



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:47 AM UTC

PDB ID : 3JRQ / pdb_00003jrq
Title : Crystal structure of (+)-ABA-bound PYL1 in complex with ABI1
Authors : Miyazono, K.; Miyakawa, T.; Sawano, Y.; Kubota, K.; Tanokura, M.
Deposited on : 2009-09-08
Resolution : 2.10 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

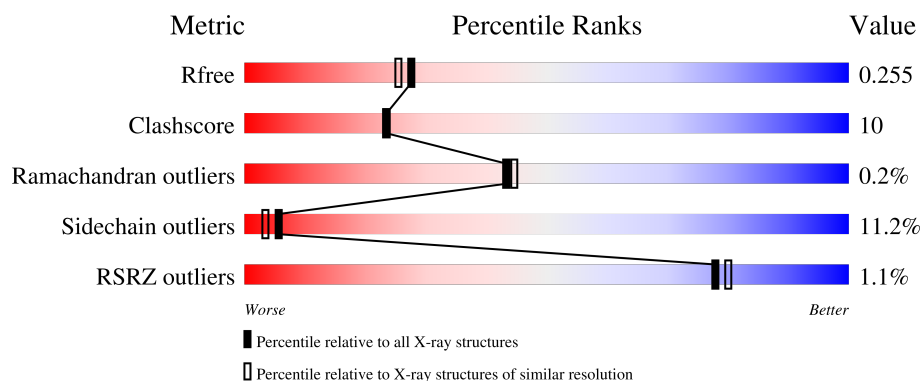
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	326	59% 19% . 17%
2	B	186	66% 21% 6% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3619 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 Protein phosphatase 2C 56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2091	1317	366	394	14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	expression tag	UNP P49597
A	105	GLY	-	expression tag	UNP P49597
A	106	SER	-	expression tag	UNP P49597
A	107	SER	-	expression tag	UNP P49597
A	108	HIS	-	expression tag	UNP P49597
A	109	HIS	-	expression tag	UNP P49597
A	110	HIS	-	expression tag	UNP P49597
A	111	HIS	-	expression tag	UNP P49597
A	112	HIS	-	expression tag	UNP P49597
A	113	HIS	-	expression tag	UNP P49597
A	114	SER	-	expression tag	UNP P49597
A	115	SER	-	expression tag	UNP P49597
A	116	GLY	-	expression tag	UNP P49597
A	117	LEU	-	expression tag	UNP P49597
A	118	VAL	-	expression tag	UNP P49597
A	119	PRO	-	expression tag	UNP P49597
A	120	ARG	-	expression tag	UNP P49597
A	121	GLY	-	expression tag	UNP P49597
A	122	SER	-	expression tag	UNP P49597
A	123	HIS	-	expression tag	UNP P49597
A	124	MET	-	expression tag	UNP P49597

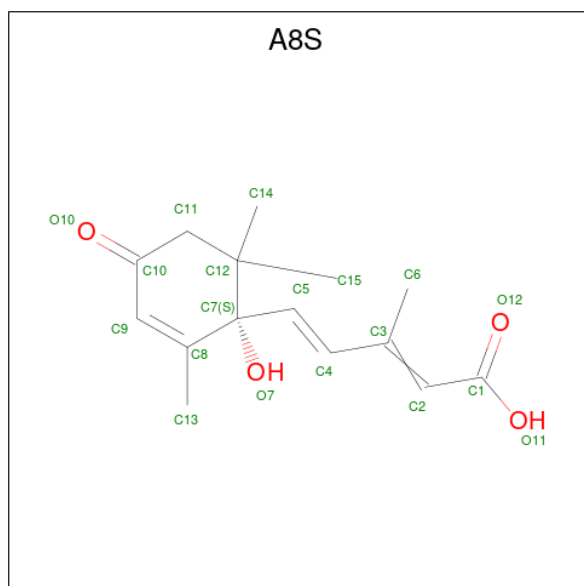
- Molecule 2 is a protein called Putative uncharacterized protein At5g46790.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1402	871	258	268	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	GLY	-	expression tag	UNP Q8VZS8
B	26	SER	-	expression tag	UNP Q8VZS8
B	27	HIS	-	expression tag	UNP Q8VZS8

- Molecule 3 is (2Z,4E)-5-[(1S)-1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl]-3-methylpenta-2,4-dienoic acid (CCD ID: A8S) (formula: C₁₅H₂₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			19	15	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	61	Total	O	0	0
			61	61		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.01Å 60.62Å 84.96Å 90.00° 104.56° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.10) 93.4 (20.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.11Å)	Xtriage
Refinement program	REFMAC refmac _5.5.0088	Depositor
R, R_{free}	0.198 , 0.249 0.203 , 0.255	Depositor DCC
R_{free} test set	1325 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3619	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: A8S

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	1.17	3/2131 (0.1%)	1.24	8/2880 (0.3%)
2	B	1.55	11/1426 (0.8%)	1.43	6/1929 (0.3%)
All	All	1.33	14/3557 (0.4%)	1.32	14/4809 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	ARG	N-CA	8.94	1.57	1.46
2	B	202	ALA	N-CA	7.92	1.55	1.46
2	B	111	ILE	CA-CB	6.67	1.60	1.54
2	B	73	TRP	C-O	6.46	1.31	1.24
2	B	132	VAL	N-CA	-6.42	1.38	1.46
2	B	196	LEU	C-O	-5.99	1.17	1.24
2	B	190	ALA	CA-CB	-5.93	1.44	1.53
1	A	407	ILE	CA-CB	5.81	1.60	1.54
2	B	204	ILE	CA-CB	5.74	1.61	1.54
2	B	105	THR	N-CA	-5.49	1.39	1.45
2	B	40	LEU	N-CA	5.41	1.53	1.46
2	B	101	ARG	C-O	5.41	1.30	1.23
1	A	187	TYR	CA-C	5.10	1.59	1.52
1	A	236	ALA	CA-CB	5.00	1.59	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	87	HIS	N-CA-C	14.48	127.06	111.28
1	A	281	PRO	CA-C-N	7.00	130.37	120.28
1	A	281	PRO	C-N-CA	7.00	130.37	120.28
1	A	250	PHE	CA-C-N	-6.74	112.69	119.56
1	A	250	PHE	C-N-CA	-6.74	112.69	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	186	THR	N-CA-C	-6.34	104.44	111.36
1	A	137	ARG	N-CA-C	5.60	118.23	111.40
1	A	237	PRO	CA-C-N	5.56	128.50	120.38
1	A	237	PRO	C-N-CA	5.56	128.50	120.38
2	B	120	ARG	N-CA-C	-5.39	100.23	109.24
2	B	85	TYR	CA-C-N	-5.23	114.82	122.19
2	B	85	TYR	C-N-CA	-5.23	114.82	122.19
1	A	324	ILE	CB-CA-C	5.14	117.83	110.84
2	B	38	THR	N-CA-C	5.00	116.73	111.28

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	2091	0	2080	46	0
2	B	1402	0	1376	26	0
3	B	19	0	19	2	0
4	A	46	0	0	2	0
4	B	61	0	0	5	0
All	All	3619	0	3475	71	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 (71) 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)
2:B:205:THR:HA	2:B:208:MET:HE2	1.40	1.03
2:B:145:ARG:HH21	2:B:145:ARG:HG3	1.41	0.85
2:B:71:THR:CG2	2:B:208:MET:HE3	2.18	0.73
2:B:208:MET:HB3	2:B:209:ASN:HA	1.70	0.73
2:B:145:ARG:HG3	2:B:145:ARG:NH2	2.07	0.69
1:A:232:ILE:HD11	1:A:316:GLY:HA2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HH12	2:B:113:GLY:H	1.46	0.63
2:B:165:ILE:HD13	4:B:231:HOH:O	1.99	0.62
2:B:155:ARG:NH2	2:B:157:GLU:OE2	2.34	0.60
1:A:420:VAL:HG22	1:A:422:LEU:HD13	1.83	0.59
2:B:71:THR:HG22	2:B:208:MET:HE3	1.82	0.59
2:B:85:TYR:O	2:B:200:LYS:HD3	2.02	0.59
1:A:232:ILE:C	1:A:232:ILE:HD12	2.27	0.59
1:A:125:SER:N	1:A:150:ARG:HH21	2.02	0.58
1:A:150:ARG:H	1:A:171:HIS:HD2	1.52	0.58
1:A:199:GLU:HG2	1:A:227:ARG:HH22	1.69	0.56
1:A:202:LYS:NZ	1:A:227:ARG:NH1	2.53	0.56
2:B:131:ARG:HD2	4:B:244:HOH:O	2.06	0.56
1:A:399:ALA:HB2	1:A:419:VAL:HG12	1.88	0.56
1:A:420:VAL:HG22	1:A:422:LEU:CD1	2.37	0.55
1:A:365:ARG:HG3	1:A:401:TYR:CD2	2.42	0.55
1:A:137:ARG:HB3	1:A:412:LYS:HA	1.89	0.55
1:A:135:CYS:SG	1:A:138:ARG:O	2.65	0.54
1:A:202:LYS:HZ2	1:A:227:ARG:NH1	2.06	0.54
1:A:227:ARG:HD3	4:A:3:HOH:O	2.06	0.54
2:B:179:GLU:H	2:B:179:GLU:CD	2.16	0.54
1:A:391:LYS:HG2	1:A:396:MET:HE2	1.90	0.53
2:B:50:TYR:O	2:B:52:LEU:HD12	2.08	0.53
2:B:144:LEU:HD22	3:B:1:A8S:H11	1.91	0.53
2:B:145:ARG:HH21	2:B:145:ARG:CG	2.17	0.53
1:A:365:ARG:HH21	1:A:368:LEU:HD12	1.74	0.52
1:A:191:ARG:O	1:A:191:ARG:HG3	2.09	0.52
1:A:405:LEU:HA	1:A:408:GLN:HE21	1.73	0.52
1:A:206:MET:HB2	1:A:209:ASP:OD1	2.10	0.51
1:A:125:SER:HB2	1:A:171:HIS:HE1	1.77	0.50
1:A:281:PRO:HG2	1:A:303:ALA:O	2.11	0.50
1:A:232:ILE:HA	1:A:235:VAL:HB	1.93	0.50
1:A:342:LEU:HB3	1:A:420:VAL:HG13	1.94	0.50
2:B:143:ARG:NH1	2:B:143:ARG:HB3	2.27	0.50
2:B:143:ARG:HH12	2:B:178:PRO:HB2	1.77	0.50
2:B:84:ILE:O	2:B:204:ILE:CD1	2.60	0.49
1:A:238:GLU:HG2	1:A:319:TYR:HB3	1.96	0.48
1:A:321:LYS:NZ	4:A:71:HOH:O	2.47	0.48
1:A:138:ARG:HG3	1:A:412:LYS:O	2.15	0.47
2:B:205:THR:HA	2:B:208:MET:CE	2.28	0.47
2:B:194:ILE:HG12	3:B:1:A8S:H2	1.97	0.47
2:B:39:GLN:NE2	4:B:236:HOH:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:HG2	1:A:285:ASP:OD2	2.16	0.46
2:B:70:GLU:H	2:B:70:GLU:CD	2.25	0.45
1:A:135:CYS:SG	1:A:139:PRO:HA	2.57	0.45
2:B:201:LEU:HD12	2:B:205:THR:HG23	1.97	0.45
1:A:327:ASP:OD1	1:A:327:ASP:N	2.48	0.44
1:A:340:ASP:OD1	1:A:423:LYS:HE2	2.17	0.44
1:A:352:VAL:HG13	1:A:409:ARG:HB2	1.99	0.44
1:A:219:LYS:HZ2	1:A:223:ASN:HD21	1.65	0.44
1:A:218:LYS:HG2	1:A:330:VAL:HG12	2.01	0.43
1:A:290:ILE:HD13	1:A:305:VAL:HG22	2.00	0.43
2:B:164:ARG:NH1	4:B:226:HOH:O	2.48	0.43
1:A:131:PHE:HA	1:A:417:VAL:O	2.19	0.42
1:A:349:VAL:HG13	1:A:353:MET:HE3	2.01	0.42
1:A:408:GLN:HE21	1:A:408:GLN:HB2	1.66	0.42
1:A:136:GLY:HA2	1:A:407:ILE:HD11	2.01	0.42
1:A:150:ARG:H	1:A:171:HIS:CD2	2.34	0.42
2:B:208:MET:O	4:B:247:HOH:O	2.21	0.42
1:A:196:LEU:HA	1:A:224:SER:OG	2.20	0.41
1:A:202:LYS:NZ	1:A:227:ARG:HH11	2.19	0.41
1:A:281:PRO:HD3	1:A:311:MET:HA	2.02	0.41
2:B:86:LYS:HB2	2:B:89:ILE:HD12	2.02	0.41
1:A:232:ILE:C	1:A:234:SER:H	2.29	0.41
1:A:360:GLU:O	1:A:364:LYS:HB2	2.21	0.40
1:A:287:ALA:O	1:A:291:GLU:HG3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	265/326 (81%)	252 (95%)	12 (4%)	1 (0%)	30 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	169/186 (91%)	162 (96%)	7 (4%)	0	100	100
All	All	434/512 (85%)	414 (95%)	19 (4%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/270 (83%)	200 (89%)	25 (11%)	6	3
2	B	158/170 (93%)	140 (89%)	18 (11%)	5	3
All	All	383/440 (87%)	340 (89%)	43 (11%)	6	3

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	THR
1	A	135	CYS
1	A	137	ARG
1	A	141	MET
1	A	150	ARG
1	A	163	ARG
1	A	190	GLU
1	A	204	LYS
1	A	215	GLU
1	A	227	ARG
1	A	232	ILE
1	A	235	VAL
1	A	266	LEU
1	A	270	LYS
1	A	309	LEU

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Mol	Chain	Res	Type
1	A	352	VAL
1	A	361	MET
1	A	364	LYS
1	A	367	LEU
1	A	407	ILE
1	A	408	GLN
1	A	413	ASP
1	A	419	VAL
1	A	420	VAL
1	A	422	LEU
2	B	32	LEU
2	B	38	THR
2	B	40	LEU
2	B	51	GLN
2	B	52	LEU
2	B	54	ASN
2	B	70	GLU
2	B	84	ILE
2	B	90	LYS
2	B	95	SER
2	B	100	MET
2	B	105	THR
2	B	114	LEU
2	B	132	VAL
2	B	144	LEU
2	B	145	ARG
2	B	170	LEU
2	B	198	LEU

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	171	HIS
1	A	223	ASN
1	A	299	GLN
1	A	408	GLN
2	B	39	GLN
2	B	54	ASN
2	B	146	ASN

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 ⓘ

1 ligand is 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
3	A8S	B	1	-	17,19,19	4.77	6 (35%)	17,29,29	6.03	9 (52%)

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	A8S	B	1	-	-	8/10/34/34	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	A8S	C2-C3	13.09	1.53	1.35
3	B	1	A8S	C11-C10	-9.30	1.34	1.51
3	B	1	A8S	C9-C10	-7.39	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	A8S	O10-C10	6.08	1.32	1.23
3	B	1	A8S	C4-C3	3.54	1.53	1.46
3	B	1	A8S	C9-C8	-3.42	1.30	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	A8S	C8-C9-C10	20.33	144.78	123.84
3	B	1	A8S	C1-C2-C3	-8.72	115.42	128.40
3	B	1	A8S	C13-C8-C9	6.49	132.57	121.05
3	B	1	A8S	C5-C4-C3	-4.98	117.80	125.53
3	B	1	A8S	C6-C3-C2	-4.38	109.70	122.84
3	B	1	A8S	C14-C12-C11	-3.16	103.08	108.50
3	B	1	A8S	C4-C3-C2	-2.86	111.21	119.15
3	B	1	A8S	C11-C10-C9	-2.56	110.99	116.70
3	B	1	A8S	O10-C10-C9	2.45	126.05	121.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	A8S	C1-C2-C3-C4
3	B	1	A8S	C1-C2-C3-C6
3	B	1	A8S	C4-C5-C7-O7
3	B	1	A8S	C4-C5-C7-C12
3	B	1	A8S	C6-C3-C4-C5
3	B	1	A8S	O11-C1-C2-C3
3	B	1	A8S	O12-C1-C2-C3
3	B	1	A8S	C4-C5-C7-C8

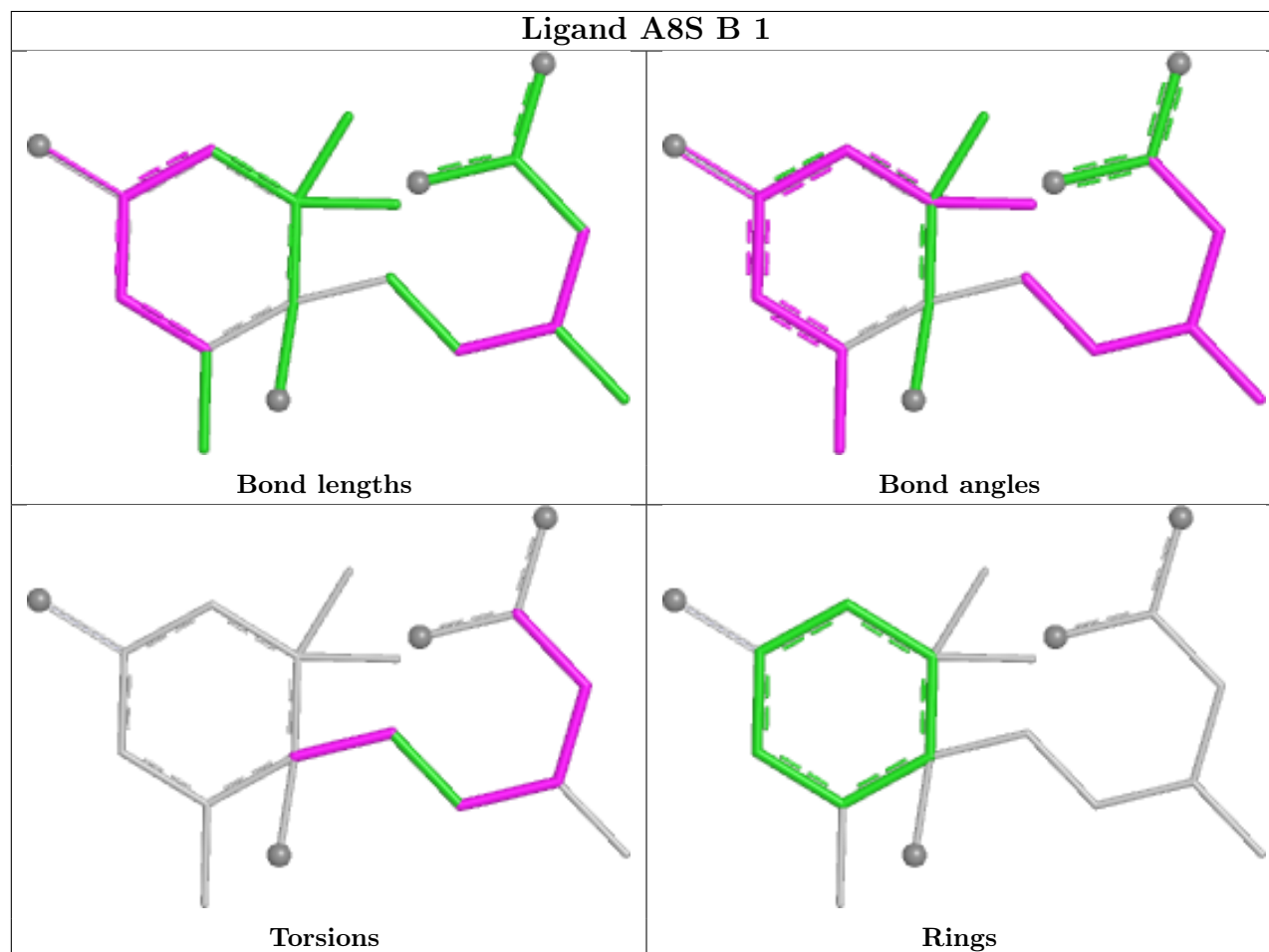
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	A8S	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	271/326 (83%)	0.03	4 (1%) 72 74	21, 31, 44, 52	0
2	B	173/186 (93%)	-0.31	1 (0%) 85 87	12, 24, 40, 54	0
All	All	444/512 (86%)	-0.10	5 (1%) 78 80	12, 29, 43, 54	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	397	SER	2.6
1	A	369	TRP	2.2
1	A	126	VAL	2.1
2	B	85	TYR	2.1
1	A	135	CYS	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](#)

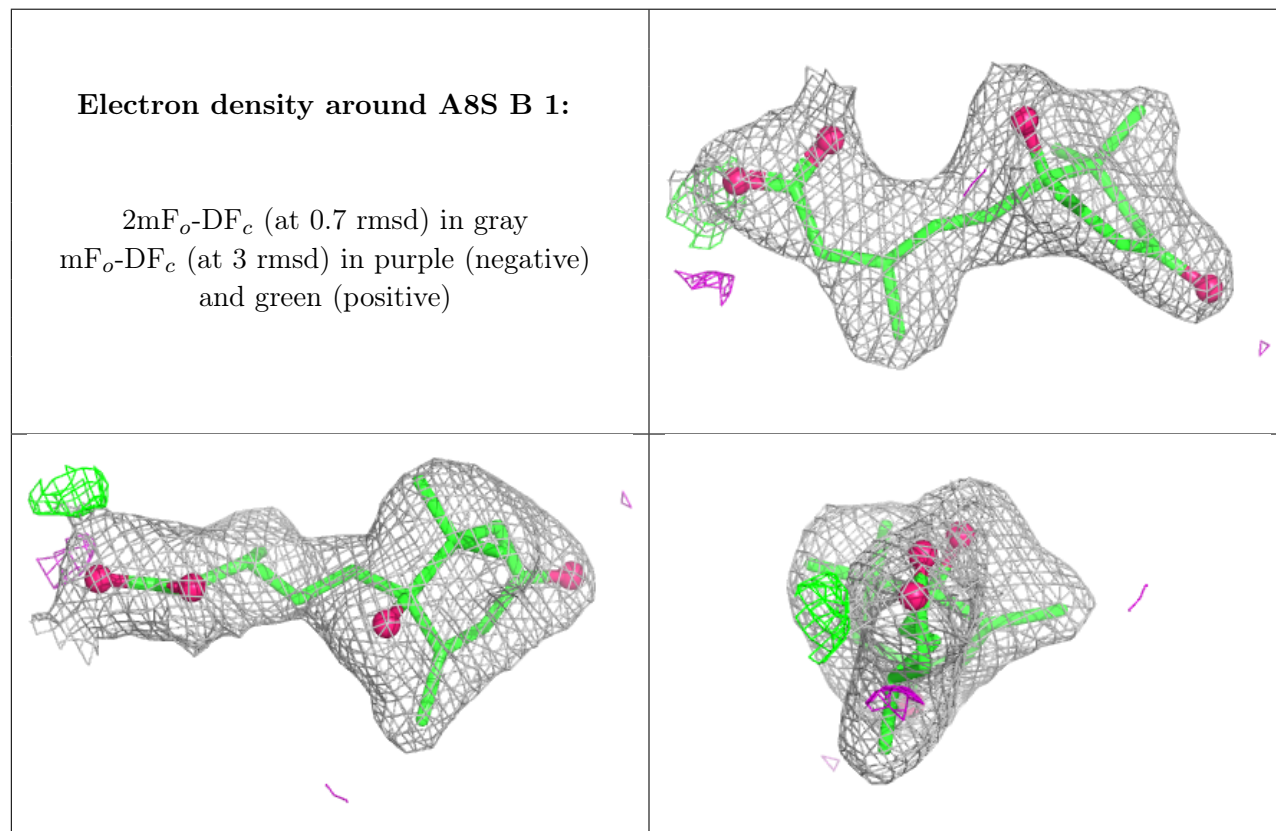
There are no oligosaccharides in this entry.

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	A8S	B	1	19/19	0.92	0.08	36,42,54,58	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.