



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:32 AM UTC

PDB ID : 4MQ6 / pdb_00004mq6
Title : Pantothenate synthase in complex with 2-(5-methoxy-2-(tosylcarbamoyl)-1H-indol-1-yl)acetic acid
Authors : Silvestre, H.L.; Blundell, T.L.
Deposited on : 2013-09-15
Resolution : 1.70 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

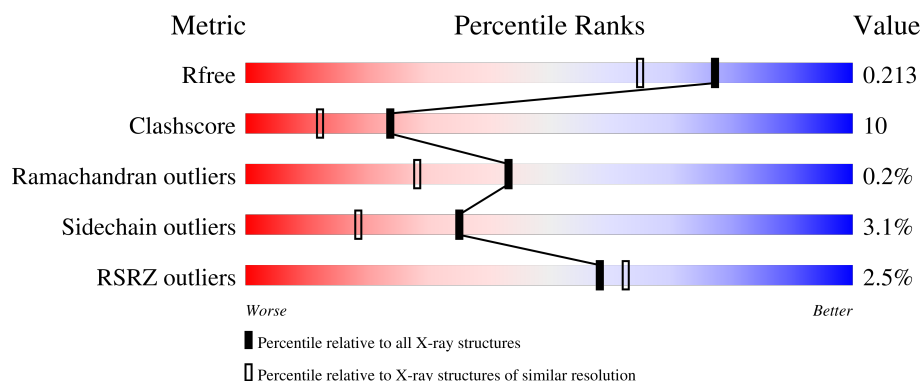
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	309	2% 73% 18% • 6%
1	B	309	2% 76% 11% • 12%

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
2	EOH	A	401	-	-	X	-
2	EOH	A	403	-	-	X	-
2	EOH	A	408	-	-	X	-
2	EOH	A	409	-	-	X	-
2	EOH	A	410	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4831 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.

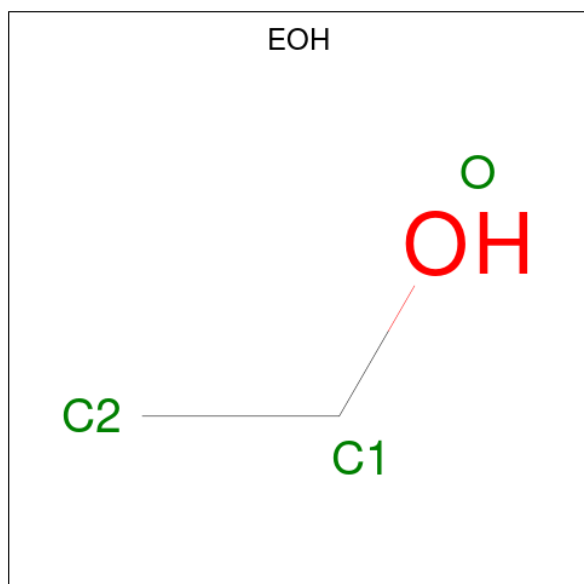
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	7	0
			2173	1371	389	407	6			
1	B	273	Total	C	N	O	S	0	7	0
			2054	1301	368	379	6			

There are 4 discrepancies between the modelled and reference sequences:

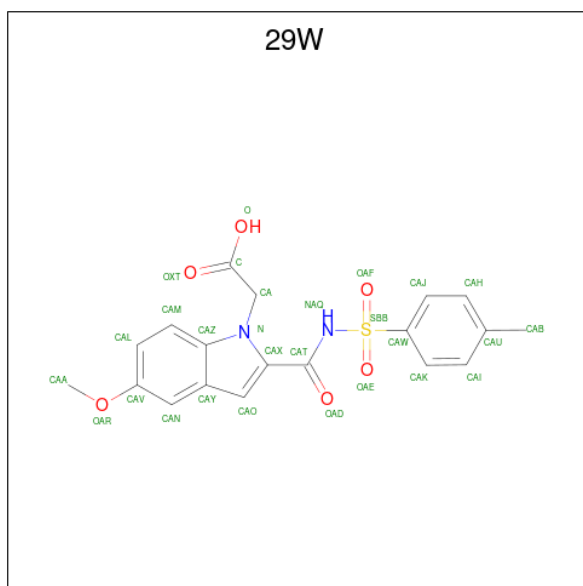
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
B	2	ALA	THR	engineered mutation	UNP P0A5R0
B	77	GLY	GLU	engineered mutation	UNP P0A5R0

- Molecule 2 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0
2	A	1	Total C O 3 2 1	0	0

- Molecule 3 is (5-methoxy-2-{[(4-methylphenyl)sulfonyl]carbamoyl}-1H-indol-1-yl)acetic acid (CCD ID: 29W) (formula: C₁₉H₁₈N₂O₆S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 28 19 2 6 1	0	0
3	A	1	Total C N O S 28 19 2 6 1	0	0
3	B	1	Total C N O S 28 19 2 6 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

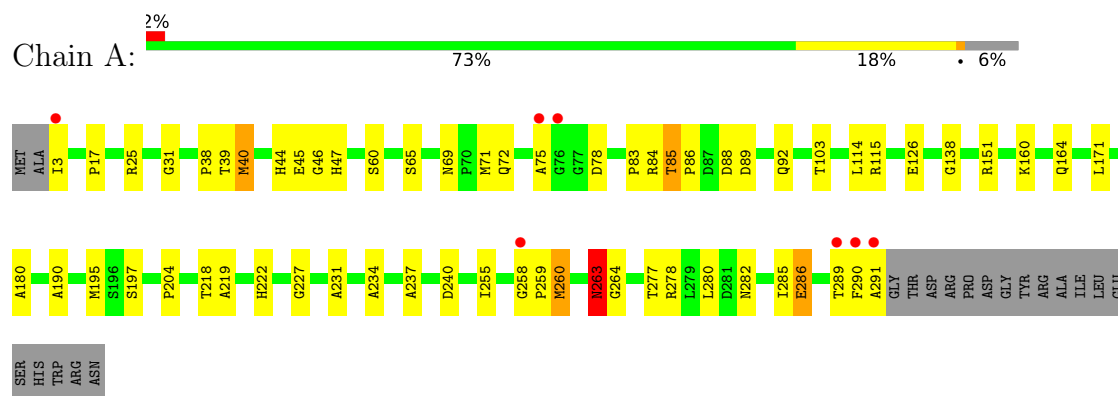
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	253	Total	O	0	0
			253	253		
5	B	227	Total	O	0	0
			227	227		

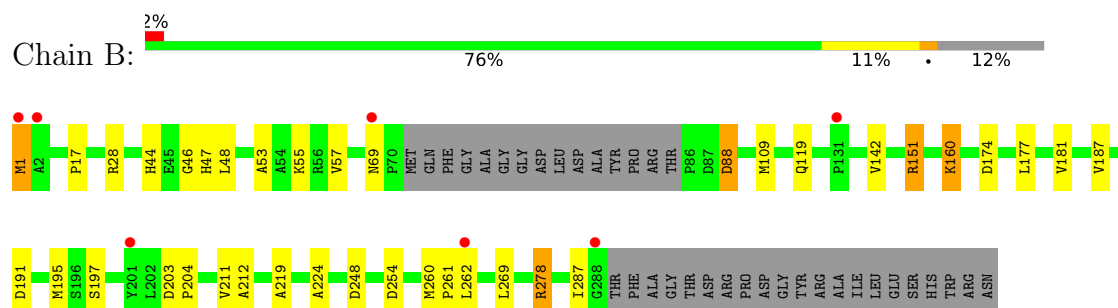
3 Residue-property plots

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: Pantothenate synthetase



• Molecule 1: Pantothenate synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.54Å 70.90Å 81.61Å 90.00° 99.36° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70 25.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-1.70) 99.9 (25.00-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.213 0.166 , 0.213	Depositor DCC
R_{free} test set	3033 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4831	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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: EDO, 29W, EOH

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	1.57	21/2212 (0.9%)	1.31	10/3022 (0.3%)
1	B	1.49	9/2094 (0.4%)	1.24	6/2859 (0.2%)
All	All	1.53	30/4306 (0.7%)	1.28	16/5881 (0.3%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	ASN	CA-C	9.85	1.59	1.53
1	A	227	GLY	N-CA	7.74	1.52	1.45
1	A	258	GLY	N-CA	7.39	1.54	1.44
1	A	237	ALA	CA-CB	7.31	1.64	1.53
1	B	151	ARG	CA-CB	7.21	1.58	1.52
1	B	181	VAL	N-CA	6.45	1.54	1.46
1	A	60	SER	C-O	6.31	1.31	1.23
1	A	85	THR	CA-CB	6.27	1.60	1.53
1	A	138	GLY	C-O	6.19	1.31	1.23
1	A	39	THR	N-CA	5.85	1.53	1.45
1	A	164	GLN	N-CA	-5.79	1.39	1.46
1	B	53	ALA	CA-CB	5.48	1.61	1.53
1	A	234	ALA	CA-C	5.41	1.59	1.52
1	A	103	THR	CA-CB	5.41	1.60	1.53
1	A	219	ALA	C-O	5.39	1.30	1.24
1	B	48	LEU	C-O	5.28	1.30	1.24
1	A	190	ALA	CA-CB	5.27	1.61	1.53
1	A	231	ALA	N-CA	5.27	1.52	1.46
1	A	240	ASP	N-CA	5.20	1.52	1.46
1	B	181	VAL	CA-CB	-5.19	1.48	1.54
1	B	109	MET	C-O	5.19	1.30	1.24
1	A	180	ALA	CA-CB	-5.17	1.46	1.53
1	B	269	LEU	C-O	-5.15	1.17	1.24
1	B	212	ALA	N-CA	5.12	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	ASP	N-CA	5.12	1.52	1.46
1	A	282	ASN	N-CA	5.10	1.51	1.46
1	A	126	GLU	CA-CB	-5.09	1.46	1.53
1	A	227	GLY	C-O	5.06	1.29	1.23
1	B	224	ALA	N-CA	5.03	1.52	1.46
1	A	277	THR	CA-CB	-5.01	1.46	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ASN	CA-C-O	6.62	121.78	117.94
1	B	197	SER	N-CA-C	-6.28	104.88	112.54
1	A	263	ASN	N-CA-C	6.11	113.79	108.78
1	A	278	ARG	NE-CZ-NH1	-5.82	115.69	121.50
1	B	219	ALA	N-CA-C	-5.75	104.92	111.07
1	A	126	GLU	CA-CB-CG	-5.69	102.72	114.10
1	B	57	VAL	CA-C-N	-5.57	114.02	119.76
1	B	57	VAL	C-N-CA	-5.57	114.02	119.76
1	A	40	MET	N-CA-C	-5.49	105.89	112.59
1	A	31	GLY	N-CA-C	5.35	122.17	115.21
1	A	85	THR	CA-C-N	5.29	125.10	119.28
1	A	85	THR	C-N-CA	5.29	125.10	119.28
1	B	278	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	285	ILE	CB-CA-C	-5.18	102.77	110.33
1	B	262	LEU	N-CA-C	5.07	117.46	111.33
1	A	171	LEU	N-CA-C	-5.01	105.71	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	2173	0	2198	42	0
1	B	2054	0	2113	39	0
2	A	24	0	48	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	56	0	34	7	0
3	B	28	0	17	3	0
4	A	4	0	6	1	0
4	B	12	0	18	0	0
5	A	253	0	0	13	0
5	B	227	0	0	7	0
All	All	4831	0	4434	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (89) 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:151:ARG:NH2	1:B:151:ARG:HH22	1.28	1.30
3:A:404:29W:H17	5:A:730:HOH:O	1.32	1.21
1:A:151:ARG:NH2	1:B:151:ARG:NH2	1.90	1.17
1:A:263:ASN:CG	1:A:264:GLY:H	1.56	1.12
1:A:83:PRO:HA	2:A:408:EOH:H22	1.31	1.08
1:A:263:ASN:OD1	1:A:264:GLY:N	1.97	0.96
1:A:291:ALA:HB1	5:A:657:HOH:O	1.65	0.95
1:A:151:ARG:CZ	1:B:151:ARG:NH2	2.34	0.91
1:A:25:ARG:HG3	1:A:25:ARG:HH21	1.39	0.88
2:A:401:EOH:H22	5:B:506:HOH:O	1.74	0.85
1:B:44:HIS:HE1	3:B:401:29W:OXT	1.61	0.84
1:A:151:ARG:CZ	1:B:151:ARG:HH22	1.90	0.84
2:A:408:EOH:C1	5:A:611:HOH:O	2.24	0.83
3:A:405:29W:H11	3:A:405:29W:CA	1.93	0.82
1:A:263:ASN:CG	1:A:264:GLY:N	2.32	0.81
2:A:408:EOH:H12	5:A:611:HOH:O	1.79	0.80
1:B:44:HIS:HD2	1:B:46:GLY:H	1.28	0.79
3:A:405:29W:H11	3:A:405:29W:H3	1.47	0.79
1:A:40:MET:SD	2:A:410:EOH:H23	2.26	0.75
1:A:72:GLN:NE2	2:A:410:EOH:H21	2.03	0.73
1:A:44:HIS:HD2	1:A:46:GLY:H	1.35	0.72
1:A:83:PRO:CA	2:A:408:EOH:H22	2.17	0.70
1:B:254:ASP:HB3	1:B:261:PRO:HD3	1.74	0.70
1:A:69:ASN:HD22	1:A:72:GLN:HE21	1.37	0.70
1:A:72:GLN:HE22	2:A:410:EOH:H21	1.56	0.69
1:B:160:LYS:HE3	5:B:617:HOH:O	1.92	0.68
1:A:84:ARG:H	2:A:408:EOH:H11	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:HIS:HD2	1:B:46:GLY:N	1.93	0.67
1:B:187:VAL:HG12	1:B:195:MET:HG3	1.78	0.65
1:A:151:ARG:HH21	1:B:151:ARG:HH22	1.41	0.65
1:A:88[B]:ASP:O	1:A:92:GLN:HG3	1.96	0.65
1:A:151:ARG:HH22	1:B:151:ARG:NH2	1.95	0.64
1:A:44:HIS:HE1	3:A:404:29W:O	1.80	0.64
2:A:410:EOH:H22	5:A:585:HOH:O	1.99	0.63
1:A:25:ARG:HG3	1:A:25:ARG:NH2	2.04	0.63
1:A:44:HIS:HD2	1:A:46:GLY:N	1.97	0.63
1:B:248:ASP:HB3	5:B:721:HOH:O	2.01	0.60
1:B:28:ARG:HD3	5:B:668:HOH:O	2.02	0.59
1:B:1:MET:HA	1:B:1:MET:CE	2.33	0.59
1:A:71:MET:HG3	1:A:114:LEU:HD13	1.84	0.58
1:B:1:MET:HA	1:B:1:MET:HE3	1.86	0.57
1:A:259:PRO:HD2	1:A:260:MET:HE2	1.87	0.57
2:A:408:EOH:H11	5:A:611:HOH:O	1.96	0.56
1:B:47:HIS:HE2	3:B:401:29W:H11	1.52	0.56
1:B:278:ARG:HG2	1:B:278:ARG:NH1	2.23	0.54
1:A:84:ARG:H	2:A:408:EOH:C1	2.20	0.54
1:A:218[B]:THR:O	1:A:222:HIS:HD2	1.92	0.53
1:A:286:GLU:O	1:A:291:ALA:HB2	2.08	0.53
1:B:88:ASP:OD1	1:B:88:ASP:N	2.40	0.52
1:A:40:MET:CG	2:A:410:EOH:H23	2.40	0.52
3:A:405:29W:OAF	1:B:119:GLN:NE2	2.43	0.52
1:A:85:THR:N	1:A:86:PRO:HD3	2.26	0.51
1:A:45:GLU:HB3	1:A:195:MET:HE3	1.92	0.51
1:B:278:ARG:HG2	1:B:278:ARG:HH11	1.76	0.50
1:A:160[A]:LYS:HE3	1:A:280:LEU:HB2	1.92	0.50
1:A:40:MET:SD	2:A:410:EOH:C2	2.99	0.50
1:A:92:GLN:HG2	5:A:731:HOH:O	2.13	0.49
1:B:55:LYS:HD3	5:B:530:HOH:O	2.12	0.48
1:A:47:HIS:HE2	3:A:404:29W:H11	1.60	0.47
1:B:44:HIS:CE1	3:B:401:29W:OXT	2.53	0.47
1:A:286:GLU:HB3	1:A:290:PHE:CB	2.44	0.47
2:A:403:EOH:H22	5:A:620:HOH:O	2.14	0.46
2:A:409:EOH:H23	1:B:177:LEU:HB3	1.98	0.46
1:B:69:ASN:OD1	1:B:142[B]:VAL:HG21	2.15	0.46
1:A:92:GLN:NE2	5:A:702:HOH:O	2.46	0.46
1:B:260:MET:HE2	1:B:287:ILE:CG1	2.47	0.45
1:B:203:ASP:OD1	1:B:203:ASP:C	2.60	0.45
1:B:260:MET:HE2	1:B:287:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:409:EOH:C2	5:B:540:HOH:O	2.64	0.44
1:A:115:ARG:O	2:A:401:EOH:H23	2.18	0.44
2:A:408:EOH:O	5:A:587:HOH:O	2.21	0.44
4:A:406:EDO:H11	1:B:174:ASP:HB3	1.99	0.44
2:A:408:EOH:H23	5:A:664:HOH:O	2.17	0.44
3:A:405:29W:H3	3:A:405:29W:NAQ	2.25	0.44
1:B:195:MET:HE3	1:B:195:MET:HB3	1.81	0.43
1:B:260:MET:SD	1:B:261:PRO:HD2	2.58	0.43
1:B:69:ASN:CG	1:B:142[B]:VAL:HG21	2.44	0.43
1:B:160:LYS:HG3	5:B:711:HOH:O	2.18	0.42
1:A:78:ASP:HB2	5:A:533:HOH:O	2.19	0.42
1:B:203:ASP:HB2	1:B:204:PRO:CD	2.49	0.42
1:A:25:ARG:NH1	1:A:151:ARG:HG3	2.33	0.42
1:B:44:HIS:CD2	1:B:46:GLY:H	2.19	0.41
1:B:55:LYS:HE3	1:B:55:LYS:HB3	1.72	0.41
2:A:401:EOH:H11	1:B:119:GLN:HE21	1.85	0.41
2:A:403:EOH:C2	5:A:620:HOH:O	2.68	0.41
1:A:38:PRO:HA	1:A:65:SER:OG	2.21	0.41
1:B:191:ASP:OD2	1:B:211[B]:VAL:HG22	2.20	0.41
1:A:84:ARG:H	2:A:408:EOH:C2	2.34	0.40
1:B:191:ASP:OD2	1:B:211[B]:VAL:CG2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/309 (95%)	284 (97%)	8 (3%)	1 (0%)	36	22
1	B	276/309 (89%)	273 (99%)	3 (1%)	0	100	100
All	All	569/618 (92%)	557 (98%)	11 (2%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ALA

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	221/231 (96%)	211 (96%)	10 (4%)	24	9
1	B	210/231 (91%)	206 (98%)	4 (2%)	50	34
All	All	431/462 (93%)	417 (97%)	14 (3%)	35	17

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	17	PRO
1	A	197[A]	SER
1	A	197[B]	SER
1	A	204	PRO
1	A	255	ILE
1	A	260	MET
1	A	263	ASN
1	A	286	GLU
1	A	289	THR
1	B	1	MET
1	B	17	PRO
1	B	88	ASP
1	B	160	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	44	HIS

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Mol	Chain	Res	Type
1	A	72	GLN
1	A	164	GLN
1	A	222	HIS
1	B	44	HIS
1	B	119	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

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	EOH	A	402	-	2,2,2	0.67	0	1,1,1	0.67	0
3	29W	B	401	-	30,30,30	2.94	13 (43%)	43,44,44	2.69	16 (37%)
3	29W	A	404	-	30,30,30	3.98	12 (40%)	43,44,44	3.59	10 (23%)
2	EOH	A	407	-	2,2,2	0.48	0	1,1,1	0.13	0
3	29W	A	405	-	30,30,30	3.47	12 (40%)	43,44,44	1.79	10 (23%)
2	EOH	A	408	-	2,2,2	0.42	0	1,1,1	0.41	0
4	EDO	B	402	-	3,3,3	0.40	0	2,2,2	0.95	0
4	EDO	B	403	-	3,3,3	0.55	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	406	-	3,3,3	0.49	0	2,2,2	0.78	0
2	EOH	A	401	-	2,2,2	0.66	0	1,1,1	0.20	0
2	EOH	A	409	-	2,2,2	0.44	0	1,1,1	0.80	0
2	EOH	A	411	-	2,2,2	0.39	0	1,1,1	0.46	0
4	EDO	B	404	-	3,3,3	0.57	0	2,2,2	0.52	0
2	EOH	A	410	-	2,2,2	0.39	0	1,1,1	0.75	0
2	EOH	A	403	-	2,2,2	0.37	0	1,1,1	0.75	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	29W	B	401	-	-	4/21/21/21	0/3/3/3
3	29W	A	404	-	-	7/21/21/21	0/3/3/3
3	29W	A	405	-	-	3/21/21/21	0/3/3/3
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	B	402	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	B	404	-	-	1/1/1/1	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	29W	CAW-SBB	-13.83	1.55	1.76
3	A	405	29W	OAE-SBB	10.73	1.56	1.43
3	A	405	29W	OAF-SBB	8.99	1.53	1.43
3	A	404	29W	CAT-NAQ	-8.85	1.29	1.38
3	A	404	29W	OAF-SBB	8.84	1.53	1.43
3	B	401	29W	OAF-SBB	7.91	1.52	1.43
3	B	401	29W	CAW-SBB	-6.58	1.66	1.76
3	A	405	29W	CAX-CAT	-5.48	1.38	1.49
3	B	401	29W	CAX-CAT	-5.40	1.38	1.49
3	A	405	29W	CA-N	5.26	1.56	1.46
3	B	401	29W	CAT-NAQ	-5.12	1.33	1.38
3	A	404	29W	CAX-CAT	-5.07	1.39	1.49
3	A	405	29W	CA-C	4.74	1.60	1.51
3	A	404	29W	CAX-N	-3.95	1.34	1.39
3	B	401	29W	OAE-SBB	3.80	1.47	1.43
3	A	404	29W	CAB-CAU	-3.49	1.40	1.51
3	A	404	29W	CAH-CAJ	3.41	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	29W	SBB-NAQ	3.39	1.72	1.64
3	A	405	29W	CAB-CAU	-3.35	1.41	1.51
3	B	401	29W	CAN-CAY	-3.30	1.35	1.40
3	B	401	29W	SBB-NAQ	-3.21	1.56	1.64
3	B	401	29W	CAZ-N	-3.21	1.33	1.39
3	A	405	29W	CAY-CAZ	-3.14	1.36	1.41
3	B	401	29W	CA-N	3.13	1.52	1.46
3	A	405	29W	CAN-CAY	-3.07	1.35	1.40
3	A	404	29W	CAY-CAZ	-2.93	1.37	1.41
3	A	404	29W	CAN-CAV	2.76	1.43	1.39
3	A	405	29W	CAW-SBB	2.74	1.80	1.76
3	A	404	29W	CA-C	-2.62	1.46	1.51
3	B	401	29W	CAB-CAU	-2.46	1.43	1.51
3	A	404	29W	OAE-SBB	-2.36	1.40	1.43
3	A	405	29W	OXT-C	2.31	1.29	1.22
3	B	401	29W	CAY-CAZ	-2.25	1.38	1.41
3	B	401	29W	CAY-CAO	-2.18	1.37	1.44
3	A	405	29W	CAM-CAZ	-2.18	1.36	1.39
3	B	401	29W	CAH-CAJ	2.14	1.42	1.38
3	A	404	29W	O-C	-2.12	1.23	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	29W	OAF-SBB-OAE	-20.39	94.76	119.52
3	B	401	29W	OAF-SBB-OAE	-10.57	106.68	119.52
3	A	405	29W	OAE-SBB-CAW	-6.26	100.09	107.98
3	B	401	29W	OAF-SBB-NAQ	4.87	120.70	106.77
3	A	404	29W	OAE-SBB-CAW	4.73	113.94	107.98
3	B	401	29W	CAY-CAN-CAV	4.64	125.72	120.46
3	B	401	29W	OAE-SBB-CAW	4.43	113.57	107.98
3	A	404	29W	CAO-CAX-N	-4.40	106.94	109.42
3	A	404	29W	OAF-SBB-NAQ	4.30	119.08	106.77
3	B	401	29W	OAF-SBB-CAW	-4.20	102.68	107.98
3	A	405	29W	CA-N-CAZ	-3.56	119.74	125.18
3	A	404	29W	C-CA-N	3.28	121.58	113.08
3	B	401	29W	CAJ-CAW-SBB	-3.25	116.18	119.76
3	A	405	29W	CA-N-CAX	3.04	132.05	127.43
3	A	405	29W	CAJ-CAH-CAU	-3.02	117.89	121.37
3	A	405	29W	CAI-CAK-CAW	-3.02	116.50	119.44
3	B	401	29W	CAK-CAW-SBB	3.02	123.08	119.76
3	B	401	29W	CAN-CAY-CAZ	-3.01	116.50	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	29W	CAM-CAL-CAV	-2.86	116.47	119.73
3	B	401	29W	OAD-CAT-NAQ	-2.73	118.00	121.94
3	B	401	29W	CA-N-CAZ	-2.67	121.09	125.18
3	B	401	29W	CAA-OAR-CAV	2.65	123.18	117.50
3	A	404	29W	CAK-CAW-CAJ	2.63	123.89	120.47
3	B	401	29W	CAL-CAV-CAN	-2.57	117.05	120.50
3	A	404	29W	OAD-CAT-NAQ	-2.57	118.23	121.94
3	B	401	29W	CAZ-CAY-CAO	2.51	109.54	107.05
3	A	405	29W	CAJ-CAW-SBB	-2.48	117.03	119.76
3	A	405	29W	OAF-SBB-OAE	-2.43	116.57	119.52
3	B	401	29W	CAW-SBB-NAQ	2.43	109.94	106.06
3	A	405	29W	CAO-CAX-N	-2.41	108.06	109.42
3	A	404	29W	CAJ-CAW-SBB	-2.37	117.15	119.76
3	A	404	29W	OXT-C-CA	-2.28	112.85	122.38
3	A	405	29W	OAE-SBB-NAQ	2.18	113.01	106.77
3	B	401	29W	CAL-CAM-CAZ	2.17	123.46	119.10
3	A	405	29W	OAF-SBB-CAW	2.14	110.67	107.98
3	A	404	29W	OAD-CAT-CAX	2.12	124.94	120.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

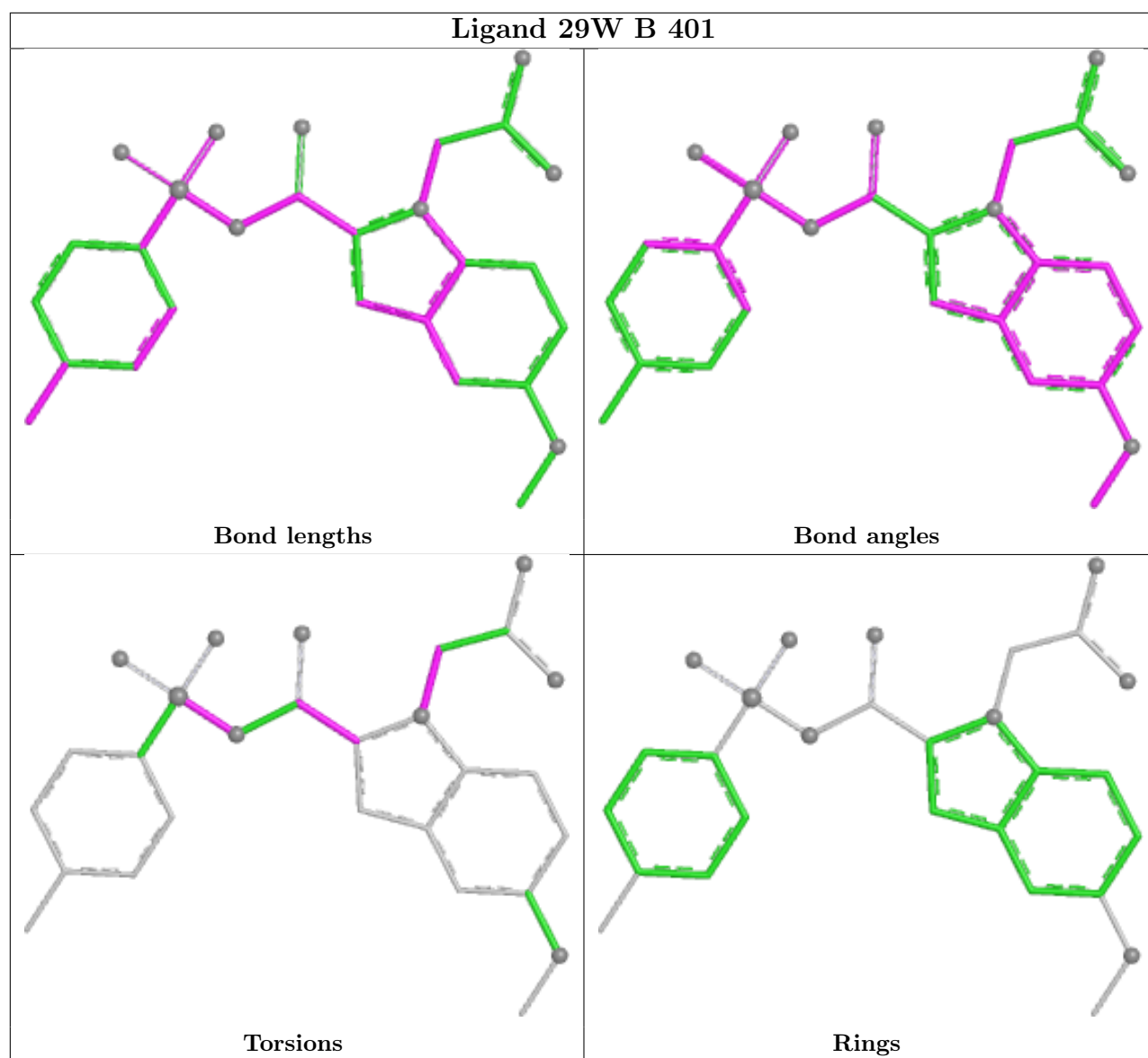
Mol	Chain	Res	Type	Atoms
3	A	404	29W	C-CA-N-CAZ
3	A	404	29W	CAT-NAQ-SBB-OAE
3	A	405	29W	OAD-CAT-CAX-N
3	A	405	29W	NAQ-CAT-CAX-N
3	B	401	29W	C-CA-N-CAZ
3	B	401	29W	C-CA-N-CAX
3	A	404	29W	CAN-CAV-OAR-CAA
3	B	401	29W	OAD-CAT-CAX-N
3	A	404	29W	CAL-CAV-OAR-CAA
4	B	404	EDO	O1-C1-C2-O2
3	A	404	29W	CAK-CAW-SBB-OAE
3	B	401	29W	CAT-NAQ-SBB-OAE
4	A	406	EDO	O1-C1-C2-O2
3	A	405	29W	NAQ-CAT-CAX-CAO
3	A	404	29W	CAJ-CAW-SBB-OAE
4	B	403	EDO	O1-C1-C2-O2
3	A	404	29W	CAT-NAQ-SBB-CAW
4	B	402	EDO	O1-C1-C2-O2

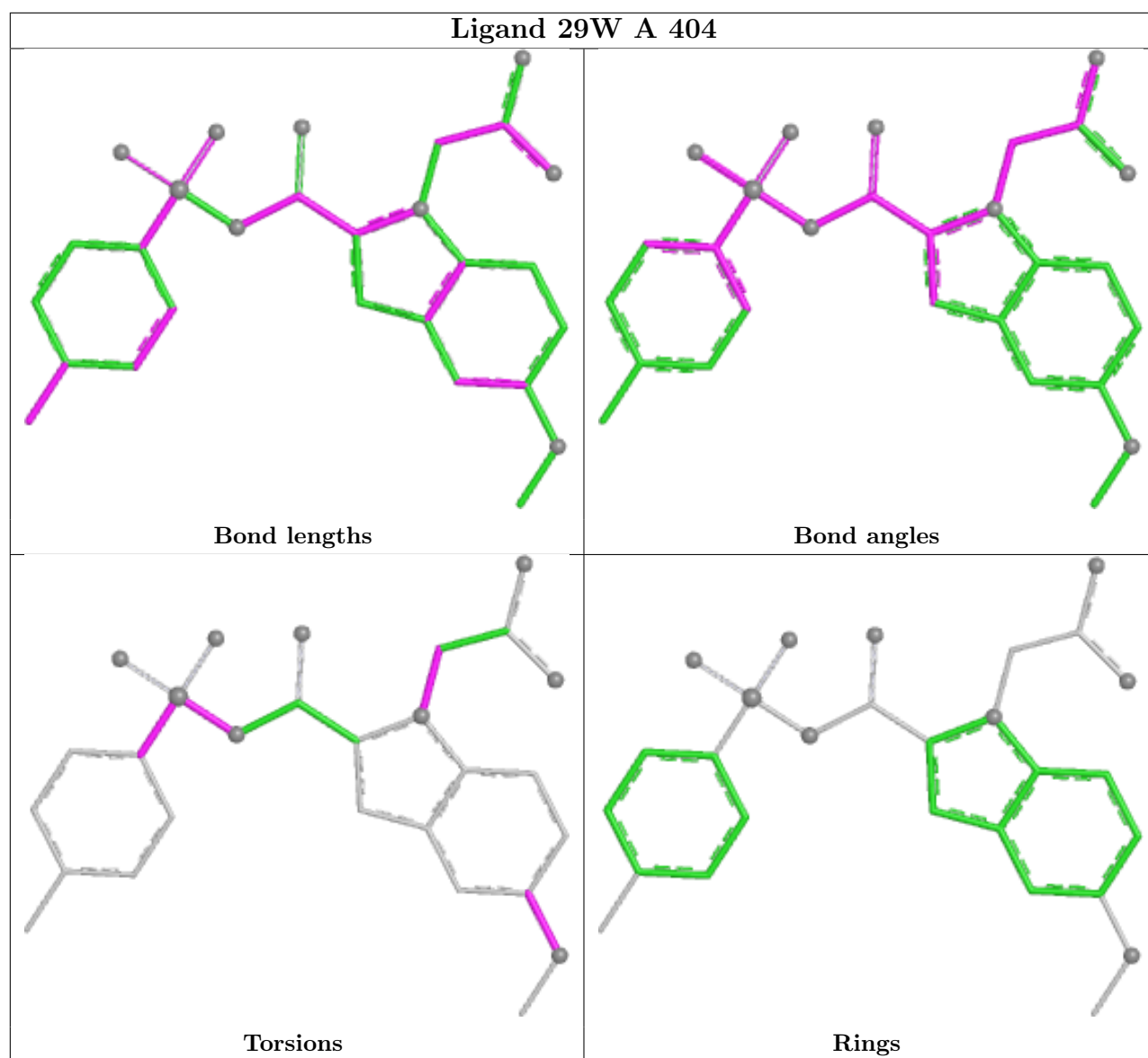
There are no ring outliers.

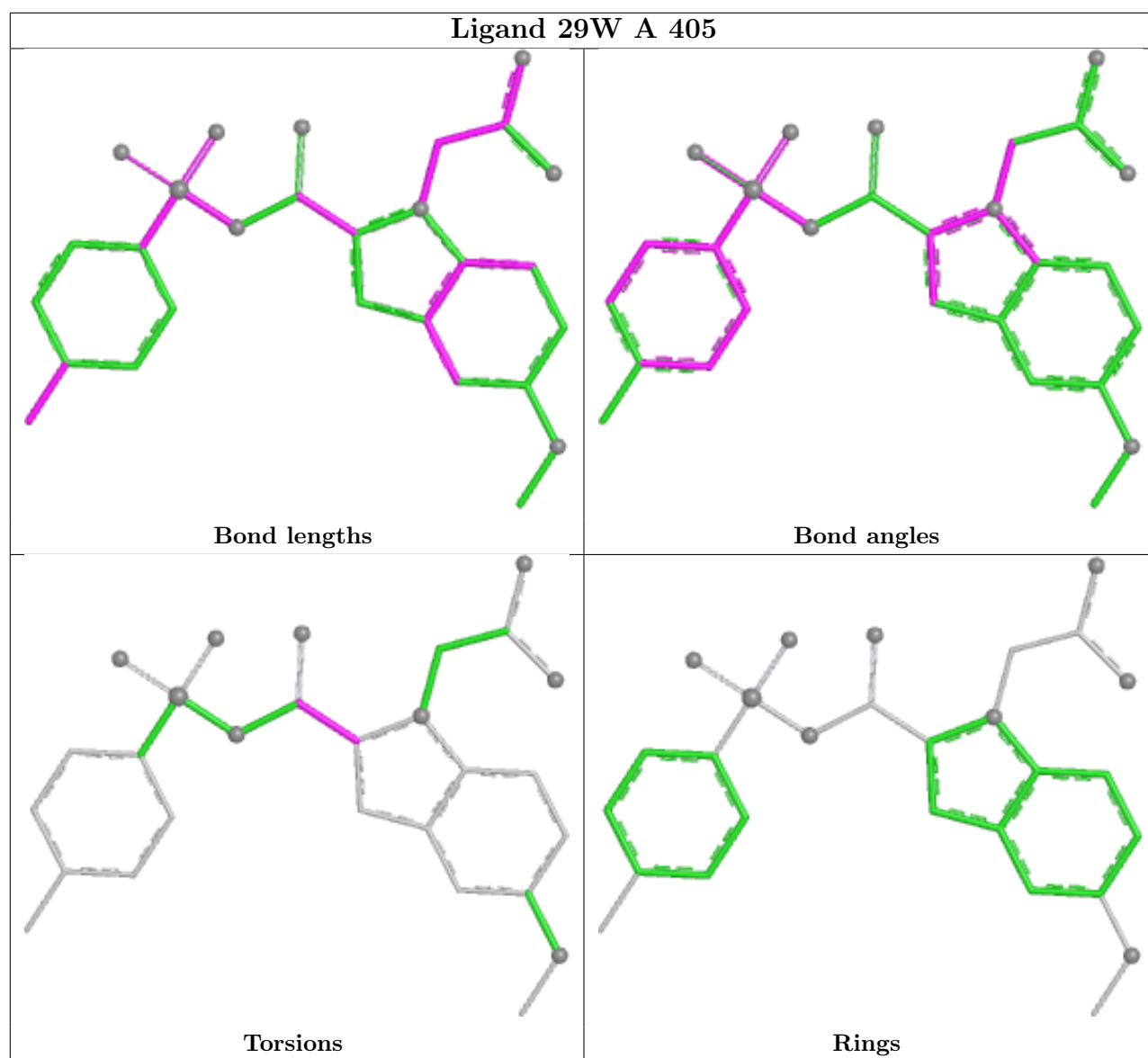
9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	29W	3	0
3	A	404	29W	3	0
3	A	405	29W	4	0
2	A	408	EOH	10	0
4	A	406	EDO	1	0
2	A	401	EOH	3	0
2	A	409	EOH	2	0
2	A	410	EOH	6	0
2	A	403	EOH	2	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.







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	289/309 (93%)	-0.23	7 (2%) 59 64	7, 21, 41, 56	8 (2%)
1	B	273/309 (88%)	-0.23	7 (2%) 57 61	7, 21, 43, 60	8 (2%)
All	All	562/618 (90%)	-0.23	14 (2%) 58 62	7, 21, 42, 60	16 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	ALA	3.2
1	A	258	GLY	3.1
1	A	3	ILE	3.1
1	A	290	PHE	3.0
1	A	291	ALA	2.8
1	B	1	MET	2.8
1	A	76	GLY	2.8
1	B	288	GLY	2.7
1	B	201	TYR	2.6
1	A	289	THR	2.6
1	B	69	ASN	2.6
1	B	262	LEU	2.3
1	B	2	ALA	2.2
1	B	131	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

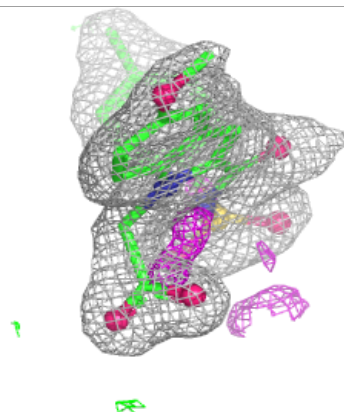
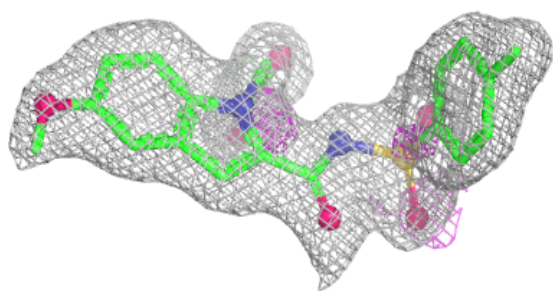
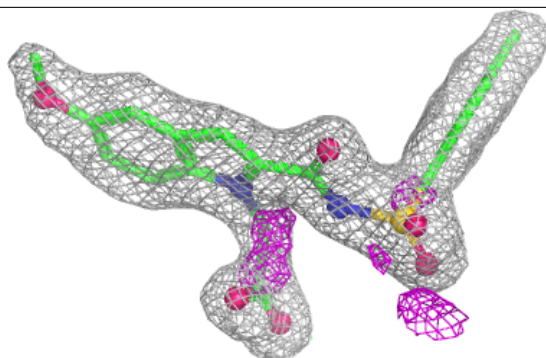
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EOH	A	402	3/3	0.72	0.18	38,38,38,40	0
2	EOH	A	401	3/3	0.85	0.14	29,29,33,33	0
2	EOH	A	403	3/3	0.85	0.14	45,45,46,46	0
2	EOH	A	409	3/3	0.89	0.10	35,35,37,38	0
2	EOH	A	411	3/3	0.90	0.12	40,40,41,42	0
2	EOH	A	410	3/3	0.91	0.12	31,31,35,37	0
3	29W	A	405	28/28	0.91	0.09	28,36,43,44	0
2	EOH	A	408	3/3	0.92	0.11	37,37,37,38	0
4	EDO	B	404	4/4	0.93	0.07	38,38,40,42	0
4	EDO	B	403	4/4	0.94	0.08	34,34,36,38	0
2	EOH	A	407	3/3	0.94	0.08	41,41,41,42	0
4	EDO	A	406	4/4	0.95	0.07	26,27,31,31	0
4	EDO	B	402	4/4	0.97	0.06	22,24,27,29	0
3	29W	B	401	28/28	0.97	0.06	17,22,31,32	0
3	29W	A	404	28/28	0.97	0.06	16,22,29,32	0

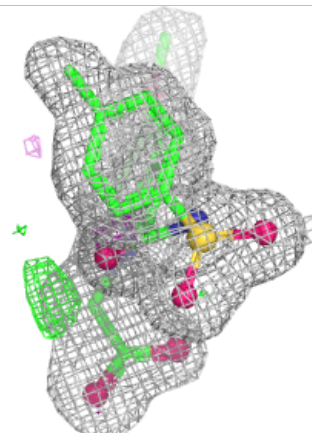
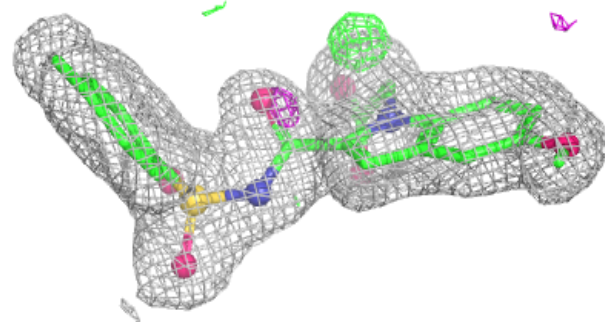
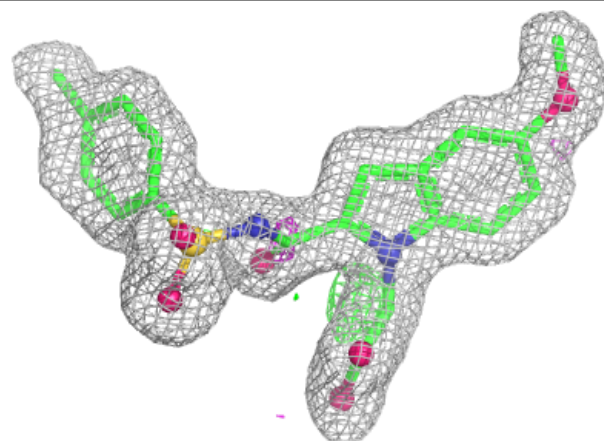
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

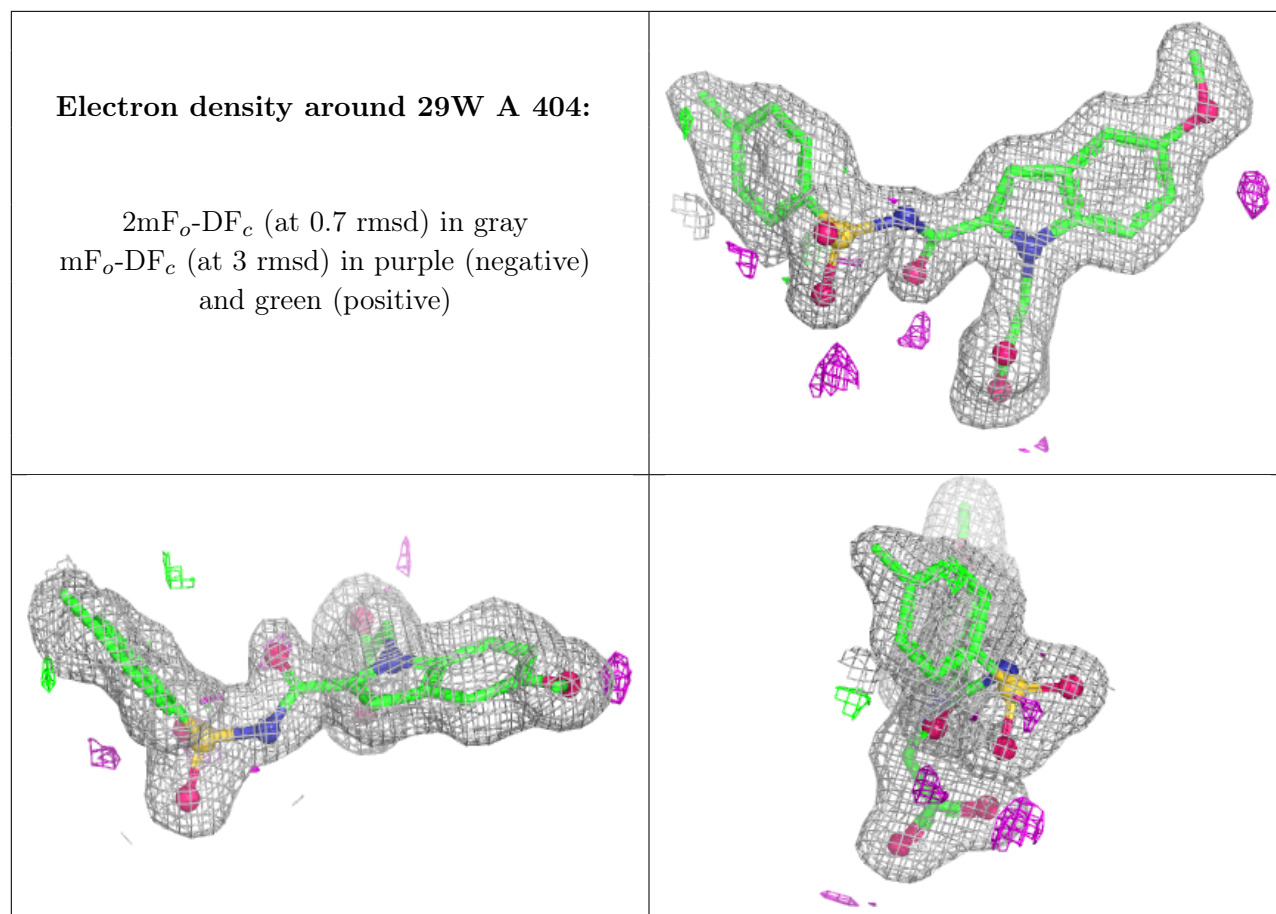
Electron density around 29W A 405:

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

**Electron density around 29W B 401:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.