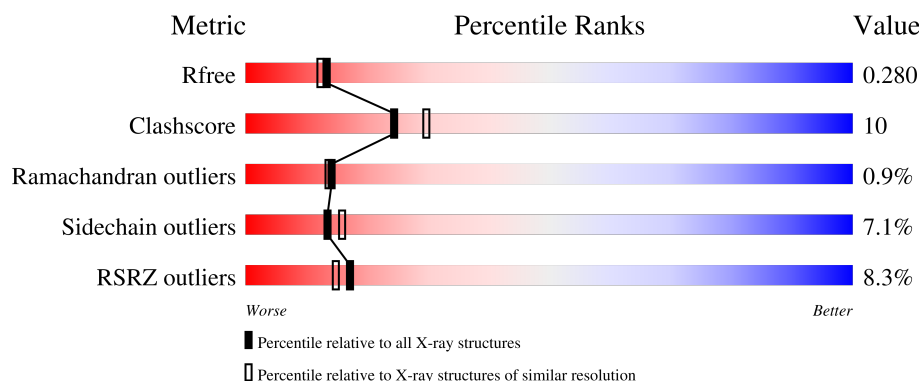
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	9% 70% 18% • 8%
1	B	638	6% 75% 15% • 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	716	-	-	X	-
4	IOD	B	713	-	-	X	-
6	SO4	B	723	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9380 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:

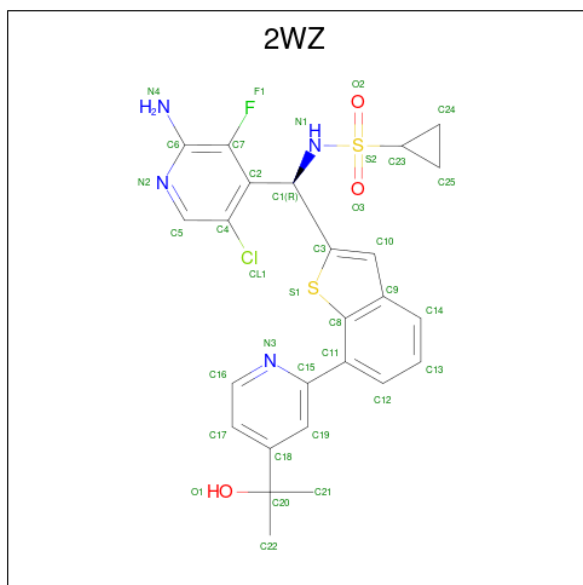
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q14397
A	-10	ALA	-	expression tag	UNP Q14397
A	-9	HIS	-	expression tag	UNP Q14397
A	-8	HIS	-	expression tag	UNP Q14397
A	-7	HIS	-	expression tag	UNP Q14397
A	-6	HIS	-	expression tag	UNP Q14397
A	-5	HIS	-	expression tag	UNP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

Continued on next page...

Continued from previous page...

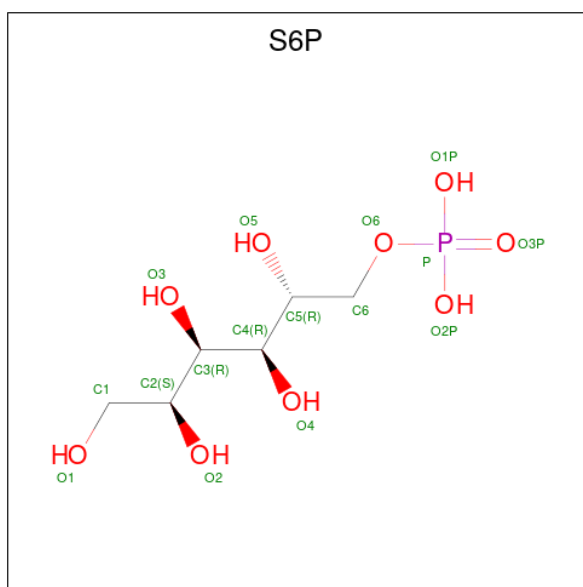
Chain	Residue	Modelled	Actual	Comment	Reference
B	626	GLY	-	expression tag	UNP Q14397

- Molecule 2 is N-[(R)-(2-amino-5-chloro-3-fluoropyridin-4-yl){7-[4-(2-hydroxypropan-2-yl)pyridin-2-yl]-1-benzothiophen-2-yl}methyl]cyclopropanesulfonamide (CCD ID: 2WZ) (formula: C₂₅H₂₄ClFN₄O₃S₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			36	25	1	1	4	3	2		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			36	25	1	1	4	3	2		

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



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

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

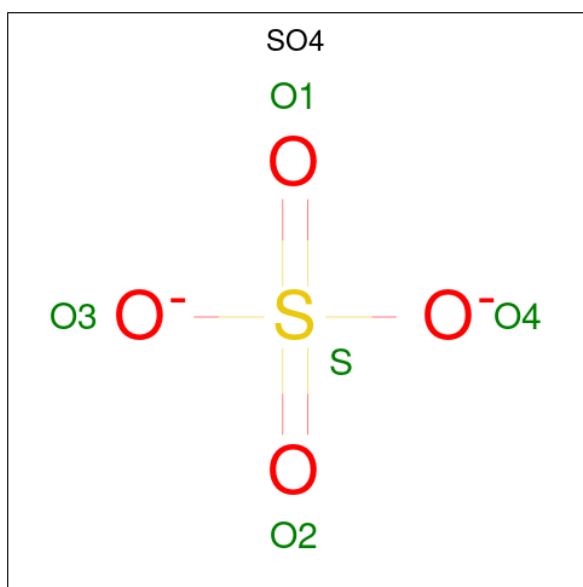
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	I	0	0
			15	15		
4	B	16	Total	I	0	0
			16	16		

- 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	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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		
6	B	1	Total	O	S	0	0
			5	4	1		

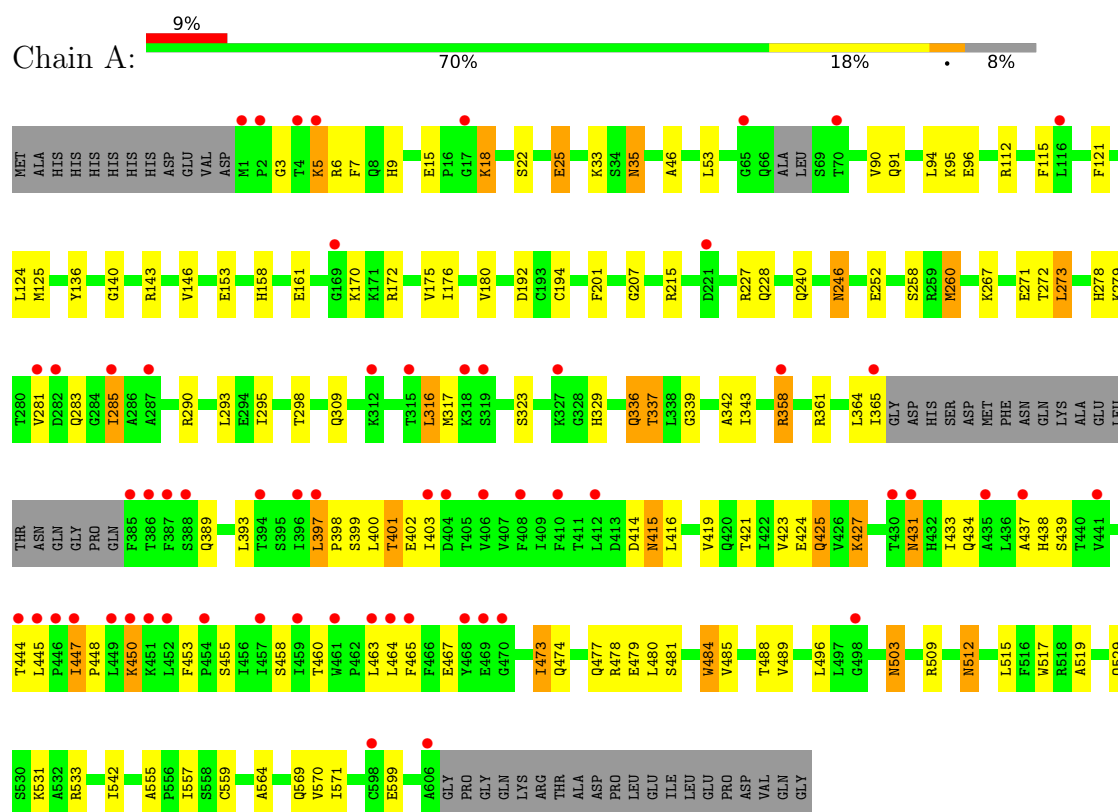
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	54	Total	O	0	0
			54	54		
7	B	73	Total	O	0	0
			73	73		

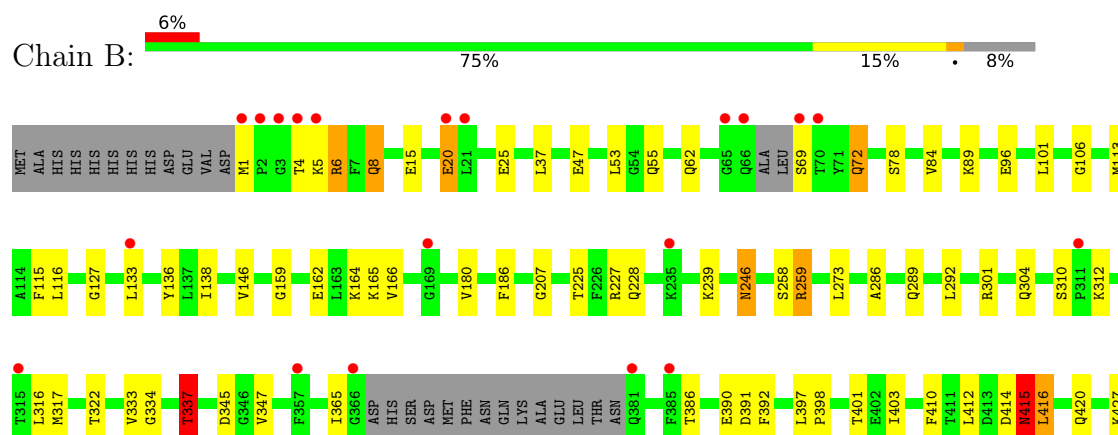
3 Residue-property plots

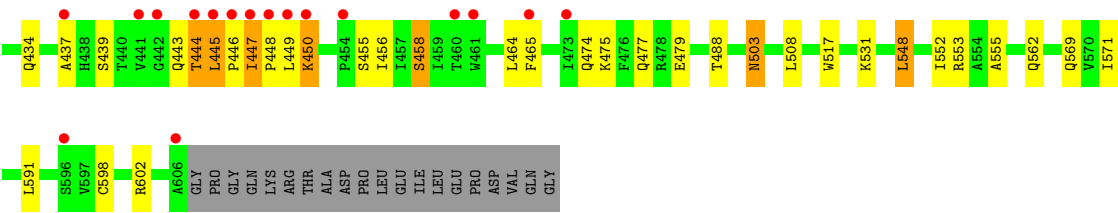
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	148.45Å 148.45Å 132.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.49 – 2.20 29.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.49-2.20) 99.8 (29.49-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.220 , 0.279 0.225 , 0.280	Depositor DCC
R_{free} test set	4161 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9380	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: GOL, S6P, 2WZ, SO4, IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	5/4603 (0.1%)	1.11	2/6228 (0.0%)
1	B	1.07	1/4637 (0.0%)	1.10	10/6274 (0.2%)
All	All	1.08	6/9240 (0.1%)	1.11	12/12502 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	ALA	C-O	-5.46	1.17	1.24
1	A	484	TRP	CA-C	-5.40	1.46	1.52
1	A	176	ILE	N-CA	-5.29	1.39	1.46
1	B	301	ARG	N-CA	5.10	1.52	1.46
1	A	542	ILE	CA-C	-5.03	1.46	1.52
1	A	112	ARG	N-CA	-5.03	1.40	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	GLY	N-CA-C	6.95	123.65	111.14
1	B	571	ILE	CA-C-N	-6.46	111.80	118.85
1	B	571	ILE	C-N-CA	-6.46	111.80	118.85
1	B	443	GLN	N-CA-C	-6.19	99.82	109.72
1	B	62	GLN	N-CA-C	5.84	118.82	110.24
1	B	310	SER	CA-C-N	-5.78	112.55	118.85
1	B	310	SER	C-N-CA	-5.78	112.55	118.85
1	B	552	ILE	N-CA-C	-5.63	105.35	110.82
1	B	115	PHE	N-CA-C	-5.20	105.52	111.14
1	A	153	GLU	N-CA-C	5.19	119.24	113.01
1	B	259	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	A	201	PHE	N-CA-C	5.05	117.73	109.59

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	108	0
1	B	4554	0	4647	75	0
2	A	36	0	24	3	0
2	B	36	0	24	4	0
3	A	16	0	13	0	0
3	B	16	0	13	1	0
4	A	15	0	0	11	0
4	B	16	0	0	5	0
5	A	6	0	8	0	0
5	B	12	0	16	2	0
6	A	5	0	0	1	0
6	B	20	0	0	2	0
7	A	54	0	0	1	0
7	B	73	0	0	0	1
All	All	9380	0	9363	184	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 10.

All (184) 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:5:LYS:HB2	4:B:710:IOD:I	2.33	0.99
1:A:400:LEU:O	1:A:401:THR:OG1	1.81	0.98
1:A:431:ASN:H	1:A:431:ASN:HD22	1.10	0.95
1:A:228:GLN:HE22	1:B:228:GLN:HE22	1.17	0.92
1:A:439:SER:OG	1:A:460:THR:HG22	1.82	0.80
1:A:431:ASN:H	1:A:431:ASN:ND2	1.82	0.77
1:A:317:MET:HE3	1:A:496:LEU:HD11	1.70	0.72
1:A:18:LYS:HD3	4:A:717:IOD:I	2.61	0.70
2:A:701:2WZ:S1	2:A:701:2WZ:N3	2.64	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:VAL:HG12	1:B:146:VAL:O	1.93	0.68
1:B:447:ILE:HA	1:B:450:LYS:HD2	1.75	0.68
1:A:272:THR:HA	1:A:295:ILE:HG21	1.76	0.67
1:B:333:VAL:CG1	1:B:365:ILE:HD11	2.24	0.66
1:A:509:ARG:NH1	7:A:836:HOH:O	2.28	0.66
1:A:480:LEU:HD21	1:A:484:TRP:CH2	2.31	0.66
1:A:90:VAL:O	1:A:94:LEU:HG	1.96	0.66
1:A:309:GLN:NE2	1:A:458:SER:O	2.29	0.65
1:A:397:LEU:O	1:A:400:LEU:HD13	1.97	0.65
1:A:228:GLN:HE22	1:B:228:GLN:NE2	1.92	0.64
1:B:458:SER:HB3	4:B:713:IOD:I	2.68	0.64
1:A:433:ILE:O	1:A:434:GLN:HG2	1.98	0.64
1:B:414:ASP:O	1:B:416:LEU:HD22	1.98	0.63
1:B:503:ASN:HD22	1:B:503:ASN:H	1.47	0.63
1:A:317:MET:CE	1:A:496:LEU:HD11	2.28	0.63
1:A:140:GLY:H	1:A:158:HIS:HE1	1.45	0.62
1:B:164:LYS:HG2	5:B:720:GOL:H32	1.80	0.62
1:A:398:PRO:HA	6:A:719:SO4:O3	2.00	0.61
1:B:447:ILE:HG22	1:B:450:LYS:CE	2.30	0.61
1:A:298:THR:HG21	1:A:473:ILE:HD11	1.82	0.60
1:A:447:ILE:HG22	1:A:450:LYS:HZ2	1.65	0.60
1:A:419:VAL:O	1:A:423:VAL:HG23	2.02	0.60
1:A:317:MET:HE3	1:A:496:LEU:CD1	2.32	0.60
1:A:9:HIS:H	1:A:9:HIS:CD2	2.19	0.59
1:B:415:ASN:C	1:B:415:ASN:HD22	2.10	0.59
1:A:146:VAL:HG12	1:A:146:VAL:O	2.03	0.59
1:A:15:GLU:H	1:A:18:LYS:HE3	1.68	0.59
1:B:259:ARG:NH2	1:B:345:ASP:OD1	2.35	0.58
1:A:337:THR:HG21	1:A:479:GLU:OE2	2.04	0.58
1:A:529:GLN:HE21	1:A:533:ARG:HE	1.50	0.58
1:A:439:SER:HG	1:A:460:THR:HG22	1.68	0.57
1:B:337:THR:HG21	1:B:479:GLU:OE1	2.04	0.57
1:A:140:GLY:H	1:A:158:HIS:CE1	2.23	0.57
1:A:215:ARG:HG3	2:A:701:2WZ:C7	2.35	0.57
1:B:84:VAL:HG13	1:B:292:LEU:CD1	2.35	0.57
1:A:246:ASN:N	1:A:246:ASN:HD22	2.03	0.56
1:B:84:VAL:HG13	1:B:292:LEU:HD12	1.87	0.56
1:A:458:SER:CB	4:A:716:IOD:I	3.23	0.56
1:A:445:LEU:HG	4:A:716:IOD:I	2.76	0.56
1:A:358:ARG:NH1	1:A:358:ARG:O	2.39	0.56
1:B:517:TRP:CG	2:B:701:2WZ:H8	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:LEU:HD22	1:B:553:ARG:HG3	1.88	0.55
2:B:701:2WZ:N3	2:B:701:2WZ:S1	2.80	0.55
1:B:598:CYS:O	1:B:602:ARG:HG3	2.07	0.54
1:A:207:GLY:O	1:A:246:ASN:HA	2.07	0.54
1:A:445:LEU:HD11	4:A:716:IOD:I	2.77	0.54
1:B:517:TRP:CD2	2:B:701:2WZ:H8	2.41	0.53
1:A:512:ASN:C	1:A:512:ASN:HD22	2.16	0.53
1:A:509:ARG:HH11	1:A:509:ARG:HB2	1.74	0.53
1:A:146:VAL:O	1:A:146:VAL:CG1	2.56	0.53
1:A:365:ILE:N	1:A:365:ILE:HD12	2.23	0.53
1:B:503:ASN:HD22	1:B:503:ASN:N	2.02	0.53
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.71	0.53
1:B:447:ILE:HG22	1:B:450:LYS:HD2	1.89	0.53
1:B:127:GLY:O	4:B:716:IOD:I	2.96	0.53
1:B:444:THR:O	1:B:446:PRO:HD3	2.08	0.53
1:A:447:ILE:HG22	1:A:450:LYS:NZ	2.24	0.53
1:A:35:ASN:C	1:A:35:ASN:HD22	2.18	0.52
1:A:124:LEU:C	1:A:124:LEU:HD23	2.34	0.52
1:A:283:GLN:HB2	1:A:285:ILE:HG22	1.91	0.52
1:B:258:SER:OG	3:B:702:S6P:H11	2.08	0.52
1:A:509:ARG:NH1	1:A:509:ARG:HB2	2.24	0.52
1:B:333:VAL:CG1	1:B:365:ILE:CD1	2.87	0.52
1:A:458:SER:HB2	4:A:716:IOD:I	2.81	0.51
1:A:474:GLN:HG3	1:A:478:ARG:HH11	1.75	0.51
1:A:246:ASN:HD22	1:A:246:ASN:H	1.57	0.51
1:A:15:GLU:H	1:A:18:LYS:CE	2.24	0.51
1:A:336:GLN:NE2	1:A:414:ASP:OD1	2.44	0.51
1:B:146:VAL:O	1:B:146:VAL:CG1	2.58	0.51
1:A:458:SER:HB3	4:A:716:IOD:I	2.81	0.51
1:B:447:ILE:HD12	1:B:448:PRO:HD3	1.94	0.50
1:A:53:LEU:HD12	1:A:488:THR:HG23	1.93	0.50
1:B:412:LEU:HD12	1:B:439:SER:HB3	1.93	0.50
1:B:101:LEU:HD12	1:B:133:LEU:O	2.12	0.50
1:B:113:MET:HE2	1:B:113:MET:N	2.26	0.50
1:A:437:ALA:O	1:A:458:SER:HA	2.12	0.49
1:A:121:PHE:O	1:A:125:MET:HG3	2.13	0.49
1:A:414:ASP:O	1:A:416:LEU:HD13	2.12	0.49
1:A:278:HIS:O	1:A:281:VAL:HG22	2.13	0.49
1:B:246:ASN:HD22	1:B:246:ASN:N	2.11	0.49
1:A:46:ALA:CB	1:A:317:MET:HE2	2.42	0.49
1:B:225:THR:H	1:B:228:GLN:HE21	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ASN:ND2	1:A:515:LEU:H	2.11	0.48
1:A:393:LEU:O	1:A:397:LEU:HB3	2.14	0.48
1:A:427:LYS:HE3	1:A:427:LYS:HA	1.95	0.48
1:A:18:LYS:HD2	1:A:22:SER:HB3	1.96	0.48
1:A:298:THR:HG21	1:A:473:ILE:CD1	2.44	0.48
1:A:339:GLY:O	1:A:342:ALA:HB3	2.13	0.48
1:A:329:HIS:HB3	1:A:358:ARG:NH1	2.28	0.48
1:A:91:GLN:HG2	1:A:281:VAL:HG13	1.95	0.47
1:A:9:HIS:H	1:A:9:HIS:HD2	1.61	0.47
1:A:273:LEU:C	1:A:273:LEU:HD23	2.40	0.47
1:A:95:LYS:HE3	1:A:281:VAL:HG12	1.97	0.47
1:B:25:GLU:OE2	1:B:25:GLU:HA	2.14	0.47
1:A:46:ALA:HA	1:A:317:MET:CE	2.44	0.47
1:A:438:HIS:HB3	1:A:478:ARG:HE	1.80	0.47
1:B:239:LYS:HB2	6:B:723:SO4:O4	2.15	0.47
1:B:162:GLU:OE1	1:B:165:LYS:HE2	2.15	0.47
1:B:531:LYS:HE3	4:B:712:IOD:I	2.85	0.46
1:A:15:GLU:O	1:A:18:LYS:HG3	2.15	0.46
1:B:180:VAL:HG11	1:B:258:SER:HB2	1.97	0.46
1:A:447:ILE:N	1:A:448:PRO:HD2	2.30	0.46
1:B:333:VAL:HG13	1:B:365:ILE:HD11	1.94	0.46
1:B:447:ILE:HG22	1:B:450:LYS:CD	2.46	0.46
1:A:364:LEU:C	1:A:365:ILE:HD12	2.41	0.46
1:B:286:ALA:HA	1:B:289:GLN:NE2	2.31	0.46
1:A:96:GLU:O	1:A:96:GLU:HG3	2.16	0.45
1:B:569:GLN:HG2	1:B:591:LEU:HD21	1.98	0.45
1:A:175:VAL:HG21	1:A:194:CYS:SG	2.57	0.45
1:B:401:THR:HG22	1:B:403:ILE:HG12	1.99	0.45
1:B:447:ILE:N	1:B:448:PRO:HD2	2.31	0.45
1:B:503:ASN:N	1:B:503:ASN:ND2	2.65	0.45
1:A:3:GLY:O	1:A:7:PHE:HD2	1.99	0.45
1:A:316:LEU:HD13	1:A:489:VAL:HG21	1.99	0.44
1:B:4:THR:O	1:B:8:GLN:HB2	2.17	0.44
1:A:474:GLN:CG	1:A:478:ARG:HH11	2.30	0.44
1:A:25:GLU:OE2	1:A:25:GLU:HA	2.16	0.44
1:A:5:LYS:HG3	4:A:709:IOD:I	2.88	0.44
1:B:414:ASP:O	1:B:416:LEU:N	2.51	0.44
1:B:164:LYS:HE3	5:B:720:GOL:H12	2.00	0.44
1:B:401:THR:HG22	1:B:403:ILE:H	1.81	0.44
1:B:420:GLN:HB3	1:B:449:LEU:HG	2.00	0.44
1:B:447:ILE:CA	1:B:450:LYS:HD2	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:HD3	1:B:555:ALA:O	2.17	0.44
1:A:424:GLU:O	1:A:427:LYS:HB2	2.17	0.43
1:A:481:SER:O	1:A:485:VAL:HG23	2.19	0.43
1:A:529:GLN:NE2	1:A:533:ARG:HE	2.16	0.43
1:A:337:THR:CG2	1:A:479:GLU:HG2	2.48	0.43
1:A:569:GLN:O	1:A:570:VAL:C	2.58	0.43
1:A:252:GLU:OE1	1:A:260:MET:HB2	2.18	0.42
1:A:323:SER:HB2	1:A:403:ILE:O	2.19	0.42
1:B:239:LYS:HG3	6:B:723:SO4:O1	2.20	0.42
1:A:6:ARG:HH11	1:A:555:ALA:C	2.28	0.42
1:A:33:LYS:HG2	4:A:710:IOD:I	2.90	0.42
1:A:421:THR:O	1:A:425:GLN:NE2	2.53	0.42
2:B:701:2WZ:H9	2:B:701:2WZ:C3	2.50	0.42
1:B:207:GLY:O	1:B:246:ASN:HA	2.20	0.42
1:A:480:LEU:CD2	1:A:484:TRP:CH2	3.00	0.42
1:B:316:LEU:O	1:B:317:MET:C	2.61	0.42
1:A:517:TRP:CE2	2:A:701:2WZ:H8	2.55	0.42
1:B:397:LEU:N	1:B:398:PRO:CD	2.83	0.42
1:B:410:PHE:O	1:B:437:ALA:HA	2.19	0.42
1:A:15:GLU:HB2	1:A:18:LYS:HG2	2.01	0.41
1:A:46:ALA:HA	1:A:317:MET:HE2	2.03	0.41
1:A:115:PHE:HD1	1:A:136:TYR:CE1	2.38	0.41
1:A:433:ILE:HD12	1:A:453:PHE:CE1	2.55	0.41
1:B:333:VAL:HG12	1:B:365:ILE:HD12	2.02	0.41
1:A:474:GLN:CG	1:A:478:ARG:NH1	2.83	0.41
1:B:446:PRO:O	1:B:450:LYS:HB3	2.21	0.41
1:B:474:GLN:HA	1:B:477:GLN:OE1	2.20	0.41
1:B:246:ASN:HD22	1:B:246:ASN:H	1.67	0.41
1:B:475:LYS:HE2	1:B:479:GLU:OE1	2.20	0.41
1:A:399:SER:C	1:A:400:LEU:HD12	2.46	0.41
1:A:503:ASN:H	1:A:503:ASN:HD22	1.69	0.41
1:A:180:VAL:HG11	1:A:258:SER:HB2	2.03	0.41
1:A:267:LYS:O	1:A:271:GLU:HB2	2.21	0.41
1:A:519:ALA:HB2	1:A:571:ILE:HD11	2.03	0.41
1:B:37:LEU:HD13	1:B:55:GLN:HG2	2.02	0.41
1:B:106:GLY:O	1:B:138:ILE:HA	2.21	0.41
1:B:445:LEU:HG	4:B:713:IOD:I	2.91	0.41
1:B:508:LEU:C	1:B:508:LEU:HD12	2.46	0.41
1:A:146:VAL:HG13	1:A:343:ILE:CG2	2.50	0.41
1:A:400:LEU:HD12	1:A:400:LEU:N	2.36	0.41
1:A:445:LEU:CD1	4:A:716:IOD:I	3.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:TYR:CD2	1:B:136:TYR:C	2.99	0.41
1:A:531:LYS:HE2	4:A:711:IOD:I	2.91	0.40
1:A:445:LEU:CG	4:A:716:IOD:I	3.39	0.40
1:B:159:GLY:HA2	1:B:186:PHE:CE1	2.56	0.40
1:B:464:LEU:O	1:B:465:PHE:C	2.64	0.40
1:B:72:GLN:HG2	1:B:78:SER:OG	2.21	0.40
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.86	0.40
1:B:273:LEU:C	1:B:273:LEU:HD23	2.47	0.40
1:B:391:ASP:O	1:B:392:PHE:C	2.63	0.40
1:B:53:LEU:HD12	1:B:488:THR:HG23	2.03	0.40
1:B:312:LYS:HD3	1:B:455:SER:O	2.21	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:860:HOH:O	7:B:864:HOH:O[5_555]	1.67	0.53

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%)	541 (93%)	32 (6%)	6 (1%)	12	11
1	B	584/638 (92%)	554 (95%)	26 (4%)	4 (1%)	18	19
All	All	1163/1276 (91%)	1095 (94%)	58 (5%)	10 (1%)	14	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	GLU
1	B	20	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	415	ASN
1	A	389	GLN
1	A	415	ASN
1	A	336	GLN
1	B	337	THR
1	A	401	THR
1	A	260	MET
1	B	456	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%)	458 (92%)	40 (8%)	11	13
1	B	501/542 (92%)	470 (94%)	31 (6%)	16	20
All	All	999/1084 (92%)	928 (93%)	71 (7%)	13	16

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	18	LYS
1	A	25	GLU
1	A	35	ASN
1	A	143	ARG
1	A	161	GLU
1	A	170	LYS
1	A	172	ARG
1	A	192	ASP
1	A	227	ARG
1	A	240	GLN
1	A	246	ASN
1	A	273	LEU
1	A	279	LYS
1	A	285	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	290	ARG
1	A	293	LEU
1	A	316	LEU
1	A	337	THR
1	A	358	ARG
1	A	361	ARG
1	A	397	LEU
1	A	415	ASN
1	A	425	GLN
1	A	427	LYS
1	A	431	ASN
1	A	444	THR
1	A	447	ILE
1	A	450	LYS
1	A	455	SER
1	A	463	LEU
1	A	464	LEU
1	A	465	PHE
1	A	467	GLU
1	A	473	ILE
1	A	503	ASN
1	A	512	ASN
1	A	557	ILE
1	A	559	CYS
1	A	599	GLU
1	B	1	MET
1	B	6	ARG
1	B	8	GLN
1	B	15	GLU
1	B	20	GLU
1	B	47	GLU
1	B	69	SER
1	B	72	GLN
1	B	89	LYS
1	B	96	GLU
1	B	166	VAL
1	B	227	ARG
1	B	246	ASN
1	B	304	GLN
1	B	322	THR
1	B	337	THR
1	B	347	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	386	THR
1	B	390	GLU
1	B	415	ASN
1	B	416	LEU
1	B	427	LYS
1	B	434	GLN
1	B	444	THR
1	B	445	LEU
1	B	447	ILE
1	B	450	LYS
1	B	458	SER
1	B	503	ASN
1	B	548	LEU
1	B	562	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	35	ASN
1	A	39	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	389	GLN
1	A	420	GLN
1	A	425	GLN
1	A	431	ASN
1	A	432	HIS
1	A	474	GLN
1	A	477	GLN
1	A	503	ASN
1	A	512	ASN
1	A	524	GLN
1	A	529	GLN
1	B	48	ASN
1	B	55	GLN
1	B	62	GLN
1	B	196	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	216	ASN
1	B	228	GLN
1	B	246	ASN
1	B	289	GLN
1	B	304	GLN
1	B	384	GLN
1	B	389	GLN
1	B	415	ASN
1	B	420	GLN
1	B	431	ASN
1	B	474	GLN
1	B	503	ASN
1	B	504	HIS
1	B	529	GLN
1	B	546	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 31 are monoatomic - leaving 12 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	720	-	5,5,5	0.26	0	5,5,5	1.01	0
6	SO4	A	719	-	4,4,4	0.36	0	6,6,6	0.90	0
6	SO4	B	724	-	4,4,4	0.61	0	6,6,6	0.31	0
2	2WZ	B	701	-	38,40,40	2.00	9 (23%)	49,62,62	2.24	16 (32%)
5	GOL	B	719	-	5,5,5	0.21	0	5,5,5	0.92	0
2	2WZ	A	701	-	38,40,40	1.83	7 (18%)	49,62,62	2.40	12 (24%)
6	SO4	B	721	-	4,4,4	0.52	0	6,6,6	0.28	0
6	SO4	B	722	-	4,4,4	0.40	0	6,6,6	0.60	0
6	SO4	B	723	-	4,4,4	0.54	0	6,6,6	0.51	0
3	S6P	A	702	-	15,15,15	1.63	1 (6%)	20,21,21	1.60	4 (20%)
5	GOL	A	718	-	5,5,5	0.48	0	5,5,5	0.56	0
3	S6P	B	702	-	15,15,15	1.19	1 (6%)	20,21,21	1.42	3 (15%)

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	720	-	-	1/4/4/4	-
2	2WZ	B	701	-	-	5/27/31/31	0/5/5/5
5	GOL	B	719	-	-	2/4/4/4	-
2	2WZ	A	701	-	-	3/27/31/31	0/5/5/5
3	S6P	A	702	-	-	2/20/20/20	-
5	GOL	A	718	-	-	2/4/4/4	-
3	S6P	B	702	-	-	0/20/20/20	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	2WZ	C3-S1	-6.63	1.64	1.75
2	B	701	2WZ	O3-S2	5.83	1.50	1.43
2	A	701	2WZ	O3-S2	5.78	1.50	1.43
2	A	701	2WZ	C11-C8	-5.18	1.36	1.41
3	A	702	S6P	P-O3P	4.38	1.64	1.50
2	B	701	2WZ	O2-S2	3.95	1.48	1.43
3	B	702	S6P	C2-C3	-2.97	1.48	1.53
2	A	701	2WZ	C11-C15	-2.95	1.41	1.48
2	B	701	2WZ	C11-C15	-2.93	1.41	1.48
2	A	701	2WZ	C21-C20	-2.86	1.49	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	2WZ	C20-C18	2.65	1.55	1.53
2	B	701	2WZ	C11-C8	-2.56	1.38	1.41
2	B	701	2WZ	C9-C10	-2.44	1.36	1.44
2	B	701	2WZ	C6-C7	-2.35	1.37	1.40
2	B	701	2WZ	S2-N1	2.33	1.66	1.61
2	A	701	2WZ	O2-S2	2.26	1.46	1.43
2	A	701	2WZ	C8-S1	-2.14	1.70	1.74
2	B	701	2WZ	C5-N2	-2.03	1.30	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2WZ	O3-S2-C23	8.71	119.59	107.98
2	A	701	2WZ	O3-S2-O2	-7.84	107.43	118.88
2	B	701	2WZ	C8-S1-C3	6.39	96.10	91.55
2	B	701	2WZ	O3-S2-C23	5.56	115.39	107.98
2	B	701	2WZ	C5-N2-C6	5.00	123.47	118.64
2	A	701	2WZ	O2-S2-C23	-4.81	101.58	107.98
2	B	701	2WZ	O3-S2-O2	-4.55	112.24	118.88
2	B	701	2WZ	C4-C5-N2	-4.21	119.55	122.78
3	A	702	S6P	O2P-P-O6	3.94	116.95	106.67
3	B	702	S6P	O6-P-O3P	3.60	116.18	106.44
2	A	701	2WZ	C7-C6-N4	-3.60	118.64	121.32
2	B	701	2WZ	C9-C8-S1	-3.58	106.31	112.82
2	A	701	2WZ	C8-S1-C3	3.51	94.05	91.55
2	A	701	2WZ	C24-C25-C23	-3.41	57.93	60.42
2	A	701	2WZ	C19-C15-N3	-3.29	117.98	122.13
2	A	701	2WZ	C8-C9-C10	3.05	113.94	110.80
2	B	701	2WZ	C19-C15-N3	-2.97	118.38	122.13
2	B	701	2WZ	C11-C8-S1	2.92	132.65	127.00
2	B	701	2WZ	C7-C6-N4	-2.80	119.23	121.32
2	A	701	2WZ	C16-N3-C15	2.79	121.15	117.24
2	B	701	2WZ	O3-S2-N1	-2.79	104.39	107.65
3	A	702	S6P	C5-C4-C3	-2.69	108.35	112.48
3	A	702	S6P	C2-C3-C4	-2.58	108.52	112.48
2	A	701	2WZ	O3-S2-N1	2.55	110.62	107.65
2	A	701	2WZ	C5-N2-C6	2.49	121.04	118.64
2	A	701	2WZ	C9-C8-S1	-2.27	108.69	112.82
2	B	701	2WZ	C8-C9-C10	2.27	113.13	110.80
2	B	701	2WZ	F1-C7-C2	2.24	123.44	120.23
2	B	701	2WZ	C10-C3-S1	-2.18	109.18	112.47
3	A	702	S6P	O6-P-O3P	-2.17	100.57	106.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	2WZ	O1-C20-C21	2.15	111.57	107.10
3	B	702	S6P	C5-C4-C3	-2.08	109.28	112.48
2	B	701	2WZ	C16-N3-C15	2.05	120.11	117.24
2	B	701	2WZ	C11-C15-N3	2.04	120.07	116.48
3	B	702	S6P	O2P-P-O3P	-2.03	102.93	110.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	2WZ	C24-C23-S2-O2
5	A	718	GOL	O1-C1-C2-O2
5	A	718	GOL	O1-C1-C2-C3
5	B	719	GOL	O1-C1-C2-C3
5	B	719	GOL	O1-C1-C2-O2
5	B	720	GOL	O1-C1-C2-O2
2	B	701	2WZ	C19-C18-C20-C22
2	B	701	2WZ	C2-C1-C3-C10
2	A	701	2WZ	N1-C1-C3-S1
2	B	701	2WZ	N1-C1-C3-S1
3	A	702	S6P	C6-O6-P-O3P
2	A	701	2WZ	C19-C18-C20-C22
3	A	702	S6P	C1-C2-C3-O3
2	A	701	2WZ	C17-C18-C20-C22
2	B	701	2WZ	C19-C18-C20-O1

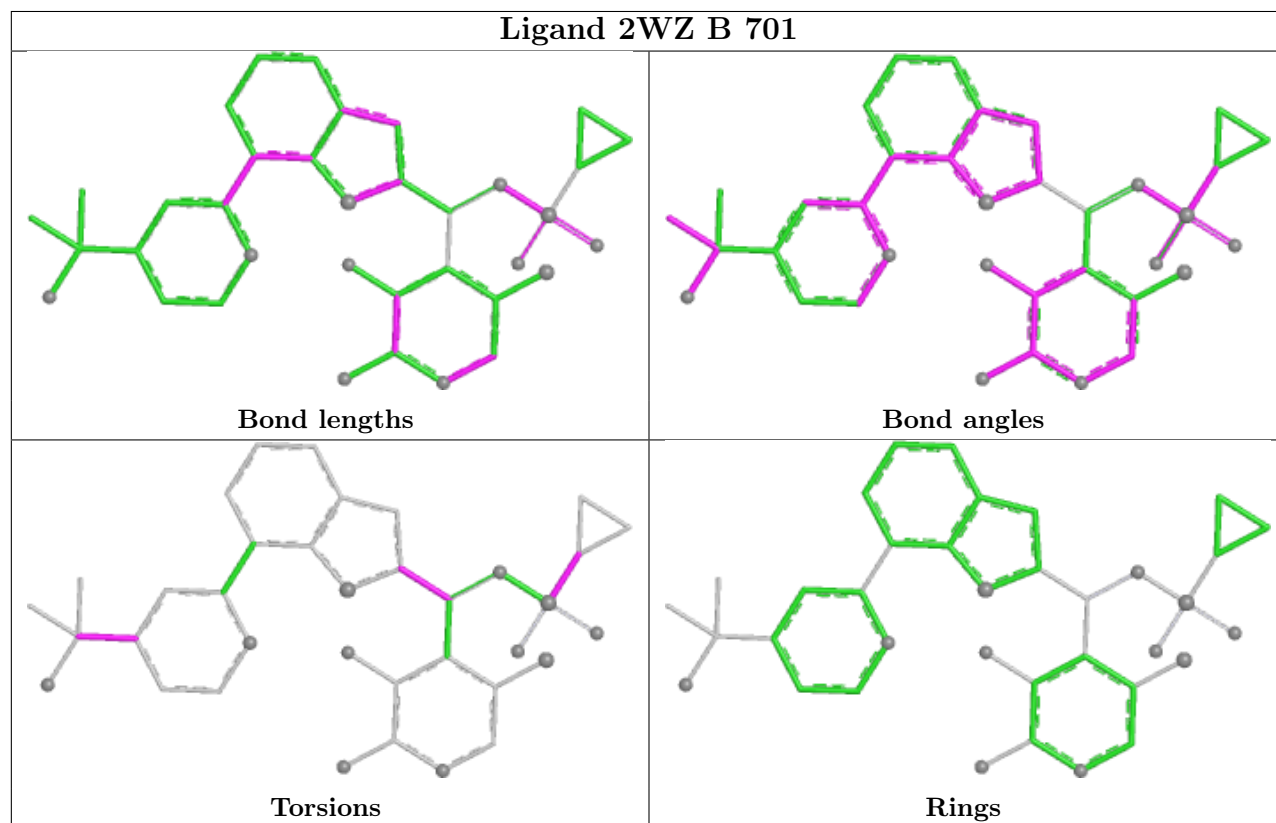
There are no ring outliers.

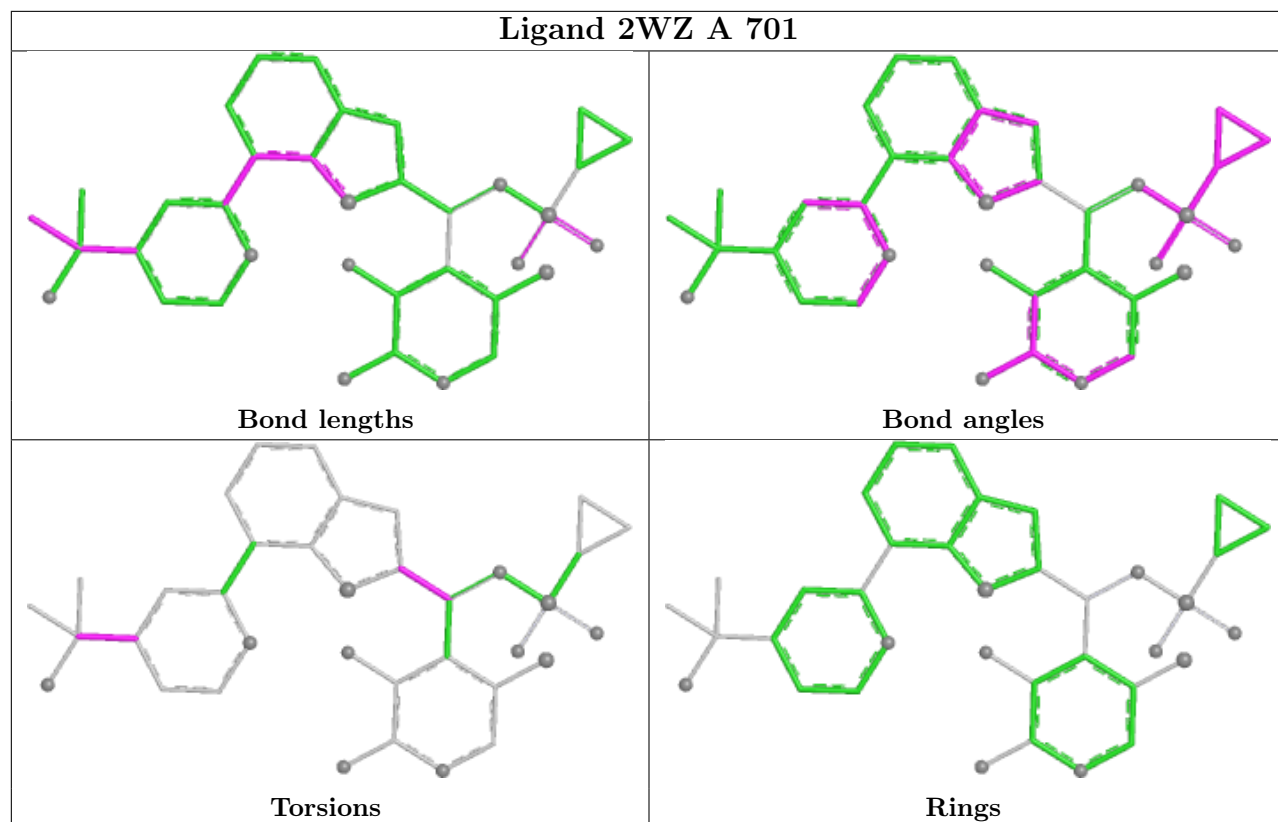
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	720	GOL	2	0
6	A	719	SO4	1	0
2	B	701	2WZ	4	0
2	A	701	2WZ	3	0
6	B	723	SO4	2	0
3	B	702	S6P	1	0

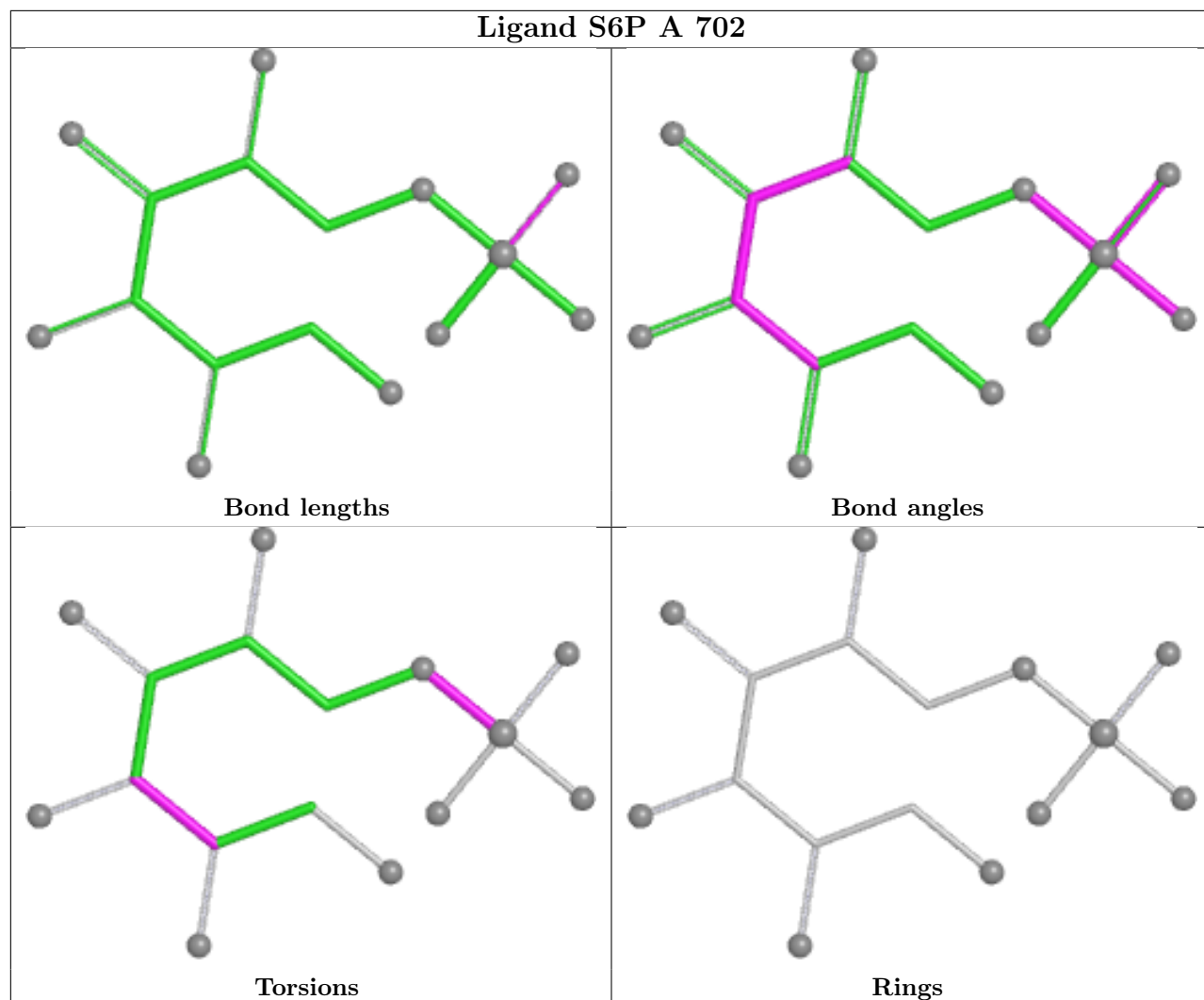
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

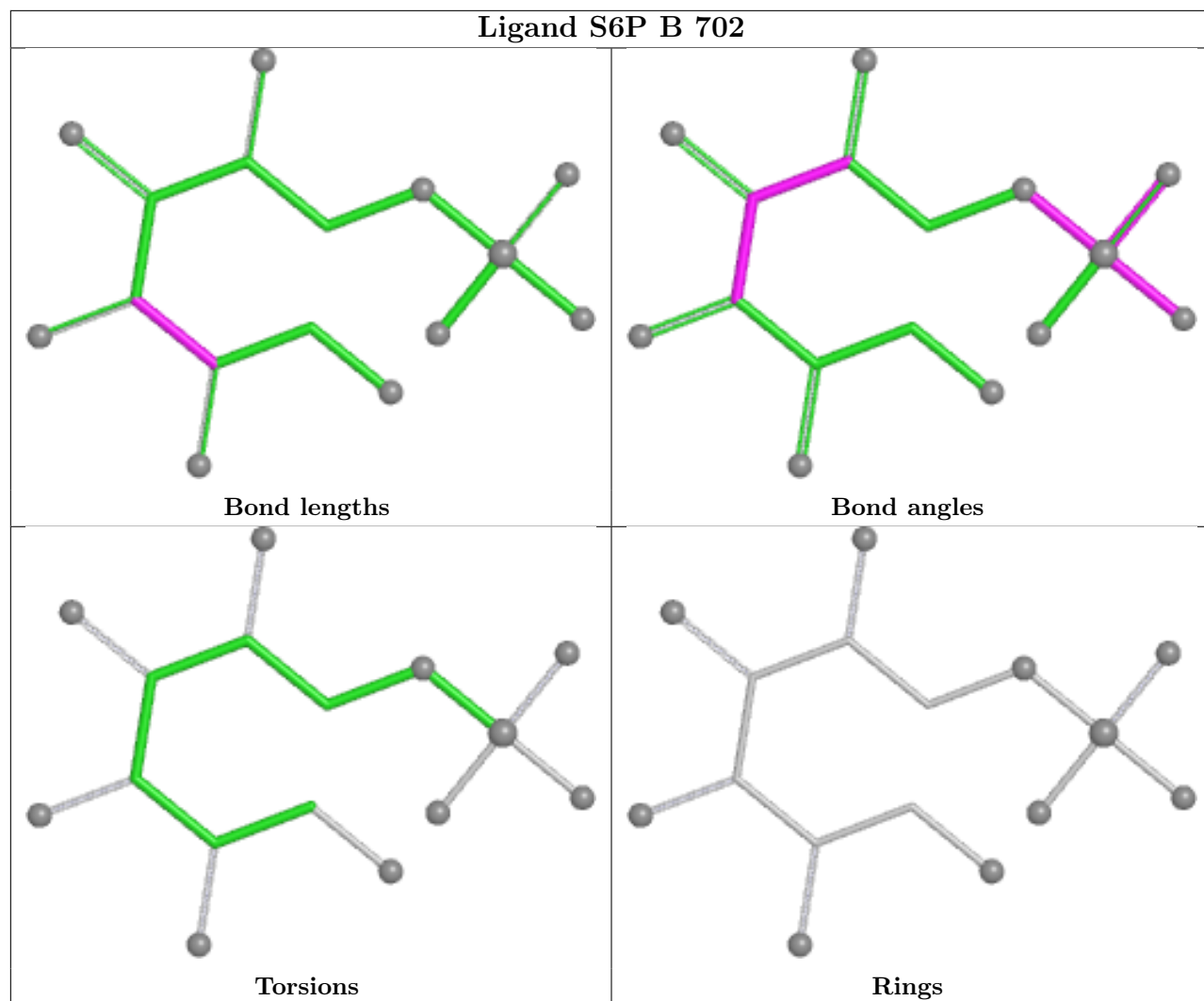
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	0.68	60 (10%) 12 9	34, 56, 90, 127	0
1	B	590/638 (92%)	0.53	37 (6%) 26 23	34, 56, 83, 126	0
All	All	1175/1276 (92%)	0.61	97 (8%) 17 15	34, 56, 88, 127	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ILE	7.3
1	A	387	PHE	5.3
1	B	4	THR	4.9
1	A	465	PHE	4.7
1	B	449	LEU	4.6
1	B	2	PRO	4.6
1	B	447	ILE	4.6
1	A	437	ALA	4.5
1	B	366	GLY	4.3
1	A	606	ALA	4.2
1	A	385	PHE	4.2
1	A	65	GLY	4.1
1	A	450	LYS	4.0
1	A	449	LEU	4.0
1	B	1	MET	3.8
1	A	446	PRO	3.8
1	A	454	PRO	3.7
1	B	70	THR	3.7
1	B	3	GLY	3.5
1	A	452	LEU	3.4
1	B	606	ALA	3.4
1	A	464	LEU	3.3
1	B	465	PHE	3.3
1	A	5	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	315	THR	3.3
1	A	412	LEU	3.2
1	A	410	PHE	3.2
1	A	441	VAL	3.2
1	B	169	GLY	3.0
1	B	66	GLN	3.0
1	A	388	SER	3.0
1	B	442	GLY	3.0
1	B	446	PRO	3.0
1	A	598	CYS	2.9
1	B	445	LEU	2.9
1	B	381	GLN	2.9
1	B	385	PHE	2.9
1	B	133	LEU	2.8
1	B	437	ALA	2.8
1	A	444	THR	2.8
1	B	69	SER	2.8
1	A	457	ILE	2.8
1	B	461	TRP	2.8
1	A	4	THR	2.7
1	B	473	ILE	2.7
1	A	431	ASN	2.7
1	B	311	PRO	2.7
1	A	312	LYS	2.7
1	A	469	GLU	2.7
1	A	386	THR	2.7
1	B	315	THR	2.7
1	B	454	PRO	2.7
1	A	397	LEU	2.6
1	A	445	LEU	2.6
1	A	358	ARG	2.6
1	B	441	VAL	2.6
1	B	596	SER	2.6
1	A	451	LYS	2.6
1	A	463	LEU	2.6
1	A	435	ALA	2.5
1	A	2	PRO	2.5
1	A	116	LEU	2.5
1	A	1	MET	2.4
1	A	282	ASP	2.4
1	A	403	ILE	2.4
1	B	235	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	5	LYS	2.4
1	B	448	PRO	2.4
1	A	287	ALA	2.4
1	B	65	GLY	2.4
1	B	444	THR	2.4
1	B	460	THR	2.4
1	A	285	ILE	2.3
1	A	221	ASP	2.3
1	A	430	THR	2.3
1	B	20	GLU	2.3
1	A	281	VAL	2.3
1	B	357	PHE	2.2
1	A	468	TYR	2.2
1	A	461	TRP	2.2
1	B	21	LEU	2.2
1	A	169	GLY	2.2
1	A	70	THR	2.2
1	A	406	VAL	2.2
1	A	394	THR	2.2
1	A	365	ILE	2.1
1	A	318	LYS	2.1
1	A	470	GLY	2.1
1	A	319	SER	2.1
1	A	327	LYS	2.1
1	A	404	ASP	2.1
1	A	459	ILE	2.1
1	A	408	PHE	2.1
1	A	17	GLY	2.1
1	A	498	GLY	2.1
1	A	396	ILE	2.0
1	B	450	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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.

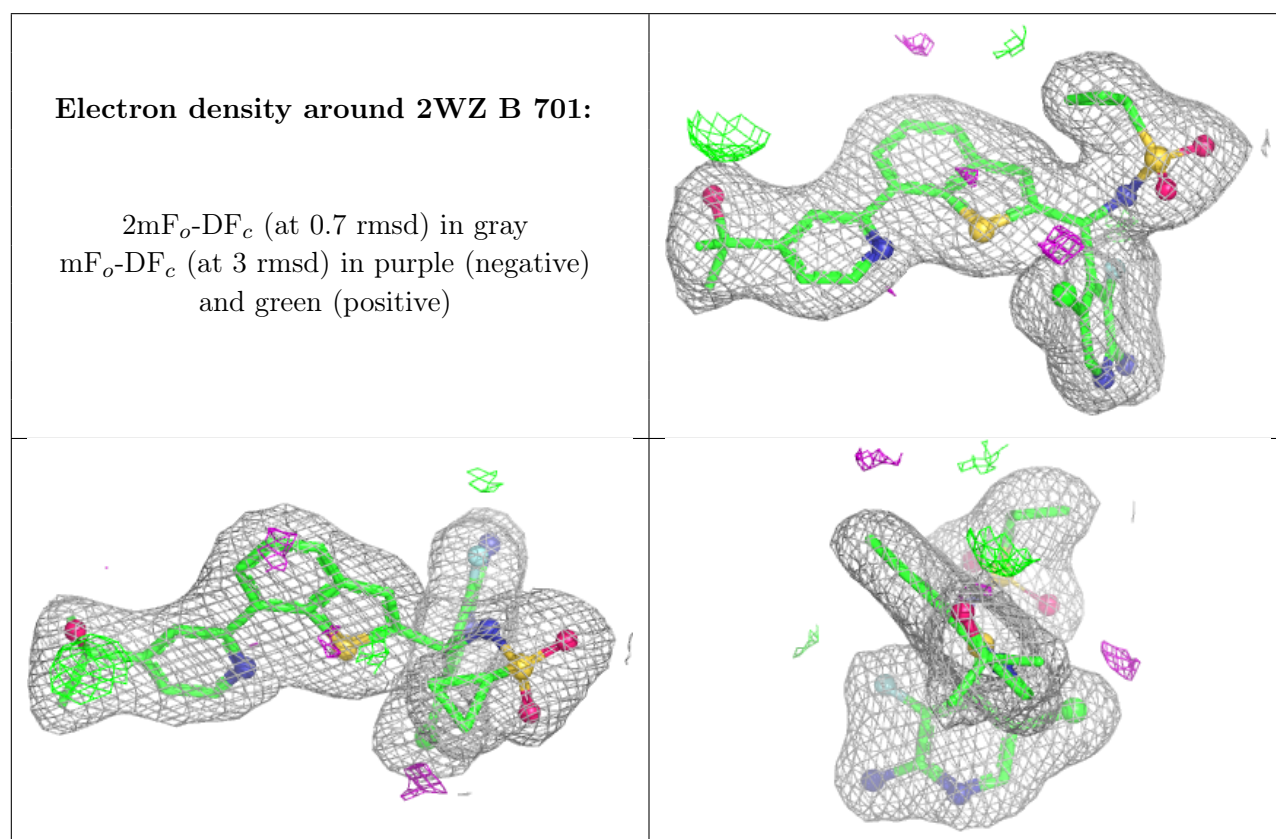
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IOD	A	711	1/1	0.75	0.21	79,79,79,79	1
4	IOD	B	712	1/1	0.75	0.17	88,88,88,88	1
6	SO4	B	723	5/5	0.78	0.20	51,57,71,73	5
5	GOL	A	718	6/6	0.83	0.12	50,60,64,80	0
6	SO4	B	724	5/5	0.85	0.13	69,78,90,95	5
4	IOD	B	713	1/1	0.86	0.11	88,88,88,88	1
5	GOL	B	720	6/6	0.87	0.12	53,57,58,78	0
6	SO4	B	721	5/5	0.87	0.10	74,74,84,91	5
4	IOD	B	717	1/1	0.87	0.12	94,94,94,94	1
4	IOD	A	715	1/1	0.87	0.17	100,100,100,100	1
6	SO4	A	719	5/5	0.88	0.18	48,54,63,75	5
4	IOD	A	706	1/1	0.88	0.16	92,92,92,92	0
4	IOD	A	717	1/1	0.89	0.10	81,81,81,81	1
4	IOD	B	718	1/1	0.90	0.11	80,80,80,80	1
4	IOD	B	710	1/1	0.91	0.14	92,92,92,92	1
4	IOD	A	716	1/1	0.91	0.09	86,86,86,86	1
4	IOD	B	709	1/1	0.91	0.10	88,88,88,88	1
4	IOD	B	715	1/1	0.91	0.09	98,98,98,98	1
5	GOL	B	719	6/6	0.92	0.11	55,61,66,71	0
4	IOD	A	709	1/1	0.92	0.12	96,96,96,96	1
4	IOD	B	716	1/1	0.92	0.09	96,96,96,96	1
4	IOD	A	703	1/1	0.92	0.09	80,80,80,80	0
4	IOD	A	713	1/1	0.92	0.09	69,69,69,69	1
4	IOD	B	707	1/1	0.92	0.11	89,89,89,89	1
4	IOD	A	712	1/1	0.93	0.09	78,78,78,78	1
4	IOD	B	703	1/1	0.93	0.08	63,63,63,63	0
4	IOD	A	708	1/1	0.93	0.16	88,88,88,88	1
4	IOD	B	714	1/1	0.94	0.09	83,83,83,83	1
4	IOD	B	711	1/1	0.94	0.21	96,96,96,96	1
6	SO4	B	722	5/5	0.94	0.09	51,54,57,59	5
4	IOD	A	714	1/1	0.94	0.09	74,74,74,74	1
4	IOD	A	710	1/1	0.94	0.28	89,89,89,89	1
4	IOD	B	706	1/1	0.95	0.07	63,63,63,63	1
4	IOD	B	708	1/1	0.95	0.09	73,73,73,73	1
4	IOD	A	707	1/1	0.96	0.07	64,64,64,64	1
4	IOD	A	705	1/1	0.97	0.06	56,56,56,56	1
2	2WZ	B	701	36/36	0.97	0.07	35,43,50,54	0

Continued on next page...

Continued from previous page...

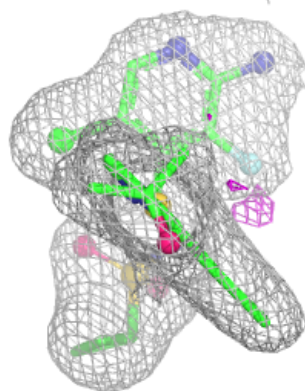
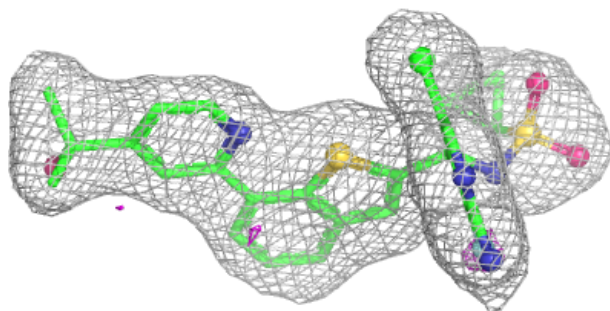
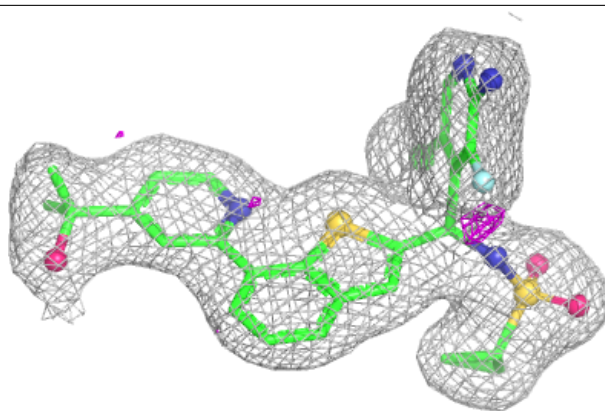
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IOD	B	705	1/1	0.97	0.08	67,67,67,67	1
2	2WZ	A	701	36/36	0.97	0.07	33,38,44,49	0
3	S6P	B	702	16/16	0.98	0.06	33,38,43,47	0
3	S6P	A	702	16/16	0.98	0.05	31,37,43,44	0
4	IOD	A	704	1/1	0.98	0.05	62,62,62,62	0
4	IOD	B	704	1/1	0.99	0.04	65,65,65,65	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.

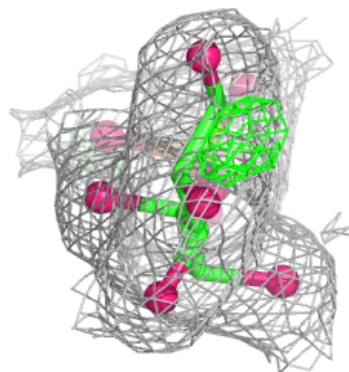
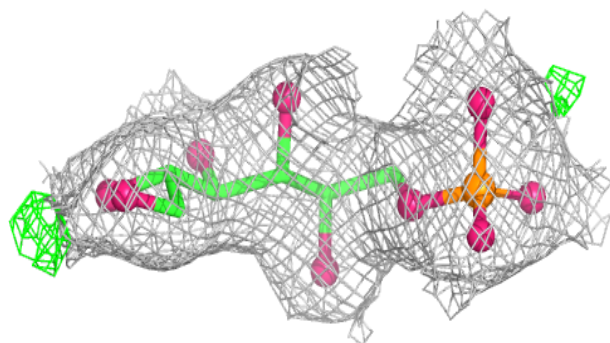
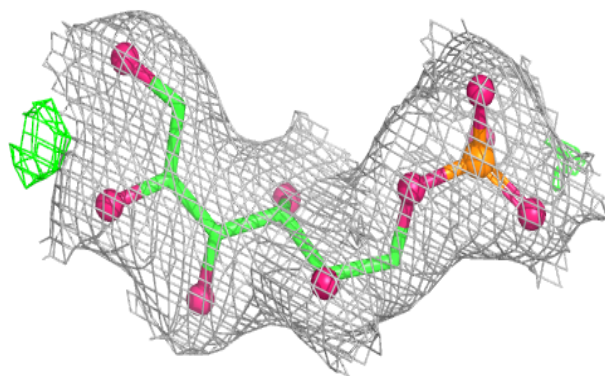


Electron density around 2WZ A 701:

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

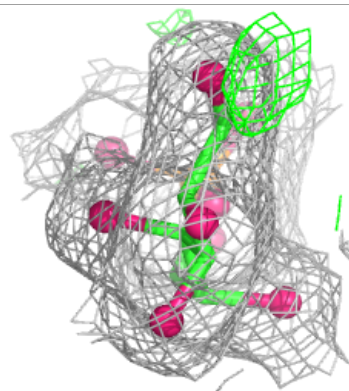
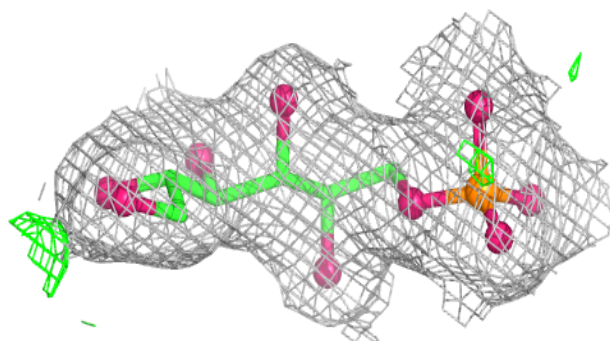
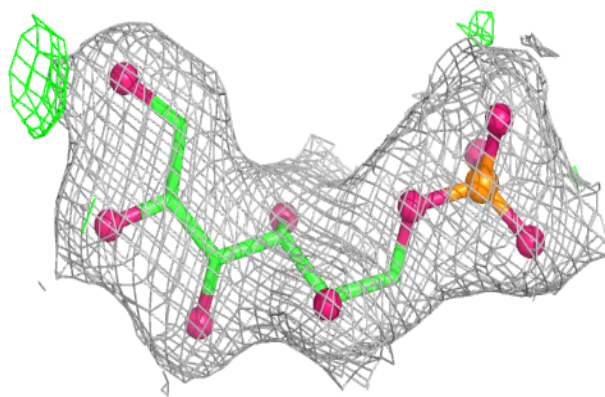
**Electron density around S6P B 702:**

$2mF_o-DF_c$ (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.