



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2024 – 12:03 AM EDT

PDB ID : 1DCN
Title : INACTIVE MUTANT H162N OF DELTA 2 CRYSTALLIN WITH BOUND ARGININOSUCCINATE
Authors : Vallee, F.; Turner, M.A.; Lindley, P.; Howell, P.L.
Deposited on : 1998-10-29
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

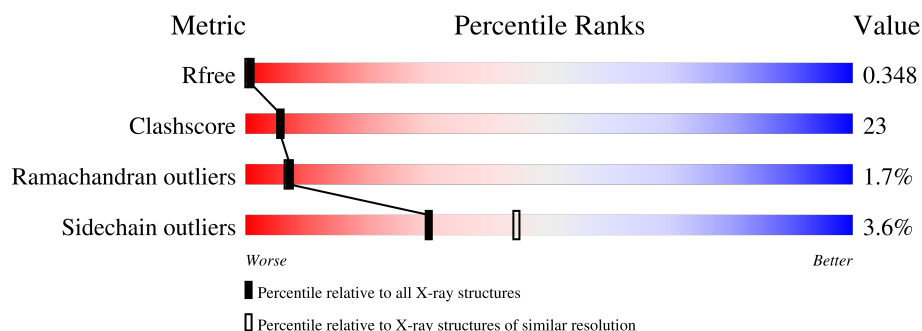
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	447	
1	B	447	
1	C	447	
1	D	447	

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	AS1	D	0	X	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13754 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.

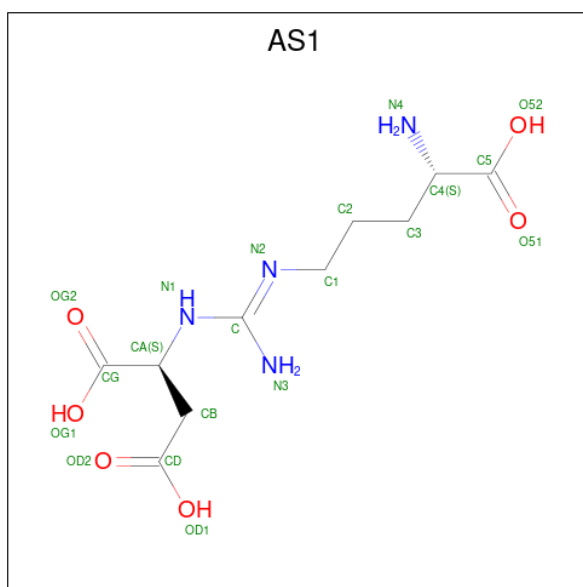
- Molecule 1 is a protein called DELTA 2 CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3287	2080	557	640	10			
1	B	418	Total	C	N	O	S	0	0	0
			3239	2050	549	629	11			
1	C	434	Total	C	N	O	S	0	0	0
			3360	2127	568	654	11			
1	D	436	Total	C	N	O	S	0	0	0
			3377	2139	571	656	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ASN	HIS	conflict	UNP P24058
A	162	ASN	HIS	engineered mutation	UNP P24058
A	302	SER	ALA	conflict	UNP P24058
A	409	ASN	LYS	conflict	UNP P24058
B	110	ASN	HIS	conflict	UNP P24058
B	162	ASN	HIS	engineered mutation	UNP P24058
B	302	SER	ALA	conflict	UNP P24058
B	409	ASN	LYS	conflict	UNP P24058
C	110	ASN	HIS	conflict	UNP P24058
C	162	ASN	HIS	engineered mutation	UNP P24058
C	302	SER	ALA	conflict	UNP P24058
C	409	ASN	LYS	conflict	UNP P24058
D	110	ASN	HIS	conflict	UNP P24058
D	162	ASN	HIS	engineered mutation	UNP P24058
D	302	SER	ALA	conflict	UNP P24058
D	409	ASN	LYS	conflict	UNP P24058

- Molecule 2 is ARGININOSUCCINATE (three-letter code: AS1) (formula: C₁₀H₁₈N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			20	10	4	6		

- Molecule 3 is water.

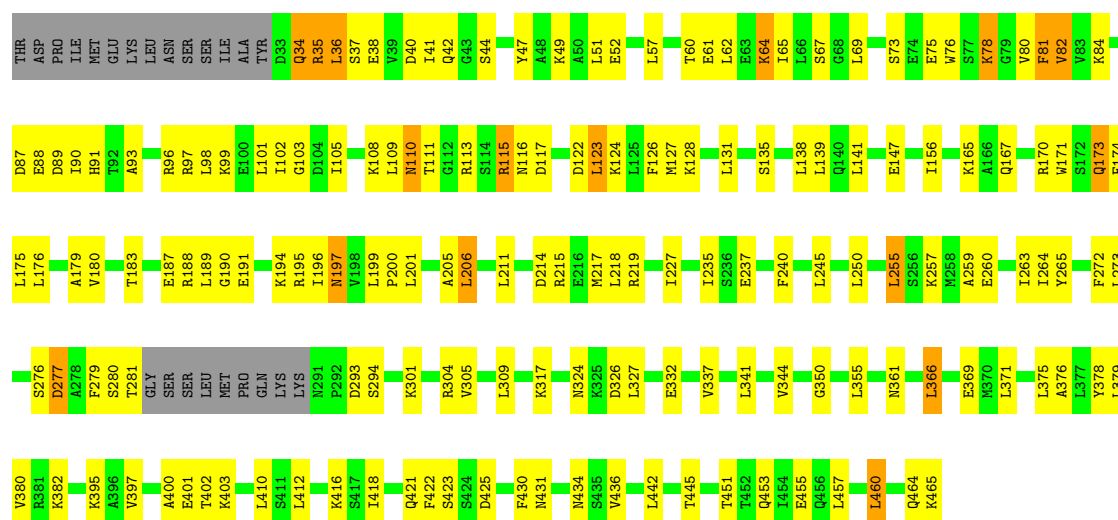
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	126	Total	O	0	0
			126	126		
3	C	110	Total	O	0	0
			110	110		
3	D	112	Total	O	0	0
			112	112		

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. 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. 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.

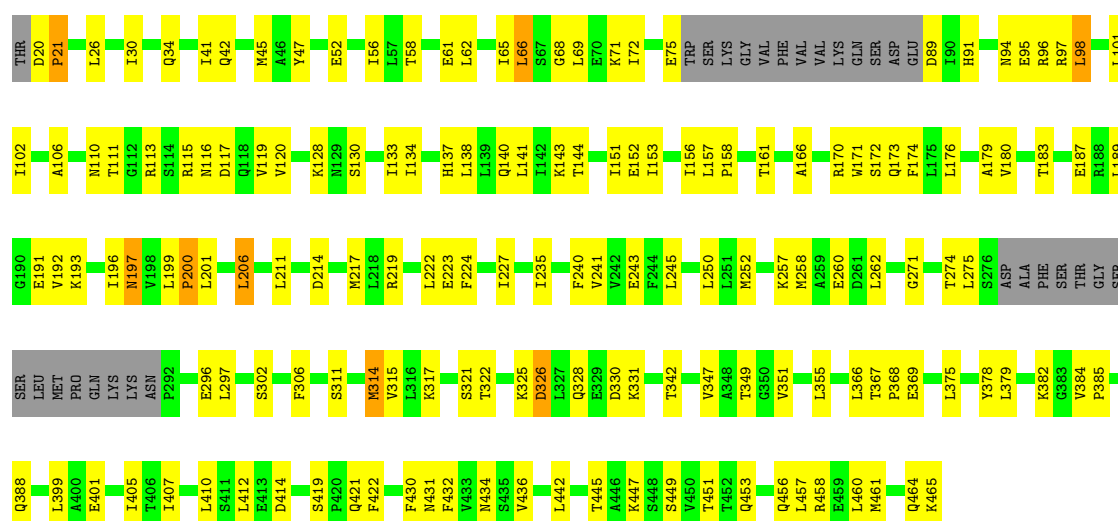
• Molecule 1: DELTA 2 CRYSTALLIN

Chain A: 



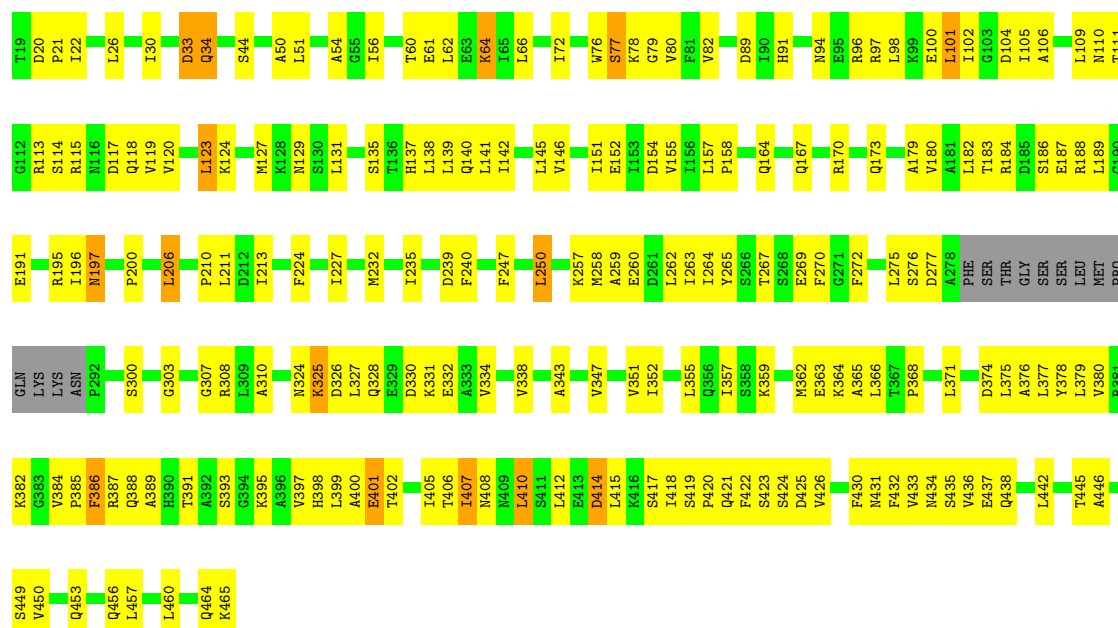
• Molecule 1: DELTA 2 CRYSTALLIN

Chain B: 



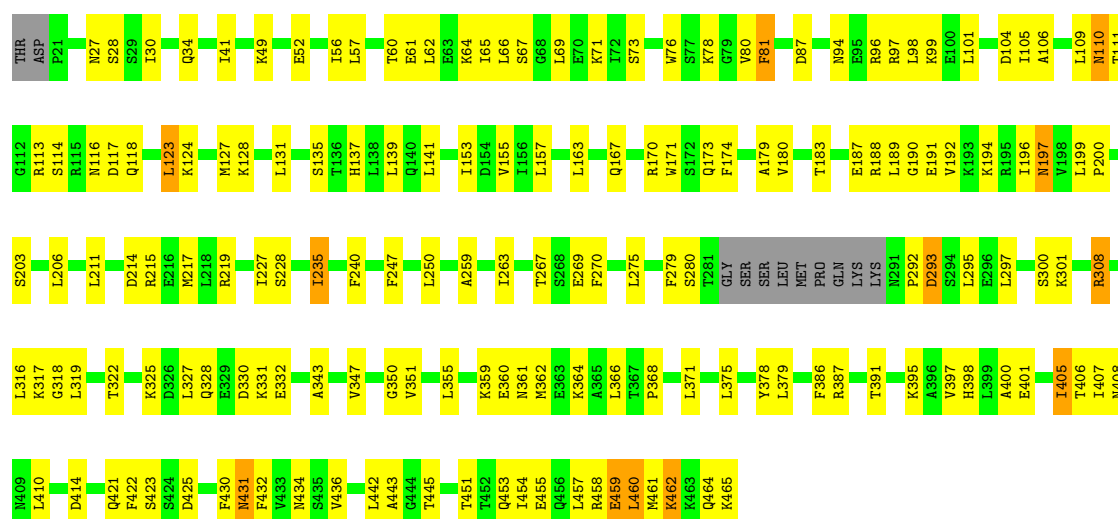
• Molecule 1: DELTA 2 CRYSTALLIN

Chain C: 



• Molecule 1: DELTA 2 CRYSTALLIN

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.58Å 99.59Å 107.14Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	82.8 (20.00-2.30) 75.8 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.27Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.229 , 0.290 0.350 , 0.348	Depositor DCC
R_{free} test set	6664 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	13754	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AS1

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	0.34	0/3326	0.60	0/4484
1	B	0.35	0/3275	0.59	0/4413
1	C	0.33	0/3400	0.60	0/4584
1	D	0.35	0/3418	0.60	0/4608
All	All	0.34	0/13419	0.60	0/18089

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3287	0	3391	165	0
1	B	3239	0	3357	138	0
1	C	3360	0	3470	195	0
1	D	3377	0	3486	145	0
2	D	20	0	13	9	0
3	A	123	0	0	9	0
3	B	126	0	0	10	0
3	C	110	0	0	11	0
3	D	112	0	0	7	0
All	All	13754	0	13717	619	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 23.

The worst 5 of 619 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:D:0:AS1:CB	2:D:0:AS1:CA	1.79	1.60
2:D:0:AS1:N2	2:D:0:AS1:C1	1.69	1.53
1:B:456:GLN:O	1:B:460:LEU:HD23	1.66	0.95
1:A:403:LYS:HE2	1:A:403:LYS:HA	1.48	0.92
1:C:131:LEU:HD22	1:C:189:LEU:HD11	1.51	0.90

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	420/447 (94%)	379 (90%)	32 (8%)	9 (2%)	5	5
1	B	412/447 (92%)	382 (93%)	27 (7%)	3 (1%)	19	23
1	C	430/447 (96%)	389 (90%)	30 (7%)	11 (3%)	4	3
1	D	432/447 (97%)	397 (92%)	29 (7%)	6 (1%)	9	9
All	All	1694/1788 (95%)	1547 (91%)	118 (7%)	29 (2%)	7	7

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PHE
1	A	82	VAL
1	A	84	LYS
1	A	88	GLU
1	A	206	LEU

5.3.2 Protein sidechains [i](#)

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	369/392 (94%)	356 (96%)	13 (4%)	31	46
1	B	364/392 (93%)	355 (98%)	9 (2%)	42	60
1	C	377/392 (96%)	360 (96%)	17 (4%)	23	34
1	D	379/392 (97%)	365 (96%)	14 (4%)	29	43
All	All	1489/1568 (95%)	1436 (96%)	53 (4%)	30	44

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	197	ASN
1	C	326	ASP
1	D	414	ASP
1	C	200	PRO
1	C	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	42	GLN
1	D	421	GLN
1	C	164	GLN
1	D	356	GLN
1	D	137	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	AS1	D	0	-	18,19,19	4.08	8 (44%)	19,24,24	8.73	11 (57%)

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	AS1	D	0	-	1/1/6/7	7/21/23/23	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	0	AS1	CB-CA	12.42	1.79	1.53
2	D	0	AS1	C1-N2	8.32	1.69	1.46
2	D	0	AS1	CB-CD	3.83	1.61	1.51
2	D	0	AS1	CA-N1	-3.77	1.38	1.45
2	D	0	AS1	C-N3	3.57	1.42	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	C2-C1-N2	34.06	170.98	110.67
2	D	0	AS1	C1-N2-C	12.09	149.61	121.86
2	D	0	AS1	CA-CB-CD	5.35	127.78	112.75
2	D	0	AS1	N1-C-N2	4.73	136.45	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	N3-C-N2	-3.99	109.01	123.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	0	AS1	C4

5 of 7 torsion outliers are listed below:

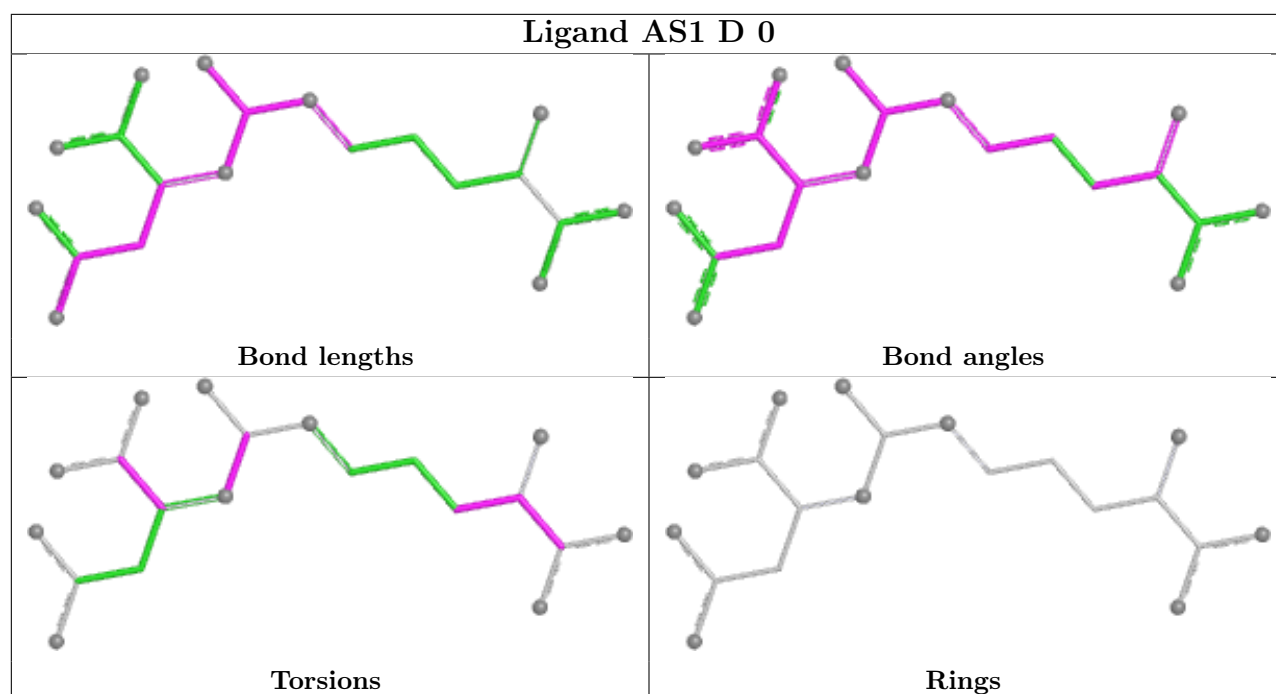
Mol	Chain	Res	Type	Atoms
2	D	0	AS1	C2-C3-C4-C5
2	D	0	AS1	CB-CA-CG-OG2
2	D	0	AS1	CB-CA-CG-OG1
2	D	0	AS1	C3-C4-C5-O52
2	D	0	AS1	N2-C-N1-CA

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	0	AS1	9	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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

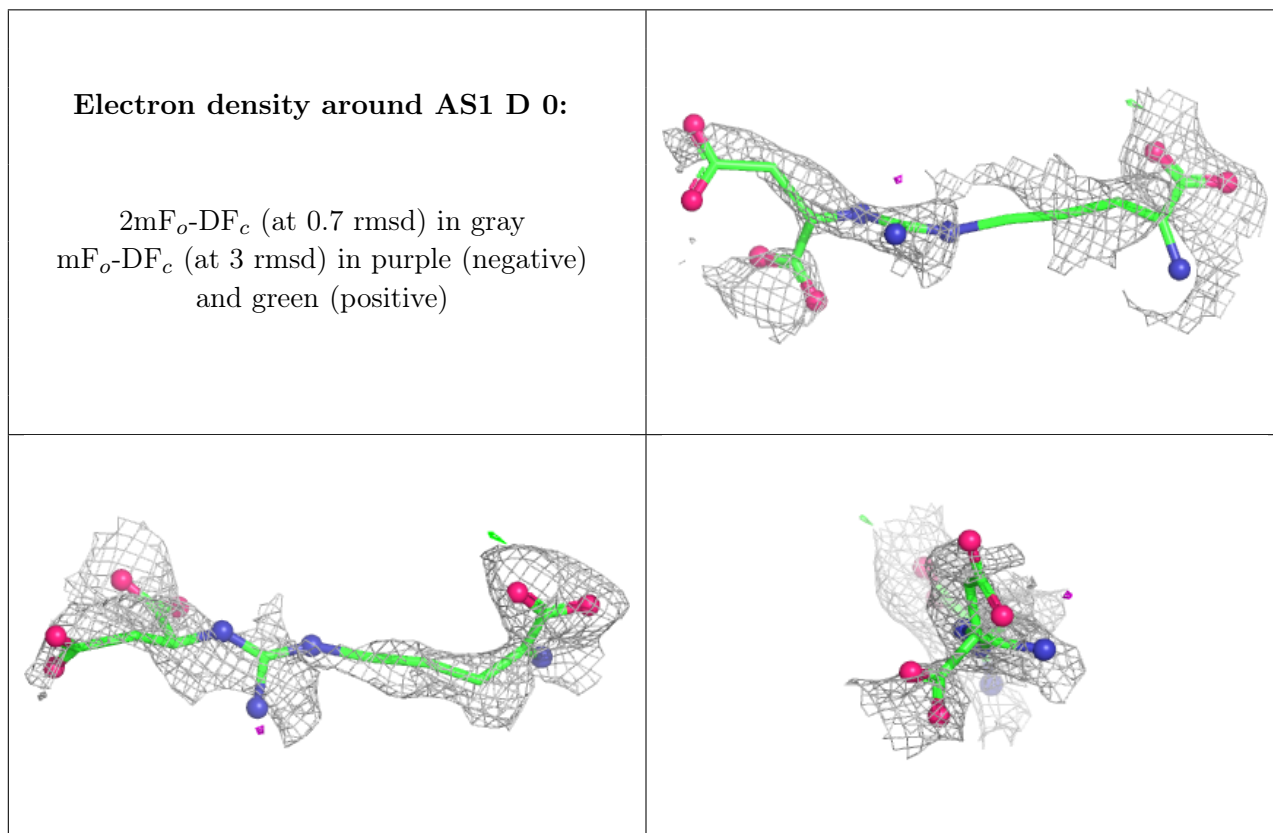
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.