



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:05 AM UTC

PDB ID : 8R56 / pdb_00008r56
Title : Crystal structure of GH31 family Sulfoquinovosidase BmSQase in covalent complex with SQ-aziridine (SQZ)
Authors : Sharma, M.; Davies, G.J.
Deposited on : 2023-11-16
Resolution : 2.45 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

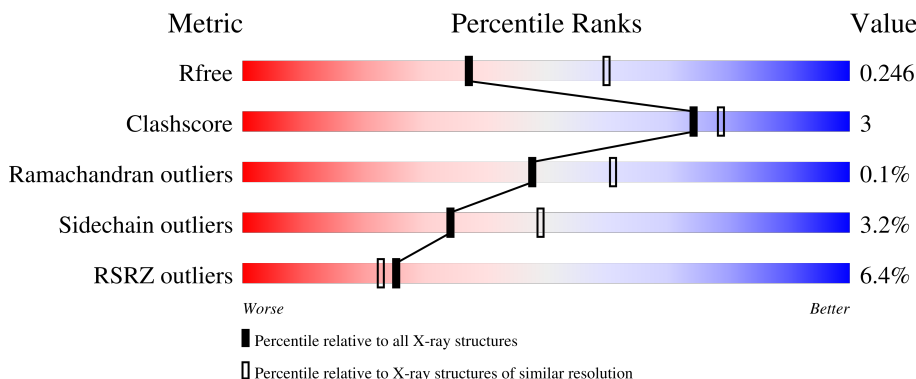
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	699	5% 86% 9% ...
1	B	699	7% 85% 9% ...
1	C	699	6% 86% 9% ...
1	D	699	7% 87% 8% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21881 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 Glycosyl hydrolase, family 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	1	0
			5300	3415	861	996	28			
1	B	669	Total	C	N	O	S	0	0	0
			5289	3414	859	988	28			
1	C	671	Total	C	N	O	S	0	0	0
			5300	3421	865	987	27			
1	D	673	Total	C	N	O	S	0	0	0
			5341	3441	874	998	28			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP D5E1T0
A	-18	GLY	-	expression tag	UNP D5E1T0
A	-17	SER	-	expression tag	UNP D5E1T0
A	-16	SER	-	expression tag	UNP D5E1T0
A	-15	HIS	-	expression tag	UNP D5E1T0
A	-14	HIS	-	expression tag	UNP D5E1T0
A	-13	HIS	-	expression tag	UNP D5E1T0
A	-12	HIS	-	expression tag	UNP D5E1T0
A	-11	HIS	-	expression tag	UNP D5E1T0
A	-10	HIS	-	expression tag	UNP D5E1T0
A	-9	SER	-	expression tag	UNP D5E1T0
A	-8	SER	-	expression tag	UNP D5E1T0
A	-7	GLY	-	expression tag	UNP D5E1T0
A	-6	LEU	-	expression tag	UNP D5E1T0
A	-5	VAL	-	expression tag	UNP D5E1T0
A	-4	PRO	-	expression tag	UNP D5E1T0
A	-3	ARG	-	expression tag	UNP D5E1T0
A	-2	GLY	-	expression tag	UNP D5E1T0
A	-1	SER	-	expression tag	UNP D5E1T0
A	0	HIS	-	expression tag	UNP D5E1T0
B	-19	MET	-	initiating methionine	UNP D5E1T0

Continued on next page...

Continued from previous page...

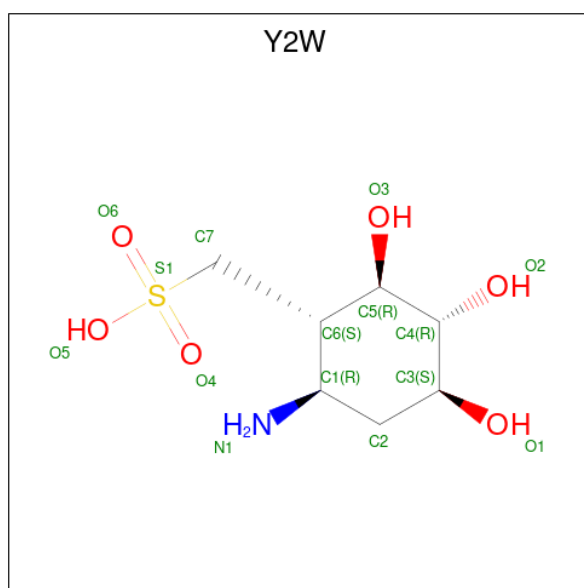
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP D5E1T0
B	-17	SER	-	expression tag	UNP D5E1T0
B	-16	SER	-	expression tag	UNP D5E1T0
B	-15	HIS	-	expression tag	UNP D5E1T0
B	-14	HIS	-	expression tag	UNP D5E1T0
B	-13	HIS	-	expression tag	UNP D5E1T0
B	-12	HIS	-	expression tag	UNP D5E1T0
B	-11	HIS	-	expression tag	UNP D5E1T0
B	-10	HIS	-	expression tag	UNP D5E1T0
B	-9	SER	-	expression tag	UNP D5E1T0
B	-8	SER	-	expression tag	UNP D5E1T0
B	-7	GLY	-	expression tag	UNP D5E1T0
B	-6	LEU	-	expression tag	UNP D5E1T0
B	-5	VAL	-	expression tag	UNP D5E1T0
B	-4	PRO	-	expression tag	UNP D5E1T0
B	-3	ARG	-	expression tag	UNP D5E1T0
B	-2	GLY	-	expression tag	UNP D5E1T0
B	-1	SER	-	expression tag	UNP D5E1T0
B	0	HIS	-	expression tag	UNP D5E1T0
C	-19	MET	-	initiating methionine	UNP D5E1T0
C	-18	GLY	-	expression tag	UNP D5E1T0
C	-17	SER	-	expression tag	UNP D5E1T0
C	-16	SER	-	expression tag	UNP D5E1T0
C	-15	HIS	-	expression tag	UNP D5E1T0
C	-14	HIS	-	expression tag	UNP D5E1T0
C	-13	HIS	-	expression tag	UNP D5E1T0
C	-12	HIS	-	expression tag	UNP D5E1T0
C	-11	HIS	-	expression tag	UNP D5E1T0
C	-10	HIS	-	expression tag	UNP D5E1T0
C	-9	SER	-	expression tag	UNP D5E1T0
C	-8	SER	-	expression tag	UNP D5E1T0
C	-7	GLY	-	expression tag	UNP D5E1T0
C	-6	LEU	-	expression tag	UNP D5E1T0
C	-5	VAL	-	expression tag	UNP D5E1T0
C	-4	PRO	-	expression tag	UNP D5E1T0
C	-3	ARG	-	expression tag	UNP D5E1T0
C	-2	GLY	-	expression tag	UNP D5E1T0
C	-1	SER	-	expression tag	UNP D5E1T0
C	0	HIS	-	expression tag	UNP D5E1T0
D	-19	MET	-	initiating methionine	UNP D5E1T0
D	-18	GLY	-	expression tag	UNP D5E1T0
D	-17	SER	-	expression tag	UNP D5E1T0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP D5E1T0
D	-15	HIS	-	expression tag	UNP D5E1T0
D	-14	HIS	-	expression tag	UNP D5E1T0
D	-13	HIS	-	expression tag	UNP D5E1T0
D	-12	HIS	-	expression tag	UNP D5E1T0
D	-11	HIS	-	expression tag	UNP D5E1T0
D	-10	HIS	-	expression tag	UNP D5E1T0
D	-9	SER	-	expression tag	UNP D5E1T0
D	-8	SER	-	expression tag	UNP D5E1T0
D	-7	GLY	-	expression tag	UNP D5E1T0
D	-6	LEU	-	expression tag	UNP D5E1T0
D	-5	VAL	-	expression tag	UNP D5E1T0
D	-4	PRO	-	expression tag	UNP D5E1T0
D	-3	ARG	-	expression tag	UNP D5E1T0
D	-2	GLY	-	expression tag	UNP D5E1T0
D	-1	SER	-	expression tag	UNP D5E1T0
D	0	HIS	-	expression tag	UNP D5E1T0

- Molecule 2 is [(1 {S},2 {R},3 {R},4 {S},6 {R})-6-azanyl-2,3,4-tris(oxidanyl)cyclohexyl]methanesulfonic acid (CCD ID: Y2W) (formula: C₇H₁₅NO₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	7	1	6	1		
2	B	1	Total	C	N	O	S	0	0
			15	7	1	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			15	7	1	6	1		
2	D	1	Total	C	N	O	S	0	0
			15	7	1	6	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		

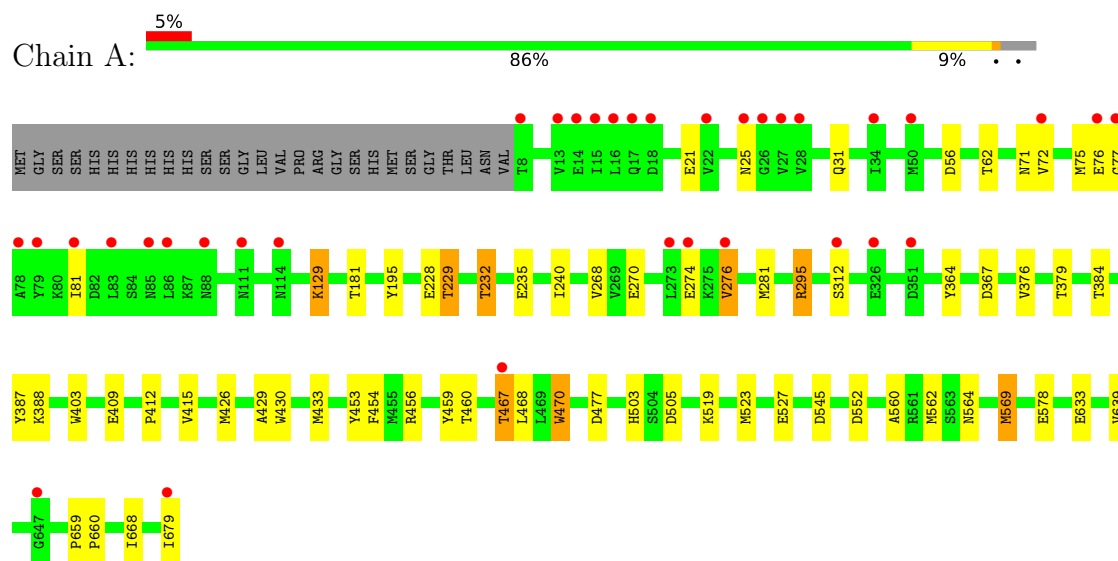
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	141	Total	O	0	0
			141	141		
4	C	135	Total	O	0	0
			135	135		
4	D	135	Total	O	0	0
			135	135		

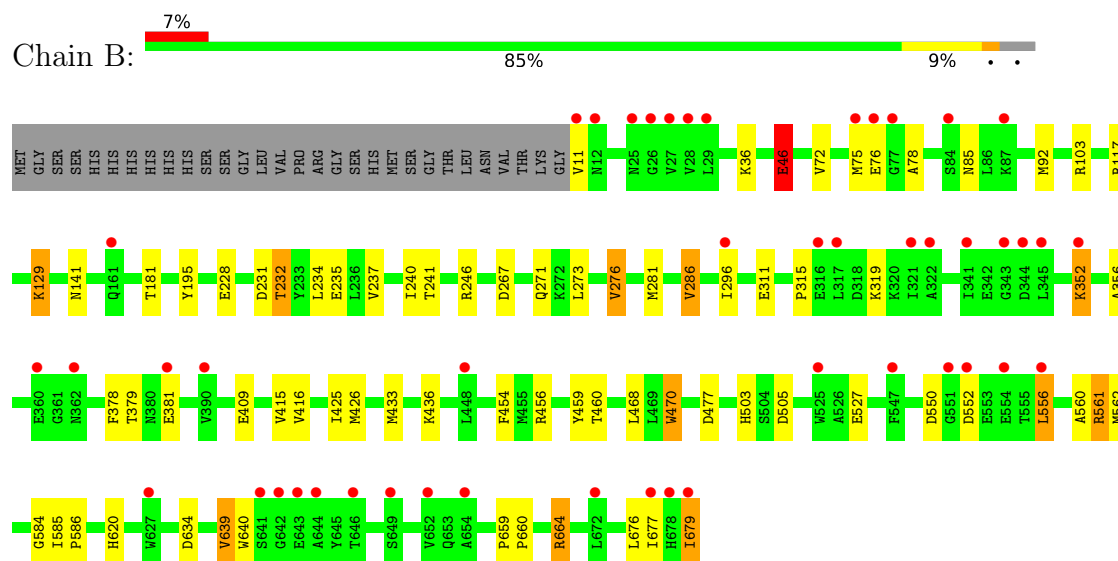
3 Residue-property plots [i](#)

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.

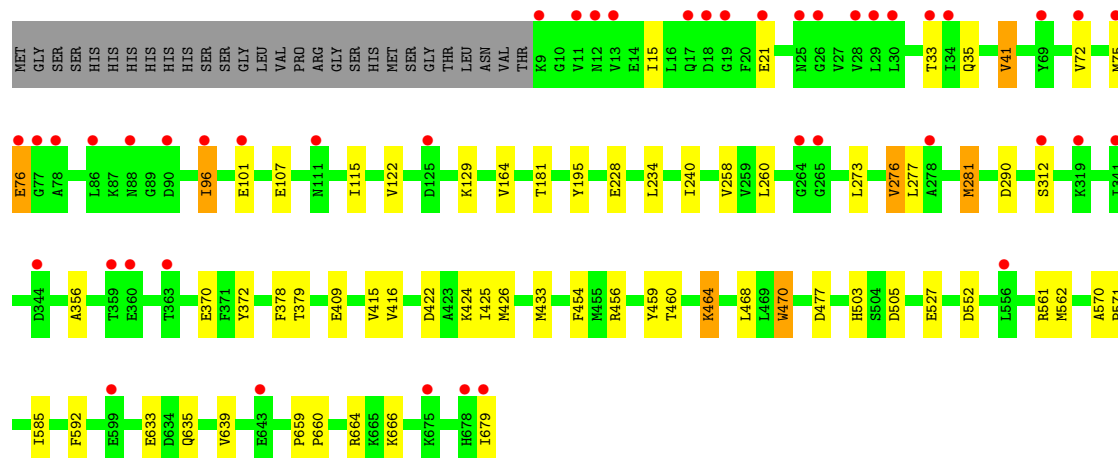
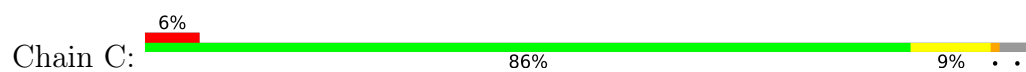
- Molecule 1: Glycosyl hydrolase, family 31



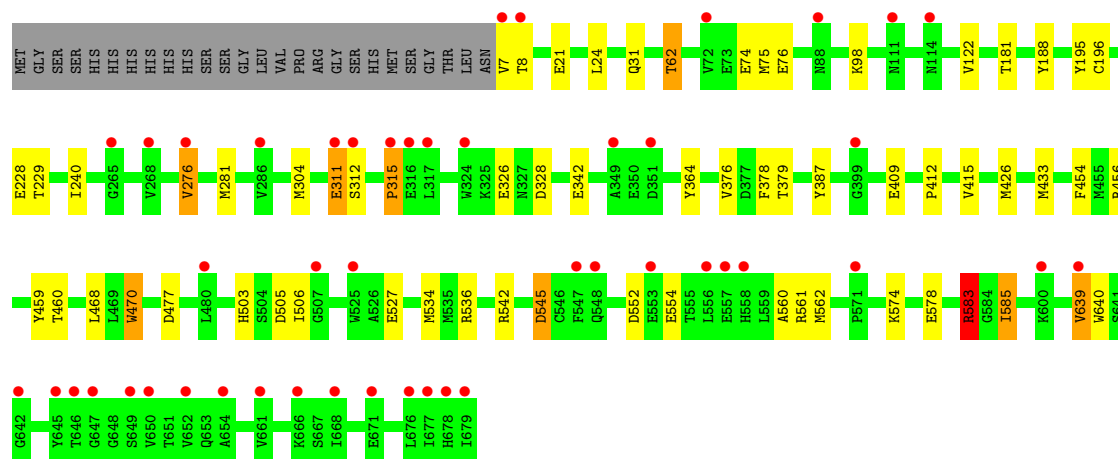
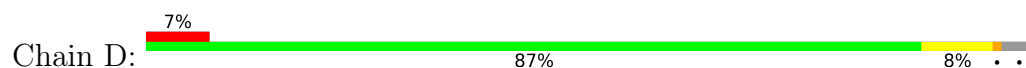
- Molecule 1: Glycosyl hydrolase, family 31



- Molecule 1: Glycosyl hydrolase, family 31



• Molecule 1: Glycosyl hydrolase, family 31



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.52Å 194.73Å 117.65Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	62.55 – 2.45 62.55 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (62.55-2.45) 99.4 (62.55-2.45)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.212 , 0.244 0.216 , 0.246	Depositor DCC
R_{free} test set	5017 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21881	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: Y2W, K

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	0.58	0/5448	1.04	13/7421 (0.2%)
1	B	0.58	0/5437	1.03	14/7402 (0.2%)
1	C	0.57	0/5447	1.04	13/7409 (0.2%)
1	D	0.57	0/5489	1.04	15/7466 (0.2%)
All	All	0.58	0/21821	1.04	55/29698 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	THR	CA-CB-OG1	-9.03	96.06	109.60
1	A	569	MET	CG-SD-CE	-7.84	83.65	100.90
1	C	101	GLU	CB-CG-CD	7.51	125.38	112.60
1	D	554	GLU	N-CA-CB	7.51	120.90	110.01
1	B	46	GLU	CB-CG-CD	7.24	124.91	112.60
1	B	286	VAL	N-CA-CB	-7.15	98.95	111.39
1	D	578	GLU	CB-CG-CD	7.12	124.70	112.60
1	D	409	GLU	CB-CG-CD	6.71	124.00	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	554	GLU	CB-CA-C	-6.60	100.52	110.88
1	B	409	GLU	CB-CG-CD	6.54	123.72	112.60
1	B	409	GLU	CB-CA-C	6.50	121.70	110.72
1	A	578	GLU	CB-CA-C	6.38	121.69	110.85
1	C	477	ASP	CA-CB-CG	6.24	118.83	112.60
1	C	666	LYS	N-CA-CB	-6.17	99.59	110.39
1	C	664	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	C	505	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	477	ASP	CA-CB-CG	6.03	118.62	112.60
1	B	319	LYS	CB-CA-C	5.96	121.64	109.67
1	D	409	GLU	CB-CA-C	5.94	120.75	110.72
1	B	267	ASP	CA-CB-CG	5.92	118.52	112.60
1	D	477	ASP	CA-CB-CG	5.86	118.46	112.60
1	D	545	ASP	CA-CB-CG	5.86	118.45	112.60
1	B	181	THR	CA-CB-OG1	-5.85	100.83	109.60
1	B	409	GLU	CG-CD-OE2	-5.81	105.04	118.40
1	D	552	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	129	LYS	CB-CG-CD	5.72	124.45	111.30
1	C	409	GLU	CB-CA-C	-5.64	101.19	110.72
1	C	561	ARG	CB-CA-C	5.60	119.67	110.88
1	A	545	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	181	THR	CA-CB-OG1	-5.55	101.28	109.60
1	C	552	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	295	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	A	505	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	552	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	464	LYS	CB-CG-CD	5.43	123.80	111.30
1	A	409	GLU	CB-CA-C	-5.41	101.58	110.72
1	B	561	ARG	CB-CA-C	5.39	119.35	110.88
1	D	181	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	477	ASP	CA-CB-CG	5.30	117.91	112.60
1	B	352	LYS	CB-CG-CD	5.27	123.42	111.30
1	B	436	LYS	CB-CG-CD	5.27	123.42	111.30
1	D	74	GLU	CB-CG-CD	5.26	121.54	112.60
1	D	505	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	561	ARG	CB-CA-C	5.22	119.07	110.88
1	B	505	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	315	PRO	N-CA-C	5.18	120.73	113.53
1	C	592	PHE	CA-CB-CG	5.15	118.95	113.80
1	C	281	MET	CG-SD-CE	-5.13	89.62	100.90
1	D	62	THR	N-CA-CB	-5.12	102.65	110.33
1	A	467	THR	N-CA-CB	-5.08	101.95	110.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	56	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	181	THR	CA-CB-OG1	-5.03	102.05	109.60
1	A	295	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	A	552	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Sidechain
1	A	456	ARG	Sidechain
1	B	456	ARG	Sidechain
1	C	456	ARG	Sidechain
1	D	456	ARG	Sidechain
1	D	583	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	5300	0	4883	33	0
1	B	5289	0	4899	39	0
1	C	5300	0	4915	31	1
1	D	5341	0	4981	25	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	176	0	0	1	0
4	B	141	0	0	3	0
4	C	135	0	0	2	0
4	D	135	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21881	0	19678	128	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 3.

All (128) 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:519:LYS:HG2	1:A:523:MET:HE2	1.38	1.03
1:A:426:MET:HE3	1:A:433:MET:HE1	1.57	0.84
1:B:425:ILE:HD11	4:B:941:HOH:O	1.82	0.78
1:C:276:VAL:CG1	1:C:281:MET:HE2	2.17	0.73
1:C:96:ILE:HG13	1:C:107:GLU:HB2	1.72	0.72
1:A:453:TYR:H	1:A:467:THR:HG21	1.55	0.72
1:A:453:TYR:O	1:A:467:THR:CG2	2.39	0.71
1:D:542:ARG:HD3	4:D:803:HOH:O	1.91	0.69
1:D:506:ILE:O	4:D:801:HOH:O	2.11	0.68
1:C:276:VAL:HG13	1:C:281:MET:HE2	1.78	0.66
1:B:550:ASP:HA	1:B:556:LEU:CD1	2.27	0.64
1:A:384:THR:O	1:A:388:LYS:HG3	1.97	0.64
1:B:550:ASP:HA	1:B:556:LEU:HD12	1.80	0.64
1:B:561:ARG:NH1	1:B:679:ILE:O	2.32	0.63
1:A:519:LYS:HG2	1:A:523:MET:CE	2.22	0.62
1:C:33:THR:HG22	1:C:35:GLN:H	1.65	0.62
1:C:96:ILE:CG1	1:C:107:GLU:HB2	2.29	0.61
1:C:276:VAL:HG11	1:C:281:MET:HE2	1.82	0.61
1:A:232:THR:HG22	1:A:235[B]:GLU:H	1.65	0.60
1:D:328:ASP:CA	4:D:908:HOH:O	2.49	0.60
1:A:232:THR:HG22	1:A:235[A]:GLU:H	1.65	0.59
1:B:620:HIS:NE2	4:B:802:HOH:O	2.32	0.58
1:C:15:ILE:HD11	1:C:72:VAL:HG11	1.85	0.57
1:B:234:LEU:HD22	1:B:585:ILE:HD13	1.85	0.57
1:C:422:ASP:OD2	1:C:424:LYS:HD2	2.04	0.57
1:A:430:TRP:HA	1:A:433:MET:HE3	1.87	0.57
1:C:260:LEU:HD21	1:C:281:MET:HE1	1.86	0.57
1:A:195:TYR:CE2	1:A:228:GLU:HB3	2.40	0.56
1:B:195:TYR:CE2	1:B:228:GLU:HB3	2.41	0.56
1:C:75:MET:O	1:C:76:GLU:C	2.49	0.55
1:C:195:TYR:CE2	1:C:228:GLU:HB3	2.42	0.55
1:D:542:ARG:CD	4:D:803:HOH:O	2.52	0.55
1:C:527:GLU:HA	1:C:562:MET:HE2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:VAL:HG12	1:D:640:TRP:CD2	2.43	0.54
1:B:46:GLU:HG3	1:B:117:ARG:HH22	1.73	0.54
1:B:561:ARG:HH12	1:B:679:ILE:C	2.15	0.54
1:D:195:TYR:CE2	1:D:228:GLU:HB3	2.42	0.54
1:A:527:GLU:HA	1:A:562:MET:HE2	1.90	0.53
1:A:453:TYR:O	1:A:467:THR:HG22	2.08	0.53
1:B:356:ALA:HB1	1:B:415:VAL:CG2	2.39	0.53
1:B:527:GLU:HA	1:B:562:MET:HE2	1.91	0.53
1:A:426:MET:CE	1:A:433:MET:HE1	2.33	0.53
1:B:639:VAL:HG12	1:B:640:TRP:CD2	2.44	0.53
1:D:527:GLU:HA	1:D:562:MET:HE2	1.91	0.52
1:A:453:TYR:O	1:A:467:THR:HG23	2.09	0.52
1:A:367:ASP:OD2	4:A:801:HOH:O	2.19	0.52
1:A:564:ASN:HB3	1:A:679:ILE:HD11	1.92	0.52
1:B:634:ASP:OD2	1:B:664:ARG:HD2	2.10	0.51
1:D:545:ASP:OD2	4:D:803:HOH:O	2.18	0.51
1:C:454:PHE:HA	1:C:468:LEU:O	2.12	0.50
1:B:276:VAL:HG13	1:B:281:MET:HB3	1.93	0.50
1:C:276:VAL:HG13	1:C:281:MET:HB3	1.93	0.50
1:B:237:VAL:HG11	1:B:586:PRO:HD3	1.94	0.50
1:D:454:PHE:HA	1:D:468:LEU:O	2.12	0.50
1:A:276:VAL:HG13	1:A:281:MET:HB3	1.92	0.50
1:C:378:PHE:HB2	1:C:433:MET:HE2	1.94	0.49
1:B:356:ALA:HB1	1:B:415:VAL:HG21	1.94	0.49
1:C:164:VAL:HG23	4:C:904:HOH:O	2.13	0.49
1:A:21:GLU:HG2	1:A:31:GLN:HG2	1.95	0.49
1:B:378:PHE:HB2	1:B:433:MET:HE2	1.94	0.49
1:C:356:ALA:HB1	1:C:415:VAL:CG2	2.42	0.48
1:A:454:PHE:HA	1:A:468:LEU:O	2.13	0.48
1:D:378:PHE:HB2	1:D:433:MET:HE2	1.96	0.48
1:A:25:ASN:HD22	1:A:229:THR:HG22	1.78	0.48
1:D:311:GLU:O	1:D:315:PRO:HA	2.14	0.48
1:D:412:PRO:O	1:D:415:VAL:HG22	2.13	0.48
1:B:454:PHE:HA	1:B:468:LEU:O	2.14	0.48
1:B:232:THR:HG22	1:B:235:GLU:H	1.79	0.47
1:C:679:ILE:C	4:C:875:HOH:O	2.57	0.47
1:D:379:THR:HG22	1:D:426:MET:HE2	1.96	0.47
1:B:241:THR:HB	1:B:246:ARG:HG2	1.96	0.47
1:A:429:ALA:CB	1:A:433:MET:HE2	2.45	0.47
1:D:21:GLU:HG2	1:D:31:GLN:HG2	1.96	0.47
1:B:11:VAL:O	1:B:11:VAL:HG13	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:415:VAL:HG22	2.15	0.46
1:D:276:VAL:HG13	1:D:281:MET:HB3	1.97	0.46
1:D:583:ARG:HH21	1:D:585:ILE:HD11	1.81	0.46
1:C:356:ALA:HB1	1:C:415:VAL:HG21	1.98	0.45
1:C:379:THR:HG22	1:C:426:MET:HE2	1.97	0.45
1:B:103:ARG:HD2	4:B:865:HOH:O	2.16	0.45
1:A:379:THR:HG22	1:A:426:MET:HE2	1.98	0.45
1:D:364:TYR:CD2	1:D:415:VAL:HG12	2.50	0.45
1:D:470:TRP:HA	1:D:503:HIS:O	2.16	0.45
1:A:470:TRP:HA	1:A:503:HIS:O	2.17	0.45
1:B:311:GLU:O	1:B:315:PRO:HA	2.17	0.45
1:B:676:LEU:HA	1:B:679:ILE:HG22	1.99	0.45
1:D:534:MET:CE	1:D:536:ARG:HD3	2.47	0.45
1:B:470:TRP:HA	1:B:503:HIS:O	2.18	0.44
1:B:46:GLU:HG3	1:B:117:ARG:NH2	2.32	0.44
1:C:273:LEU:HD12	1:C:273:LEU:HA	1.79	0.44
1:C:234:LEU:HD22	1:C:585:ILE:HD13	1.99	0.44
1:C:470:TRP:HA	1:C:503:HIS:O	2.17	0.44
1:C:41:VAL:HG11	1:C:115:ILE:HD13	2.00	0.44
1:A:25:ASN:HB2	1:A:229:THR:HG21	2.00	0.44
1:B:659:PRO:HA	1:B:660:PRO:HD3	1.88	0.44
1:C:459:TYR:O	1:C:460:THR:C	2.60	0.44
1:D:281:MET:HG3	1:D:560:ALA:HA	1.99	0.44
1:D:188:TYR:CE2	1:D:196:CYS:HB3	2.54	0.43
1:B:639:VAL:O	1:B:677:ILE:HD13	2.18	0.43
1:B:459:TYR:O	1:B:460:THR:C	2.62	0.43
1:C:258:VAL:CG1	1:C:281:MET:HE3	2.49	0.42
1:B:46:GLU:CG	1:B:117:ARG:HH22	2.31	0.42
1:A:281:MET:HG3	1:A:560:ALA:HA	2.01	0.42
1:B:129:LYS:HE2	1:B:141:ASN:HD21	1.85	0.42
1:A:403:TRP:O	1:A:453:TYR:HA	2.20	0.42
1:A:426:MET:HE3	1:A:433:MET:CE	2.39	0.42
1:B:85:ASN:CG	1:B:92:MET:HE1	2.44	0.42
1:C:260:LEU:HD21	1:C:281:MET:CE	2.47	0.42
1:B:415:VAL:HG22	1:B:416:VAL:N	2.35	0.42
1:B:237:VAL:HG12	1:B:584:GLY:O	2.20	0.42
1:C:659:PRO:HA	1:C:660:PRO:HD3	1.89	0.42
1:B:76:GLU:C	1:B:78:ALA:H	2.28	0.42
1:C:570:ALA:HB3	1:C:571:PRO:HD3	2.02	0.42
1:A:364:TYR:CD2	1:A:415:VAL:HG12	2.55	0.41
1:C:415:VAL:HG22	1:C:416:VAL:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:MET:O	1:A:77:GLY:N	2.53	0.41
1:A:659:PRO:HA	1:A:660:PRO:HD3	1.87	0.41
1:B:379:THR:HG22	1:B:426:MET:HE2	2.01	0.41
1:C:258:VAL:HG11	1:C:281:MET:HE3	2.02	0.41
1:D:376:VAL:HG21	1:D:387:TYR:CE1	2.55	0.41
1:A:376:VAL:HG21	1:A:387:TYR:CE1	2.55	0.41
1:A:459:TYR:O	1:A:460:THR:C	2.63	0.41
1:D:304:MET:HE1	1:D:342:GLU:HB2	2.03	0.41
1:B:561:ARG:NH1	1:B:679:ILE:C	2.78	0.40
1:D:24:LEU:HD23	1:D:229:THR:HG23	2.02	0.40
1:D:459:TYR:O	1:D:460:THR:C	2.62	0.40
1:B:273:LEU:HD12	1:B:273:LEU:HA	1.91	0.40
1:B:281:MET:HG3	1:B:560:ALA:HA	2.04	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)
1:C:372:TYR:OH	1:C:635:GLN:OE1[1_655]	1.72	0.48

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	671/699 (96%)	647 (96%)	23 (3%)	1 (0%)	48	61
1	B	667/699 (95%)	643 (96%)	24 (4%)	0	100	100
1	C	669/699 (96%)	647 (97%)	21 (3%)	1 (0%)	48	61
1	D	671/699 (96%)	649 (97%)	20 (3%)	2 (0%)	36	45
All	All	2678/2796 (96%)	2586 (97%)	88 (3%)	4 (0%)	48	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	76	GLU
1	D	76	GLU
1	A	76	GLU
1	D	8	THR

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	526/602 (87%)	508 (97%)	18 (3%)	32	47
1	B	525/602 (87%)	506 (96%)	19 (4%)	31	45
1	C	523/602 (87%)	508 (97%)	15 (3%)	37	52
1	D	537/602 (89%)	522 (97%)	15 (3%)	38	54
All	All	2111/2408 (88%)	2044 (97%)	67 (3%)	34	49

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
1	A	71	ASN
1	A	72	VAL
1	A	81	ILE
1	A	129	LYS
1	A	229	THR
1	A	232	THR
1	A	240	ILE
1	A	268	VAL
1	A	270	GLU
1	A	274	GLU
1	A	276	VAL
1	A	312	SER
1	A	470	TRP
1	A	569	MET
1	A	633	GLU
1	A	639	VAL
1	A	668	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	36	LYS
1	B	46	GLU
1	B	72	VAL
1	B	75	MET
1	B	129	LYS
1	B	231	ASP
1	B	232	THR
1	B	240	ILE
1	B	271	GLN
1	B	276	VAL
1	B	286	VAL
1	B	296	ILE
1	B	352	LYS
1	B	381	GLU
1	B	470	TRP
1	B	556	LEU
1	B	639	VAL
1	B	664	ARG
1	B	679	ILE
1	C	21	GLU
1	C	41	VAL
1	C	96	ILE
1	C	122	VAL
1	C	129	LYS
1	C	240	ILE
1	C	276	VAL
1	C	277	LEU
1	C	312	SER
1	C	370	GLU
1	C	425	ILE
1	C	464	LYS
1	C	470	TRP
1	C	633	GLU
1	C	639	VAL
1	D	7	VAL
1	D	62	THR
1	D	75	MET
1	D	98	LYS
1	D	122	VAL
1	D	240	ILE
1	D	276	VAL
1	D	311	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	312	SER
1	D	326	GLU
1	D	470	TRP
1	D	574	LYS
1	D	583	ARG
1	D	585	ILE
1	D	639	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	A	292	GLN
1	A	474	GLN
1	A	580	ASN
1	A	635	GLN
1	A	653	GLN
1	B	102	ASN
1	B	139	HIS
1	B	292	GLN
1	B	580	ASN
1	B	653	GLN
1	C	12	ASN
1	C	292	GLN
1	C	474	GLN
1	C	653	GLN
1	D	263	GLN
1	D	289	GLN
1	D	292	GLN
1	D	624	GLN
1	D	653	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
2	Y2W	A	701	1	13,15,15	0.44	0	20,23,23	1.15	2 (10%)
2	Y2W	C	701	1	13,15,15	0.62	0	20,23,23	0.95	1 (5%)
2	Y2W	B	701	1	13,15,15	0.63	0	20,23,23	1.16	1 (5%)
2	Y2W	D	701	1	13,15,15	0.43	0	20,23,23	1.25	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
2	Y2W	A	701	1	-	0/5/25/25	0/1/1/1
2	Y2W	C	701	1	-	0/5/25/25	0/1/1/1
2	Y2W	B	701	1	-	0/5/25/25	0/1/1/1
2	Y2W	D	701	1	-	0/5/25/25	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	Y2W	C3-C2-C1	3.13	119.05	112.65
2	C	701	Y2W	C3-C2-C1	2.95	118.70	112.65
2	A	701	Y2W	C3-C2-C1	2.76	118.29	112.65
2	D	701	Y2W	C2-C1-C6	2.51	114.83	111.67
2	D	701	Y2W	C3-C2-C1	2.33	117.41	112.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	Y2W	O4-S1-C7	-2.18	103.50	106.76
2	D	701	Y2W	O5-S1-C7	-2.03	102.05	105.97

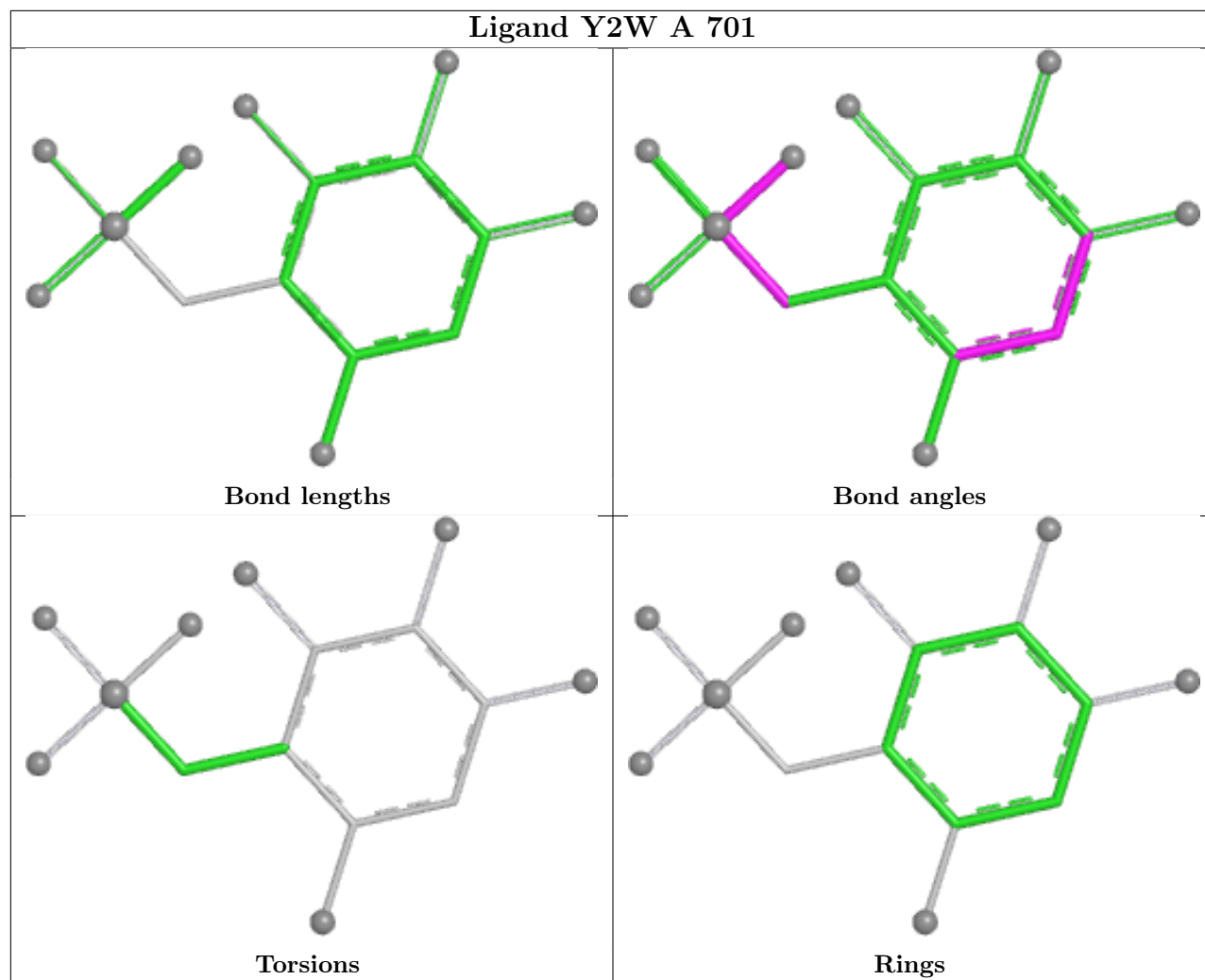
There are no chirality outliers.

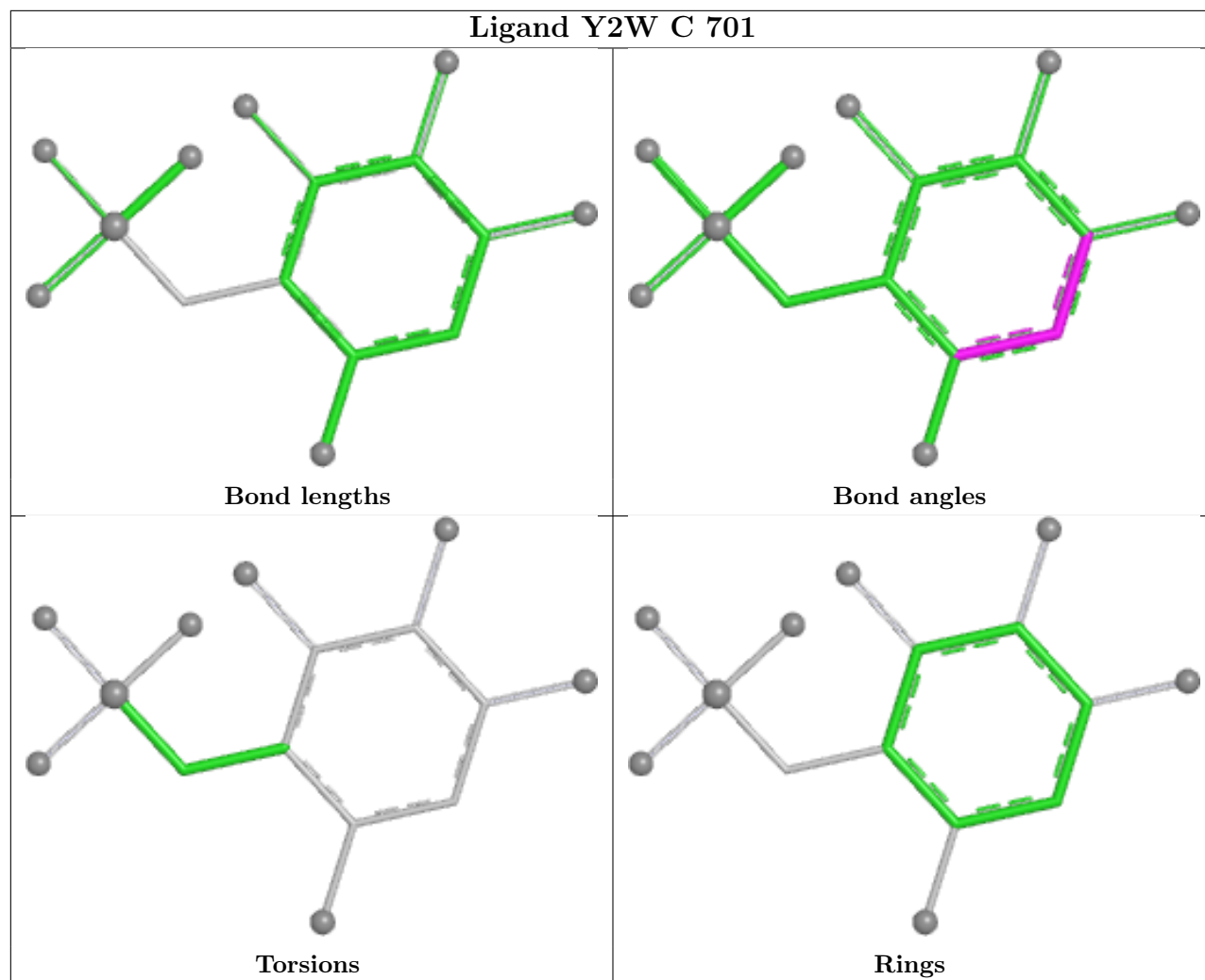
There are no torsion outliers.

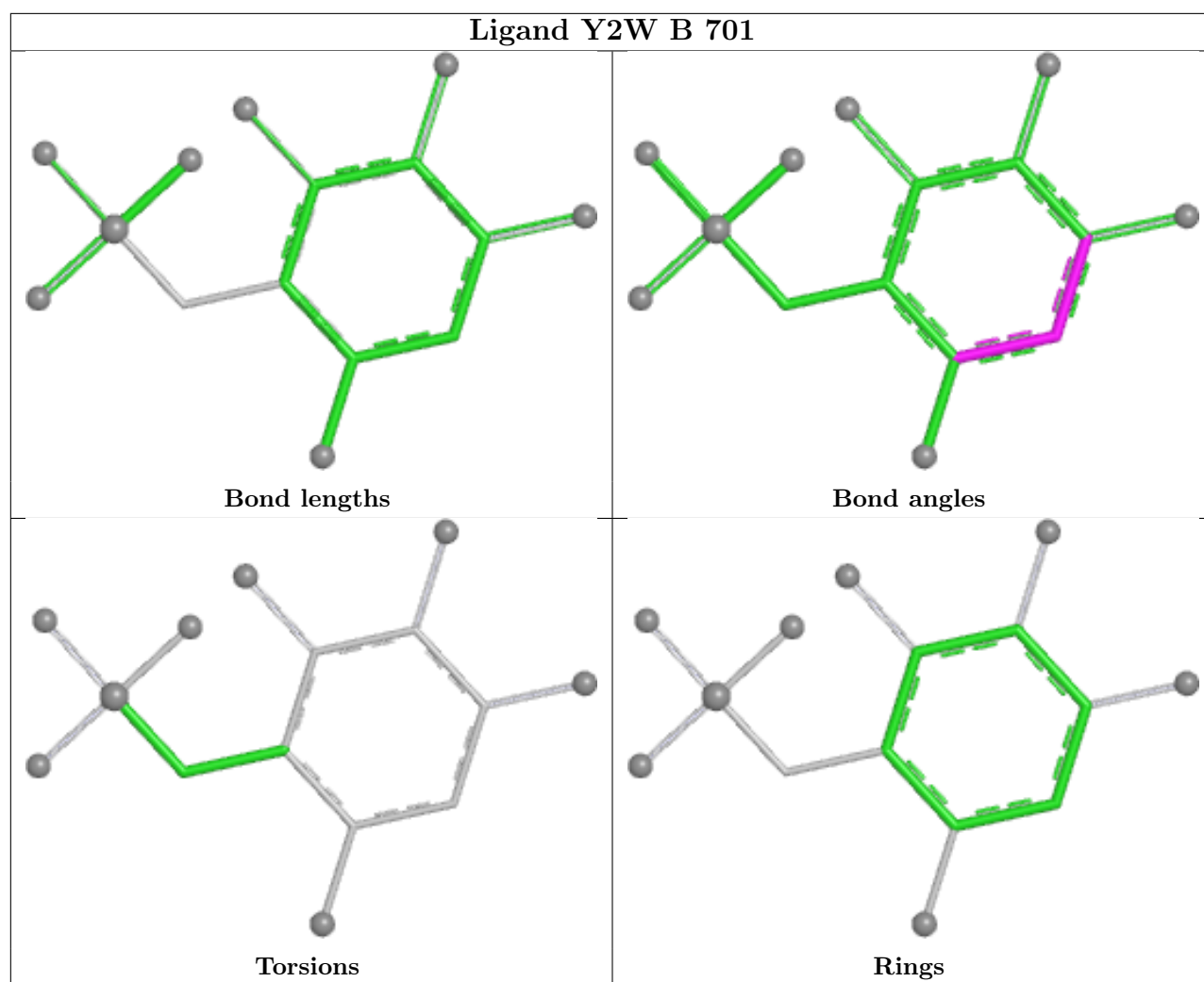
There are no ring outliers.

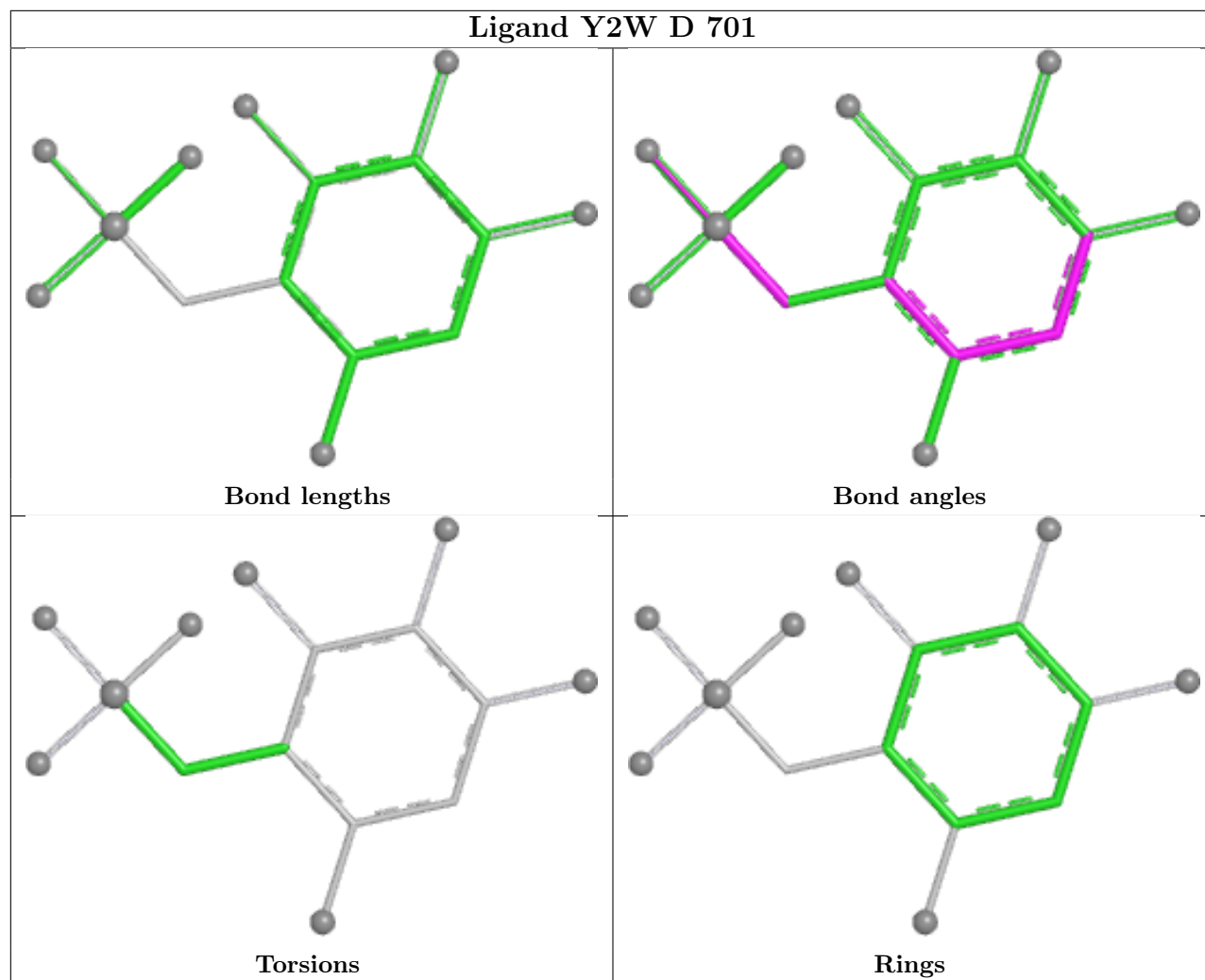
No monomer is involved in short contacts.

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.









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	672/699 (96%)	0.63	35 (5%)	33	30	13, 27, 50, 90	1 (0%)
1	B	669/699 (95%)	0.77	47 (7%)	22	20	16, 30, 49, 75	0
1	C	671/699 (95%)	0.76	44 (6%)	24	22	15, 30, 52, 86	0
1	D	673/699 (96%)	0.86	47 (6%)	22	20	17, 32, 52, 87	0
All	All	2685/2796 (96%)	0.76	173 (6%)	25	23	13, 30, 52, 90	1 (0%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	GLY	6.7
1	D	7	VAL	5.7
1	B	26	GLY	5.0
1	B	11	VAL	4.8
1	D	8	THR	4.7
1	C	18	ASP	4.5
1	A	81	ILE	4.4
1	D	556	LEU	4.4
1	B	25	ASN	4.4
1	B	677	ILE	4.3
1	C	76	GLU	4.3
1	C	13	VAL	4.1
1	D	668	ILE	3.8
1	B	551	GLY	3.8
1	C	19	GLY	3.8
1	B	646	THR	3.8
1	A	78	ALA	3.7
1	A	79	TYR	3.7
1	C	17	GLN	3.7
1	A	114	ASN	3.6
1	A	88	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	33	THR	3.5
1	A	8	THR	3.5
1	A	111	ASN	3.4
1	D	678	HIS	3.4
1	C	86	LEU	3.4
1	C	679	ILE	3.3
1	C	12	ASN	3.3
1	C	111	ASN	3.3
1	D	649	SER	3.2
1	D	315	PRO	3.2
1	B	679	ILE	3.2
1	A	76	GLU	3.1
1	A	679	ILE	3.1
1	C	34	ILE	3.1
1	A	28	VAL	3.1
1	D	311	GLU	3.1
1	D	312	SER	3.1
1	B	12	ASN	3.1
1	A	26	GLY	3.1
1	B	654	ALA	3.0
1	C	125	ASP	3.0
1	A	13	VAL	3.0
1	D	88	ASN	3.0
1	C	341	ILE	2.9
1	B	84	SER	2.9
1	D	324	TRP	2.9
1	D	114	ASN	2.9
1	B	341	ILE	2.9
1	C	678	HIS	2.9
1	C	319	LYS	2.8
1	C	360	GLU	2.8
1	C	28	VAL	2.8
1	C	72	VAL	2.8
1	A	18	ASP	2.8
1	B	547	PHE	2.8
1	D	679	ILE	2.8
1	B	644	ALA	2.8
1	A	274	GLU	2.8
1	D	316	GLU	2.7
1	B	643	GLU	2.7
1	B	552	ASP	2.7
1	B	87	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	111	ASN	2.7
1	C	556	LEU	2.7
1	A	14	GLU	2.7
1	D	276	VAL	2.6
1	A	25	ASN	2.6
1	D	676	LEU	2.6
1	B	360	GLU	2.6
1	C	599	GLU	2.6
1	C	77	GLY	2.6
1	A	22	VAL	2.6
1	D	639	VAL	2.6
1	D	646	THR	2.6
1	A	34	ILE	2.5
1	D	647	GLY	2.5
1	D	525	TRP	2.5
1	C	29	LEU	2.5
1	B	76	GLU	2.5
1	B	296	ILE	2.5
1	A	17	GLN	2.5
1	B	75	MET	2.5
1	B	448	LEU	2.5
1	A	467	THR	2.5
1	D	600	LYS	2.4
1	D	480	LEU	2.4
1	A	276	VAL	2.4
1	D	553	GLU	2.4
1	B	77	GLY	2.4
1	D	642	GLY	2.4
1	C	75	MET	2.4
1	C	96	ILE	2.4
1	C	278	ALA	2.4
1	C	9	LYS	2.4
1	A	83	LEU	2.4
1	B	29	LEU	2.4
1	D	547	PHE	2.4
1	A	72	VAL	2.4
1	C	25	ASN	2.4
1	A	647	GLY	2.3
1	A	86	LEU	2.3
1	C	90	ASP	2.3
1	D	349	ALA	2.3
1	D	571	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	677	ILE	2.3
1	D	351	ASP	2.3
1	A	27	VAL	2.3
1	D	645	TYR	2.3
1	C	26	GLY	2.3
1	B	352	LYS	2.3
1	A	326	GLU	2.3
1	D	661	VAL	2.3
1	B	678	HIS	2.3
1	B	556	LEU	2.3
1	B	627	TRP	2.3
1	D	317	LEU	2.3
1	B	28	VAL	2.3
1	D	650	VAL	2.3
1	A	273	LEU	2.2
1	B	316	GLU	2.2
1	B	554	GLU	2.2
1	C	643	GLU	2.2
1	D	557	GLU	2.2
1	B	27	VAL	2.2
1	D	548	GLN	2.2
1	C	675	LYS	2.2
1	D	265	GLY	2.2
1	D	666	LYS	2.2
1	D	268	VAL	2.2
1	D	558	HIS	2.2
1	C	363	THR	2.2
1	C	21	GLU	2.2
1	D	652	VAL	2.2
1	C	78	ALA	2.2
1	B	161	GLN	2.2
1	B	345	LEU	2.2
1	C	264	GLY	2.2
1	A	351	ASP	2.2
1	B	322	ALA	2.1
1	B	321	ILE	2.1
1	B	641	SER	2.1
1	B	652	VAL	2.1
1	D	72	VAL	2.1
1	C	88	ASN	2.1
1	B	642	GLY	2.1
1	B	672	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	359	THR	2.1
1	A	312	SER	2.1
1	C	344	ASP	2.1
1	B	390	VAL	2.1
1	B	525	TRP	2.1
1	D	654	ALA	2.1
1	C	69	TYR	2.1
1	A	85	ASN	2.1
1	C	30	LEU	2.1
1	B	343	GLY	2.1
1	D	399	GLY	2.1
1	C	101	GLU	2.1
1	A	15	ILE	2.1
1	C	312	SER	2.1
1	C	11	VAL	2.0
1	D	286	VAL	2.0
1	A	16	LEU	2.0
1	B	317	LEU	2.0
1	B	362	ASN	2.0
1	B	381	GLU	2.0
1	B	344	ASP	2.0
1	A	50	MET	2.0
1	B	649	SER	2.0
1	D	671	GLU	2.0
1	C	265	GLY	2.0
1	D	507	GLY	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

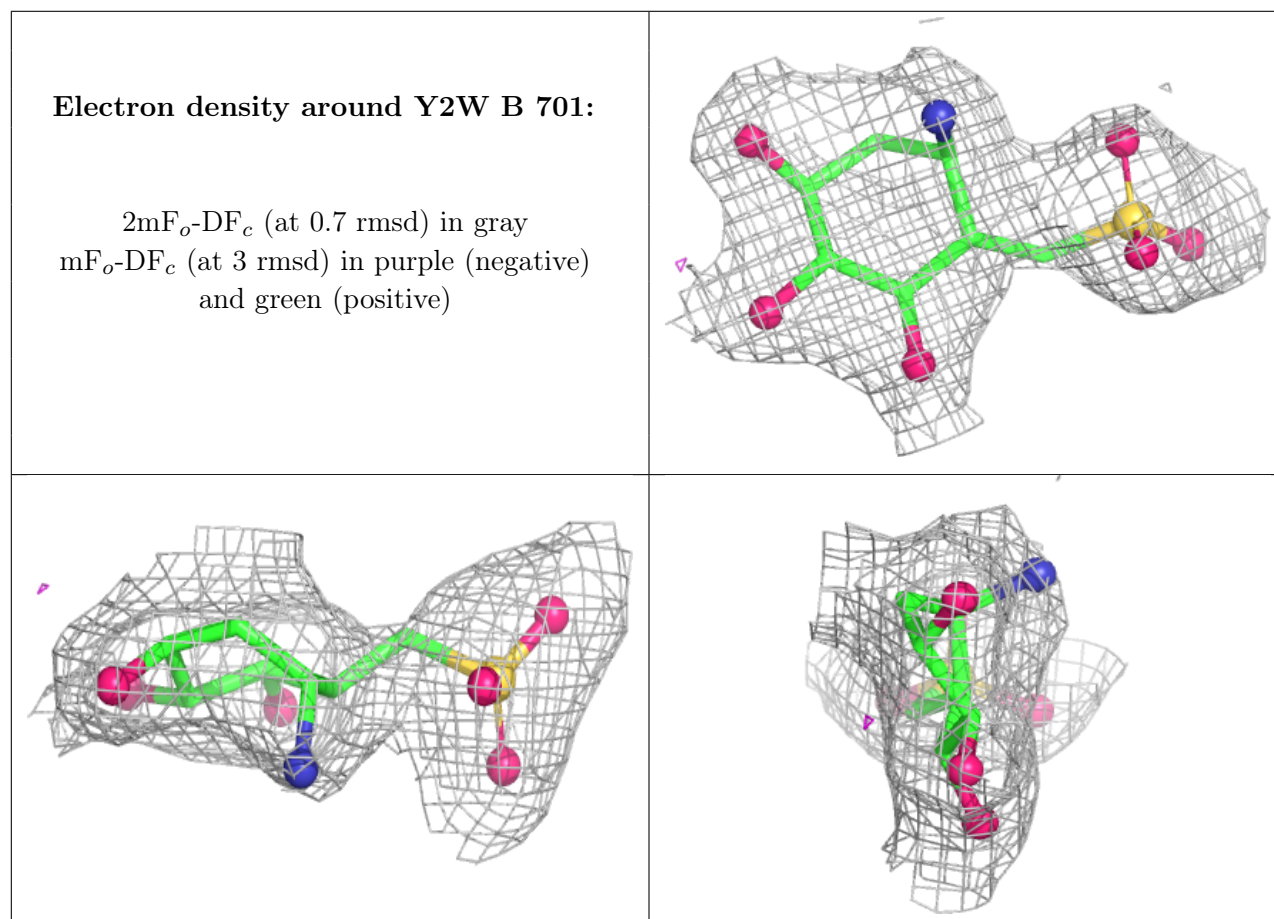
There are no oligosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

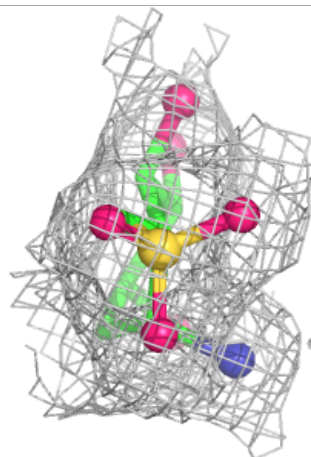
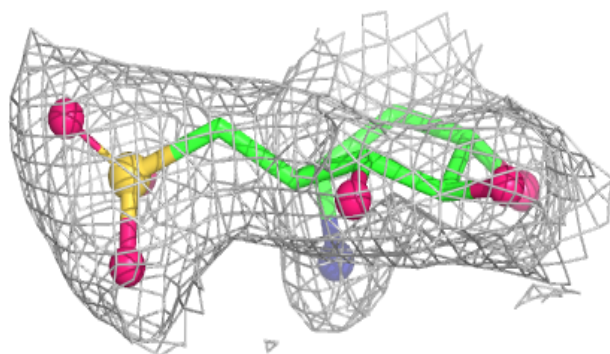
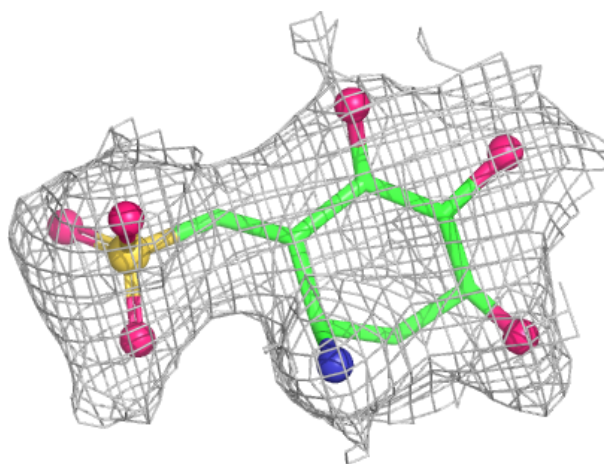
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	B	702	1/1	0.82	0.10	44,44,44,44	0
3	K	A	702	1/1	0.86	0.09	48,48,48,48	0
3	K	D	702	1/1	0.91	0.10	44,44,44,44	0
2	Y2W	B	701	15/15	0.92	0.10	23,26,34,34	0
3	K	C	702	1/1	0.93	0.06	33,33,33,33	0
2	Y2W	C	701	15/15	0.94	0.10	18,21,23,23	0
2	Y2W	D	701	15/15	0.94	0.09	22,29,33,39	0
2	Y2W	A	701	15/15	0.96	0.08	15,19,22,23	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.



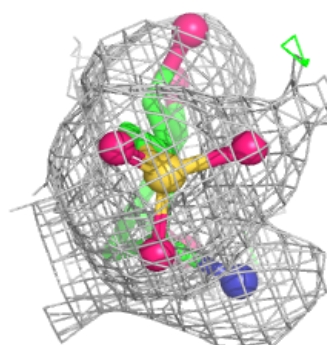
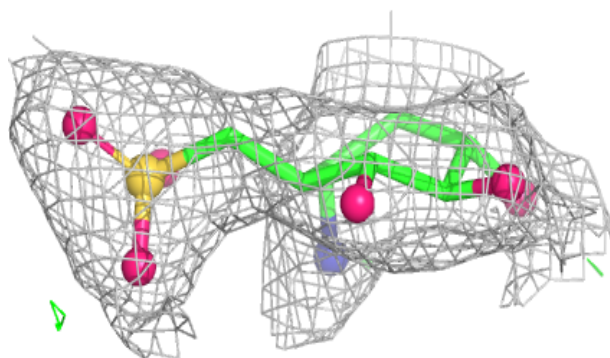
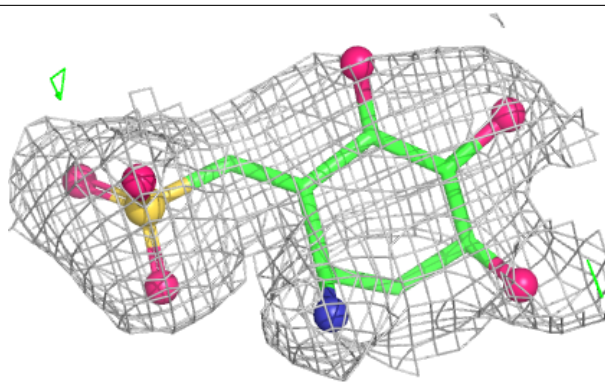
Electron density around Y2W C 701:

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

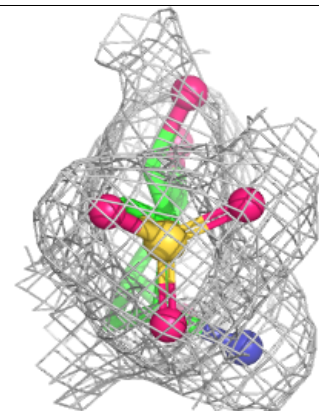
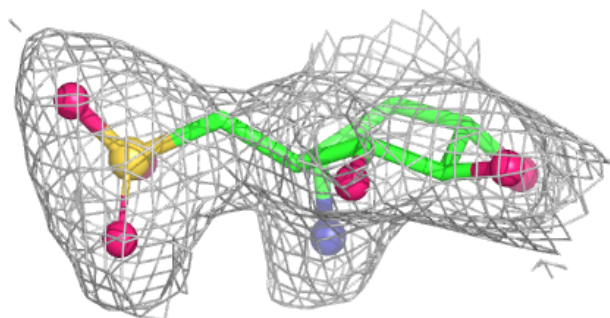
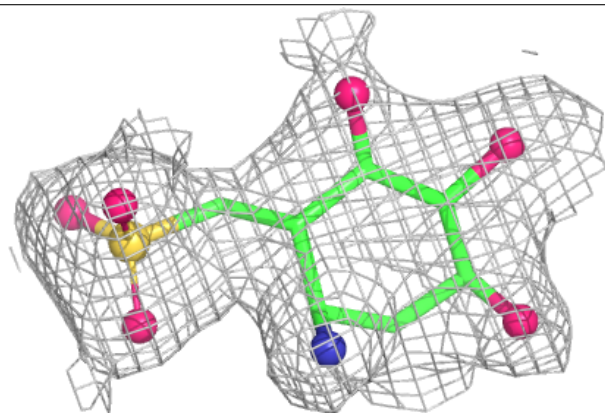


Electron density around Y2W D 701:

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

**Electron density around Y2W 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.