



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:10 PM UTC

PDB ID : 3KB3 / pdb_00003kb3
Title : Crystal structure of abscisic acid-bound PYL2 in complex with HAB1
Authors : Zhou, X.E.; Melcher, K.; Soon, F.-F.; Ng, L.-M.; Xu, Y.; Suino-Powell, K.M.;
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Deposited on : 2009-10-20
Resolution : 1.95 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

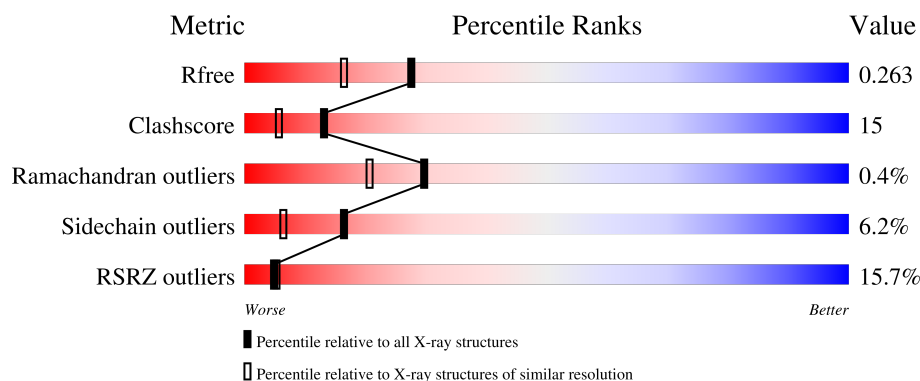
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	176	5% 74% 23% .
2	B	321	21% 66% 22% . 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3933 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 Putative uncharacterized protein At2g26040.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1395	876	243	272	4			

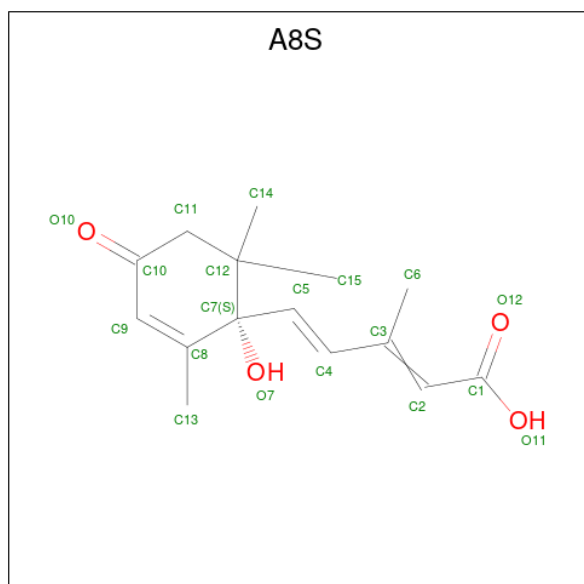
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	SER	-	expression tag	UNP O80992

- Molecule 2 is a protein called Protein phosphatase 2C 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	294	Total	C	N	O	S	0	0	0
			2286	1441	408	421	16			

- 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	A	1	Total	C	O	0	0
			19	15	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		

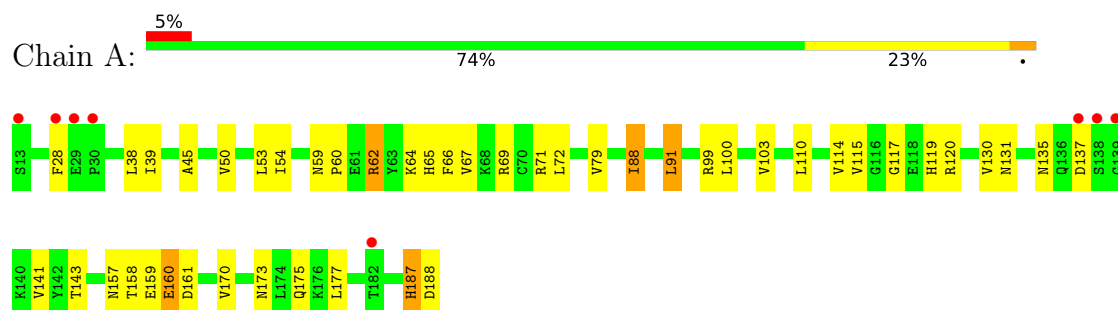
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O	0	0
			118	118		
5	B	112	Total	O	0	0
			112	112		

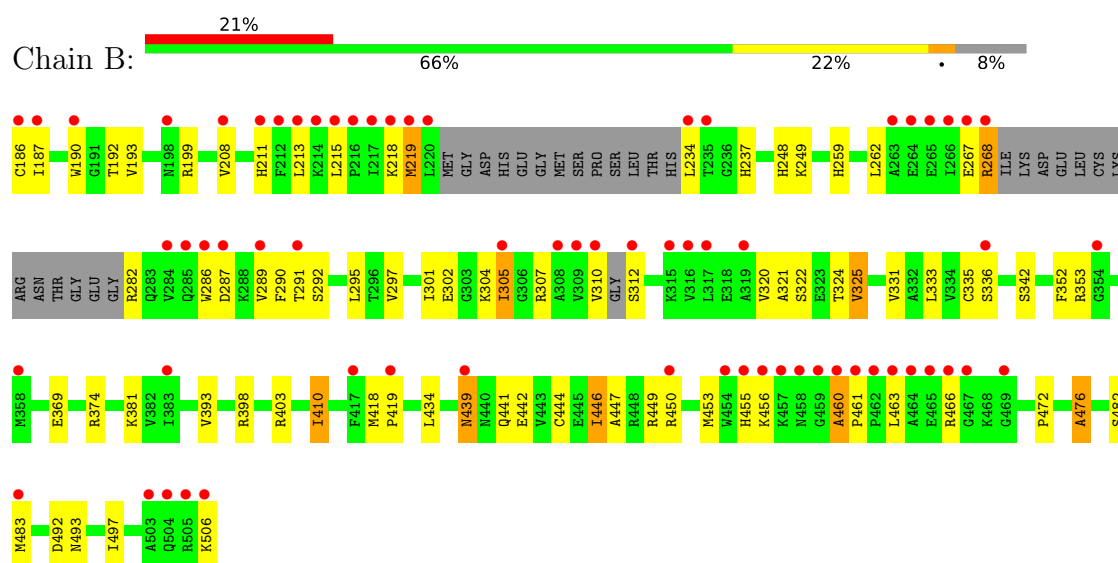
3 Residue-property plots [i](#)

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: Putative uncharacterized protein At2g26040



- Molecule 2: Protein phosphatase 2C 16



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.32Å 67.47Å 143.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.52 – 1.95 29.52 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.52-1.95) 94.2 (29.52-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.93Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.259 0.218 , 0.263	Depositor DCC
R_{free} test set	2918 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3933	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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: MG, 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	1.46	6/1423 (0.4%)	1.18	5/1933 (0.3%)
2	B	1.20	3/2328 (0.1%)	1.06	3/3139 (0.1%)
All	All	1.30	9/3751 (0.2%)	1.11	8/5072 (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	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	193	VAL	C-O	-7.09	1.17	1.24
2	B	476	ALA	CA-CB	6.87	1.64	1.53
1	A	54	ILE	CA-CB	-6.64	1.45	1.54
1	A	50	VAL	CA-CB	-6.25	1.46	1.54
2	B	447	ALA	CA-CB	5.57	1.62	1.53
1	A	131	ASN	CG-ND2	5.47	1.44	1.33
1	A	115	VAL	N-CA	-5.41	1.40	1.46
1	A	173	ASN	N-CA	-5.16	1.40	1.46
1	A	67	VAL	CA-CB	-5.10	1.48	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	ARG	N-CA-C	5.95	117.98	110.24
2	B	456	LYS	N-CA-C	-5.80	106.12	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LEU	N-CA-C	-5.75	105.10	111.36
1	A	115	VAL	N-CA-C	-5.57	107.36	113.43
2	B	493	ASN	N-CA-C	-5.50	102.87	110.35
1	A	45	ALA	N-CA-C	-5.50	103.27	108.22
1	A	117	GLY	N-CA-C	5.45	117.60	112.04
1	A	99	ARG	NE-CZ-NH2	5.19	123.87	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	HIS	Peptide

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	1395	0	1382	31	0
2	B	2286	0	2286	81	0
3	A	19	0	19	1	0
4	B	3	0	0	0	0
5	A	118	0	0	5	0
5	B	112	0	0	10	0
All	All	3933	0	3687	110	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 15.

All (110) 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:158:THR:HG23	1:A:161:ASP:H	1.27	0.99
2:B:449:ARG:HD2	2:B:453:MET:HE3	1.47	0.95
2:B:192:THR:HG22	2:B:497:ILE:HD12	1.48	0.95
2:B:287:ASP:O	2:B:291:THR:HG23	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:ARG:HD2	2:B:453:MET:CE	2.05	0.86
2:B:442:GLU:O	2:B:446:ILE:HD13	1.81	0.81
2:B:301:ILE:HG12	2:B:320:VAL:HG11	1.65	0.76
2:B:418:MET:HE3	2:B:419:PRO:HD2	1.68	0.76
2:B:321:ALA:HB1	2:B:325:VAL:HG11	1.67	0.76
1:A:65:HIS:O	2:B:324:THR:HG21	1.86	0.74
2:B:301:ILE:HG23	2:B:320:VAL:CG1	2.17	0.74
2:B:460:ALA:CB	2:B:461:PRO:HA	2.17	0.74
2:B:190:TRP:CZ3	2:B:208:VAL:HG11	2.24	0.72
2:B:460:ALA:HB1	2:B:461:PRO:CA	2.19	0.72
2:B:187:ILE:HG23	2:B:187:ILE:O	1.90	0.72
2:B:192:THR:CG2	2:B:497:ILE:HD12	2.19	0.71
2:B:310:VAL:HG22	2:B:312:SER:O	1.93	0.69
2:B:286:TRP:HA	2:B:289:VAL:HG12	1.74	0.69
2:B:310:VAL:HG13	2:B:312:SER:HA	1.75	0.69
2:B:439:ASN:HD22	2:B:441:GLN:H	1.41	0.69
2:B:460:ALA:CB	2:B:461:PRO:CA	2.72	0.68
2:B:213:LEU:HD13	2:B:215:LEU:HD21	1.75	0.68
2:B:374:ARG:HH21	2:B:374:ARG:HG3	1.59	0.68
2:B:460:ALA:HB1	2:B:461:PRO:HA	1.74	0.67
1:A:66:PHE:O	1:A:88:ILE:HD12	1.96	0.66
2:B:213:LEU:HD13	2:B:215:LEU:CD2	2.26	0.66
2:B:460:ALA:HB1	2:B:461:PRO:C	2.21	0.66
2:B:301:ILE:HA	2:B:320:VAL:HG12	1.78	0.65
2:B:410:ILE:H	2:B:410:ILE:HD13	1.61	0.65
2:B:219:MET:HE1	2:B:335:CYS:SG	2.39	0.62
1:A:120:ARG:HH12	1:A:157:ASN:ND2	1.99	0.61
2:B:322:SER:O	2:B:325:VAL:HG12	2.01	0.59
1:A:39:ILE:HD12	1:A:170:VAL:HB	1.84	0.58
1:A:187:HIS:HD2	1:A:188:ASP:HA	1.68	0.57
2:B:449:ARG:CD	2:B:453:MET:HE3	2.29	0.56
1:A:79:VAL:CG2	1:A:103:VAL:HG22	2.34	0.56
2:B:463:LEU:HD12	2:B:466:ARG:HB3	1.89	0.55
2:B:398:ARG:HG2	2:B:410:ILE:HD13	1.88	0.54
1:A:69:ARG:NE	5:A:259:HOH:O	2.41	0.54
1:A:130:VAL:HG13	1:A:143:THR:HG21	1.89	0.54
1:A:91:LEU:HD13	2:B:393:VAL:HG13	1.90	0.54
2:B:352:PHE:CG	2:B:444:CYS:HB3	2.44	0.53
1:A:114:VAL:HG11	1:A:119:HIS:CE1	2.44	0.53
2:B:186:CYS:N	2:B:237:HIS:HE1	2.08	0.52
2:B:403:ARG:HG3	5:B:45:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:CD2	1:A:188:ASP:HA	2.46	0.51
2:B:449:ARG:NH2	5:B:29:HOH:O	2.43	0.51
2:B:455:HIS:C	5:B:55:HOH:O	2.53	0.51
2:B:213:LEU:CD1	2:B:215:LEU:HD21	2.41	0.50
2:B:301:ILE:CA	2:B:320:VAL:HG12	2.41	0.50
1:A:88:ILE:N	1:A:88:ILE:HD13	2.27	0.50
2:B:398:ARG:HG2	2:B:410:ILE:CD1	2.41	0.50
1:A:69:ARG:CZ	5:A:259:HOH:O	2.59	0.50
1:A:158:THR:OG1	1:A:160:GLU:OE1	2.30	0.50
2:B:460:ALA:HB3	2:B:461:PRO:HA	1.91	0.50
2:B:187:ILE:O	2:B:187:ILE:CG2	2.59	0.50
2:B:439:ASN:HD22	2:B:441:GLN:N	2.08	0.50
2:B:301:ILE:HG23	2:B:320:VAL:HG12	1.92	0.49
2:B:211:HIS:H	2:B:237:HIS:HD2	1.61	0.49
1:A:39:ILE:HD12	1:A:170:VAL:CG1	2.43	0.48
2:B:295:LEU:HD21	5:B:520:HOH:O	2.13	0.48
2:B:302:GLU:HG3	2:B:403:ARG:HD3	1.96	0.48
2:B:186:CYS:HB2	2:B:336:SER:HB3	1.95	0.48
2:B:450:ARG:CZ	2:B:476:ALA:HB1	2.44	0.48
2:B:304:LYS:C	2:B:305:ILE:HD12	2.39	0.47
1:A:79:VAL:HG23	1:A:103:VAL:HG22	1.95	0.47
2:B:322:SER:O	2:B:325:VAL:CG1	2.63	0.47
2:B:259:HIS:HD2	5:B:9:HOH:O	1.98	0.47
2:B:267:GLU:N	2:B:267:GLU:OE2	2.47	0.46
2:B:267:GLU:O	2:B:268:ARG:C	2.58	0.46
2:B:262:LEU:HD21	2:B:333:LEU:HD11	1.98	0.46
2:B:290:PHE:HZ	2:B:333:LEU:HD13	1.81	0.46
2:B:324:THR:HG23	5:B:44:HOH:O	2.15	0.46
2:B:353:ARG:HH12	2:B:418:MET:HE2	1.81	0.46
2:B:482:SER:OG	2:B:483:MET:HE2	2.16	0.46
3:A:189:A8S:H5	3:A:189:A8S:H6	1.70	0.45
1:A:175:GLN:NE2	5:A:288:HOH:O	2.49	0.45
2:B:307:ARG:HD3	5:B:72:HOH:O	2.16	0.45
1:A:66:PHE:C	1:A:88:ILE:HD12	2.41	0.45
2:B:374:ARG:HH21	2:B:374:ARG:CG	2.23	0.45
2:B:310:VAL:HG13	2:B:312:SER:OG	2.16	0.45
2:B:463:LEU:HA	2:B:466:ARG:HB2	1.98	0.45
2:B:211:HIS:H	2:B:237:HIS:CD2	2.35	0.44
2:B:310:VAL:HG13	2:B:312:SER:CA	2.46	0.44
2:B:301:ILE:HA	2:B:320:VAL:CG1	2.46	0.44
1:A:135:ASN:ND2	1:A:137:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:ARG:CZ	5:B:29:HOH:O	2.65	0.44
1:A:28:PHE:HD1	5:A:296:HOH:O	1.99	0.44
2:B:248:HIS:CE1	2:B:249:LYS:HD2	2.53	0.44
2:B:374:ARG:CZ	2:B:410:ILE:HD12	2.48	0.44
2:B:262:LEU:CD2	2:B:333:LEU:HD11	2.48	0.43
2:B:331:VAL:CG2	2:B:342:SER:HB3	2.49	0.43
1:A:59:ASN:OD1	1:A:62:ARG:HG3	2.19	0.43
1:A:88:ILE:CD1	1:A:88:ILE:H	2.31	0.43
1:A:91:LEU:CD1	2:B:393:VAL:HG13	2.48	0.43
1:A:130:VAL:HG13	1:A:143:THR:CG2	2.49	0.43
2:B:472:PRO:HG2	5:B:182:HOH:O	2.19	0.43
1:A:66:PHE:HA	1:A:88:ILE:HD12	2.01	0.42
2:B:305:ILE:N	2:B:305:ILE:CD1	2.82	0.42
2:B:292:SER:HB2	5:B:180:HOH:O	2.20	0.42
1:A:60:PRO:HB2	1:A:64:LYS:HD2	2.02	0.42
2:B:305:ILE:HD12	2:B:305:ILE:N	2.35	0.42
1:A:88:ILE:N	1:A:88:ILE:CD1	2.83	0.41
1:A:110:LEU:C	1:A:110:LEU:HD23	2.46	0.41
1:A:159:GLU:HG2	5:A:225:HOH:O	2.20	0.41
2:B:321:ALA:HB1	2:B:325:VAL:CG1	2.44	0.41
1:A:66:PHE:CA	1:A:88:ILE:HD12	2.50	0.41
2:B:286:TRP:HA	2:B:289:VAL:CG1	2.48	0.41
2:B:286:TRP:CE3	2:B:289:VAL:HG11	2.56	0.40
2:B:302:GLU:HG2	2:B:304:LYS:HG2	2.02	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	174/176 (99%)	168 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	286/321 (89%)	273 (96%)	11 (4%)	2 (1%)	18	10
All	All	460/497 (93%)	441 (96%)	17 (4%)	2 (0%)	30	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	219	MET
2	B	460	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	161/161 (100%)	151 (94%)	10 (6%)	16	6
2	B	245/267 (92%)	230 (94%)	15 (6%)	17	7
All	All	406/428 (95%)	381 (94%)	25 (6%)	16	6

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	53	LEU
1	A	62	ARG
1	A	71	ARG
1	A	72	LEU
1	A	88	ILE
1	A	91	LEU
1	A	100	LEU
1	A	141	VAL
1	A	160	GLU
2	B	218	LYS
2	B	234	LEU
2	B	268	ARG
2	B	282	ARG

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Mol	Chain	Res	Type
2	B	297	VAL
2	B	305	ILE
2	B	325	VAL
2	B	369	GLU
2	B	381	LYS
2	B	410	ILE
2	B	434	LEU
2	B	439	ASN
2	B	446	ILE
2	B	492	ASP
2	B	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	41	GLN
1	A	44	HIS
1	A	131	ASN
1	A	135	ASN
1	A	157	ASN
1	A	187	HIS
2	B	198	ASN
2	B	237	HIS
2	B	248	HIS
2	B	259	HIS
2	B	285	GLN
2	B	439	ASN
2	B	475	GLN
2	B	487	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A8S	A	189	-	17,19,19	2.53	6 (35%)	17,29,29	3.24	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	A	189	-	-	0/10/34/34	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	189	A8S	C7-C12	-6.57	1.47	1.57
3	A	189	A8S	C15-C12	5.57	1.64	1.53
3	A	189	A8S	C9-C10	2.97	1.51	1.45
3	A	189	A8S	C11-C10	2.39	1.55	1.51
3	A	189	A8S	C11-C12	-2.14	1.48	1.54
3	A	189	A8S	C9-C8	2.04	1.36	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	189	A8S	C15-C12-C11	-9.47	92.24	108.50
3	A	189	A8S	C8-C9-C10	-4.77	118.92	123.84
3	A	189	A8S	C6-C3-C4	-3.60	112.59	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	189	A8S	C4-C3-C2	2.99	127.44	119.15
3	A	189	A8S	C11-C10-C9	2.80	122.95	116.70
3	A	189	A8S	O11-C1-C2	2.54	120.95	113.40
3	A	189	A8S	O12-C1-C2	-2.37	116.76	124.02
3	A	189	A8S	C14-C12-C11	2.30	112.44	108.50
3	A	189	A8S	C15-C12-C14	-2.29	104.05	107.37

There are no chirality outliers.

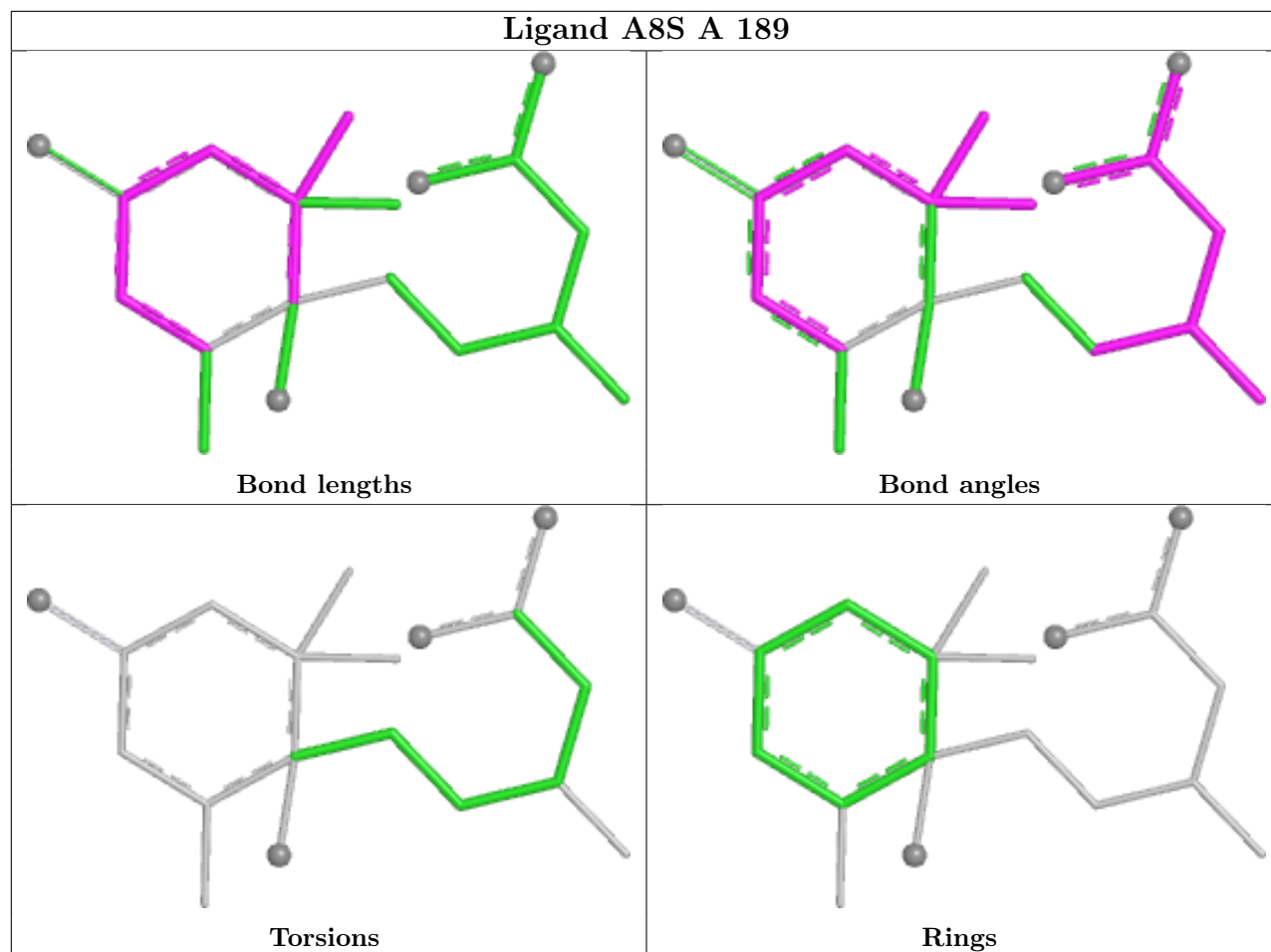
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	189	A8S	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.



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	176/176 (100%)	0.17	8 (4%) 38 44	22, 32, 74, 87	0
2	B	294/321 (91%)	1.18	66 (22%) 2 2	25, 47, 124, 170	0
All	All	470/497 (94%)	0.80	74 (15%) 5 5	22, 41, 109, 170	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	217	ILE	7.8
2	B	215	LEU	6.4
2	B	220	LEU	6.3
2	B	460	ALA	6.1
2	B	463	LEU	5.8
1	A	28	PHE	5.8
2	B	464	ALA	5.8
2	B	234	LEU	5.4
2	B	219	MET	5.4
2	B	457	LYS	5.4
2	B	266	ILE	5.4
2	B	284	VAL	5.1
2	B	216	PRO	5.0
2	B	212	PHE	5.0
2	B	462	PRO	4.7
2	B	286	TRP	4.4
2	B	417	PHE	4.1
2	B	214	LYS	4.1
2	B	213	LEU	3.9
2	B	461	PRO	3.8
2	B	317	LEU	3.6
2	B	309	VAL	3.6
2	B	285	GLN	3.5
2	B	450	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	336	SER	3.3
2	B	308	ALA	3.2
2	B	187	ILE	3.2
2	B	467	GLY	3.2
2	B	218	LYS	3.2
2	B	211	HIS	3.1
2	B	310	VAL	3.1
2	B	316	VAL	3.1
2	B	459	GLY	3.1
2	B	268	ARG	3.0
2	B	458	ASN	3.0
2	B	455	HIS	3.0
2	B	305	ILE	3.0
2	B	289	VAL	2.9
2	B	235	THR	2.8
2	B	186	CYS	2.8
1	A	138	SER	2.7
2	B	506	LYS	2.7
2	B	190	TRP	2.6
2	B	456	LYS	2.6
1	A	30	PRO	2.6
2	B	483	MET	2.6
2	B	503	ALA	2.6
1	A	13	SER	2.6
2	B	358	MET	2.5
2	B	264	GLU	2.5
2	B	465	GLU	2.5
2	B	319	ALA	2.5
2	B	419	PRO	2.5
2	B	466	ARG	2.4
2	B	312	SER	2.4
2	B	291	THR	2.4
2	B	469	GLY	2.3
1	A	29	GLU	2.3
2	B	263	ALA	2.3
2	B	354	GLY	2.3
2	B	505	ARG	2.3
2	B	287	ASP	2.3
2	B	454	TRP	2.3
2	B	198	ASN	2.3
2	B	439	ASN	2.2
1	A	139	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	267	GLU	2.1
2	B	504	GLN	2.1
2	B	383	ILE	2.1
1	A	137	ASP	2.1
1	A	182	THR	2.1
2	B	265	GLU	2.1
2	B	315	LYS	2.1
2	B	208	VAL	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](#)

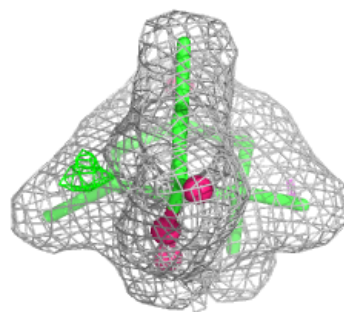
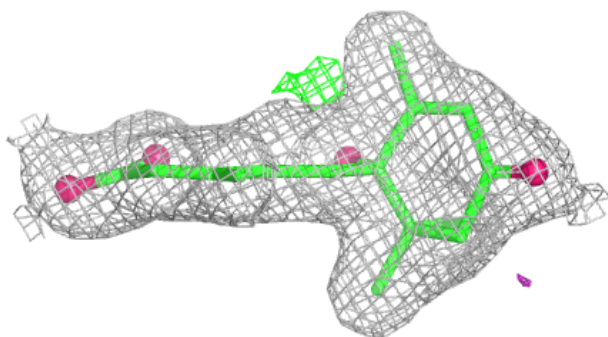
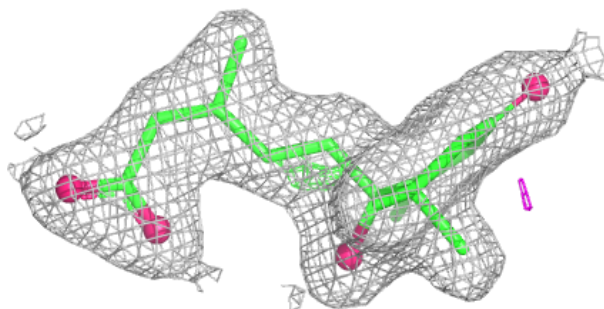
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	MG	B	997	1/1	0.91	0.10	47,47,47,47	0
3	A8S	A	189	19/19	0.93	0.07	18,24,28,35	0
4	MG	B	998	1/1	0.97	0.14	42,42,42,42	0
4	MG	B	999	1/1	0.99	0.11	37,37,37,37	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 A8S A 189:

$2mF_o-DF_c$ (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.