



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 02:10 PM EDT

PDB ID : 9Y5Z / pdb_00009y5z
Title : Crystal structure of ternary complex Helios-ZF2:CRBN:DDB1 in complex with BMS-986449, a molecular glue degrader
Authors : Zhu, J.; Pagarigan, B.E.; Tran, E.T.
Deposited on : 2025-09-05
Resolution : 3.53 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

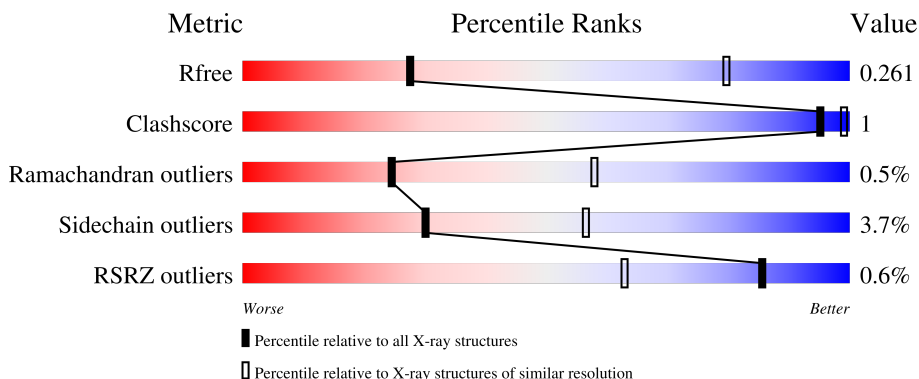
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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	856	86% 6% 7%
2	B	426	85% 5% 10%
3	C	31	87% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18588 atoms, of which 9164 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	796	Total	C	H	N	O	S	5990	0	0
			12122	3894	5990	1023	1180	35			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	ASP	-	expression tag	UNP Q16531
A	-10	GLU	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	385	Total	C	H	N	O	S	2939	0	0
			5978	1932	2939	512	571	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	expression tag	UNP Q96SW2
B	18	ASP	-	expression tag	UNP Q96SW2
B	19	TRP	-	expression tag	UNP Q96SW2
B	20	SER	-	expression tag	UNP Q96SW2
B	21	HIS	-	expression tag	UNP Q96SW2
B	22	PRO	-	expression tag	UNP Q96SW2
B	23	GLN	-	expression tag	UNP Q96SW2
B	24	PHE	-	expression tag	UNP Q96SW2
B	25	GLU	-	expression tag	UNP Q96SW2
B	26	LYS	-	expression tag	UNP Q96SW2
B	27	SER	-	expression tag	UNP Q96SW2
B	28	ALA	-	expression tag	UNP Q96SW2
B	29	VAL	-	expression tag	UNP Q96SW2
B	30	ASP	-	expression tag	UNP Q96SW2
B	31	GLU	-	expression tag	UNP Q96SW2
B	32	ASN	-	expression tag	UNP Q96SW2
B	33	LEU	-	expression tag	UNP Q96SW2
B	34	TYR	-	expression tag	UNP Q96SW2
B	35	PHE	-	expression tag	UNP Q96SW2
B	36	GLN	-	expression tag	UNP Q96SW2
B	37	GLY	-	expression tag	UNP Q96SW2
B	38	GLY	-	expression tag	UNP Q96SW2
B	39	GLY	-	expression tag	UNP Q96SW2
B	40	ARG	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Zinc finger protein Helios.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	28	Total	C	H	N	O	S	214	0	0
			436	137	214	46	37	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	133	GLY	-	expression tag	UNP Q9UKS7

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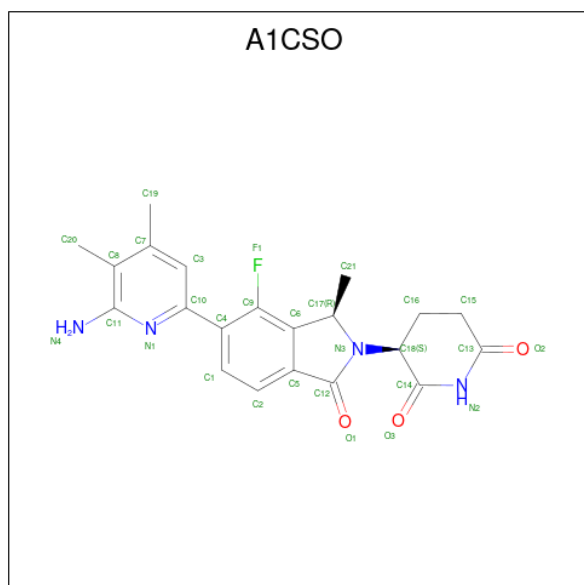
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Chain	Residue	Modelled	Actual	Comment	Reference
C	134	SER	-	expression tag	UNP Q9UKS7

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (3S)-3-[(3R,5M)-5-(6-amino-4,5-dimethylpyridin-2-yl)-4-fluoro-3-methyl-1-oxo-1,3-dihydro-2H-isoindol-2-yl]piperidine-2,6-dione (CCD ID: A1CSO) (formula: C₂₁H₂₁FN₄O₃) (labeled as "Ligand of Interest" by depositor).

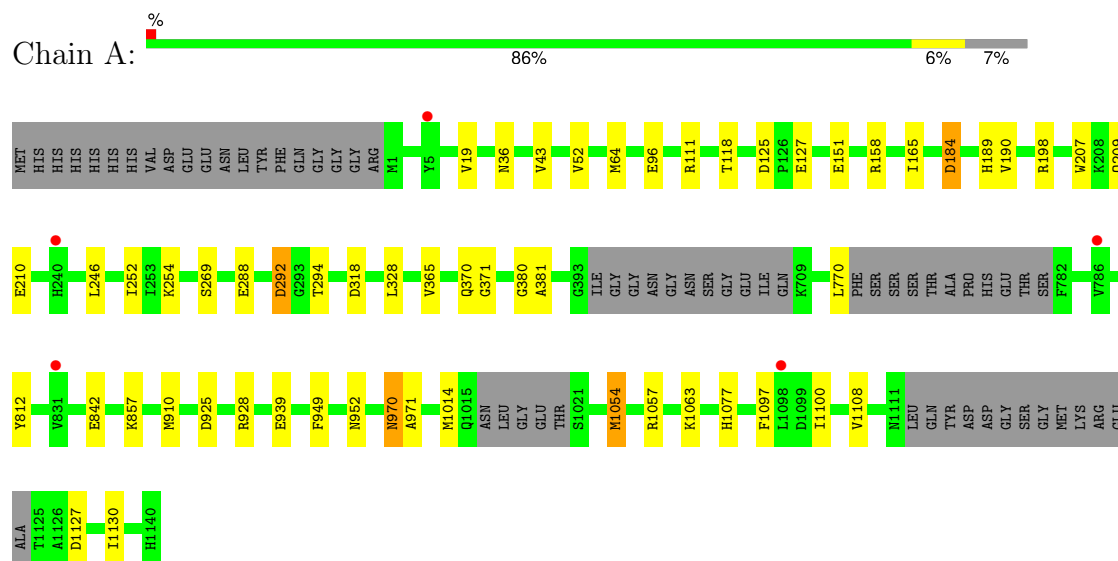


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	F	H	N	O	21	0
			50	21	1	21	4	3		

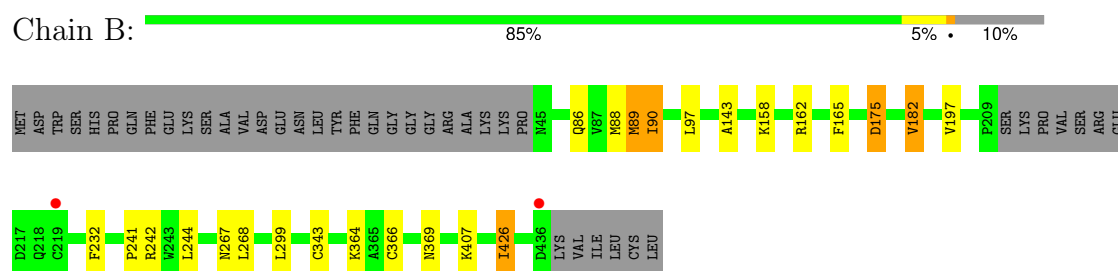
3 Residue-property plots [i](#)

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.

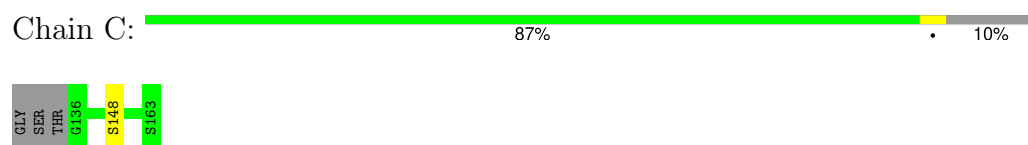
• Molecule 1: DNA damage-binding protein 1



• Molecule 2: Protein cereblon



• Molecule 3: Zinc finger protein Helios



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	259.89Å 259.89Å 124.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.20 – 3.53 37.20 – 3.53	Depositor EDS
% Data completeness (in resolution range)	67.4 (37.20-3.53) 67.3 (37.20-3.53)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 3.49Å)	Xtriage
Refinement program	BUSTER 2.11.8 (10-JUL-2024)	Depositor
R, R_{free}	0.229 , 0.236 0.249 , 0.261	Depositor DCC
R_{free} test set	1012 reflections (3.29%)	wwPDB-VP
Wilson B-factor (Å ²)	146.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18588	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: ZN, A1CSO

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	0.73	1/6242 (0.0%)	0.94	4/8462 (0.0%)
2	B	0.79	1/3111 (0.0%)	0.98	2/4235 (0.0%)
3	C	0.77	0/227	1.00	0/302
All	All	0.75	2/9580 (0.0%)	0.96	6/12999 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	426	ILE	CA-CB	5.64	1.59	1.53
1	A	184	ASP	CA-C	5.08	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	90	ILE	CB-CA-C	6.57	117.87	111.23
1	A	925	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	949	PHE	CA-CB-CG	5.59	119.39	113.80
2	B	175	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	292	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	207	TRP	N-CA-C	5.11	117.01	108.99

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	6132	5990	5993	18	0
2	B	3039	2939	2939	6	1
3	C	222	214	214	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	29	21	0	0	0
All	All	9424	9164	9146	22	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (22) 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:118:THR:HG21	1:A:165:ILE:O	1.98	0.62
1:A:125:ASP:OD2	1:A:127:GLU:HG2	2.03	0.58
1:A:19:VAL:HG22	1:A:64:MET:HE3	1.88	0.55
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.89	0.54
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.92	0.52
1:A:190:VAL:O	1:A:209:GLN:HA	2.10	0.52
1:A:910:MET:HE1	2:B:244:LEU:HD11	1.92	0.52
1:A:328:LEU:HD22	1:A:381:ALA:HB3	1.93	0.51
1:A:118:THR:O	1:A:118:THR:HG22	2.10	0.51
1:A:971:ALA:HB3	1:A:1077:HIS:O	2.11	0.51
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.93	0.51
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.13	0.49
1:A:1127:ASP:HA	1:A:1130:ILE:HD12	1.95	0.47
1:A:812:TYR:CZ	2:B:241:PRO:HB3	2.50	0.47
2:B:89:MET:HE2	2:B:97:LEU:HD13	1.98	0.45
1:A:1057:ARG:HD3	1:A:1108:VAL:O	2.19	0.43
1:A:1054:MET:HE3	1:A:1054:MET:HA	2.01	0.43
1:A:184:ASP:OD1	1:A:189:HIS:NE2	2.49	0.42
2:B:232:PHE:O	2:B:242:ARG:HG2	2.18	0.42
1:A:328:LEU:O	1:A:380:GLY:HA2	2.19	0.42
1:A:952:ASN:OD1	1:A:970:ASN:HB3	2.20	0.41
1:A:1054:MET:HE2	1:A:1108:VAL:HG12	2.02	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ASN:ND2	2:B:369:ASN:HD21[9_555]	1.26	0.34

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	786/856 (92%)	749 (95%)	32 (4%)	5 (1%)	21	55
2	B	381/426 (89%)	360 (94%)	20 (5%)	1 (0%)	36	66
3	C	26/31 (84%)	23 (88%)	3 (12%)	0	100	100
All	All	1193/1313 (91%)	1132 (95%)	55 (5%)	6 (0%)	24	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLN
1	A	970	ASN
1	A	318	ASP
1	A	371	GLY
1	A	36	ASN
2	B	197	VAL

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	664/744 (89%)	642 (97%)	22 (3%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	333/385 (86%)	318 (96%)	15 (4%)	24	51
3	C	24/26 (92%)	23 (96%)	1 (4%)	26	52
All	All	1021/1155 (88%)	983 (96%)	38 (4%)	30	56

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLU
1	A	111	ARG
1	A	151	GLU
1	A	158	ARG
1	A	198	ARG
1	A	210	GLU
1	A	246	LEU
1	A	252	ILE
1	A	254	LYS
1	A	269	SER
1	A	288	GLU
1	A	292	ASP
1	A	294	THR
1	A	365	VAL
1	A	770	LEU
1	A	842	GLU
1	A	857	LYS
1	A	928	ARG
1	A	939	GLU
1	A	1014	MET
1	A	1054	MET
1	A	1063	LYS
2	B	86	GLN
2	B	88	MET
2	B	89	MET
2	B	90	ILE
2	B	162	ARG
2	B	175	ASP
2	B	182	VAL
2	B	267	ASN
2	B	268	LEU
2	B	299	LEU
2	B	343	CYS
2	B	364	LYS

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Mol	Chain	Res	Type
2	B	366	CYS
2	B	407	LYS
2	B	426	ILE
3	C	148	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	234	GLN
1	A	711	HIS
1	A	797	HIS
1	A	950	ASN
1	A	991	HIS
1	A	993	GLN
1	A	1034	ASN
1	A	1059	ASN
1	A	1106	GLN
2	B	218	GLN
2	B	225	GLN
2	B	228	GLN
2	B	267	ASN
2	B	297	GLN
2	B	327	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

Of 3 ligands modelled in this entry, 2 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$
5	A1CSO	B	502	-	32,32,32	0.42	0	41,49,49	0.58	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
5	A1CSO	B	502	-	-	0/8/37/37	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

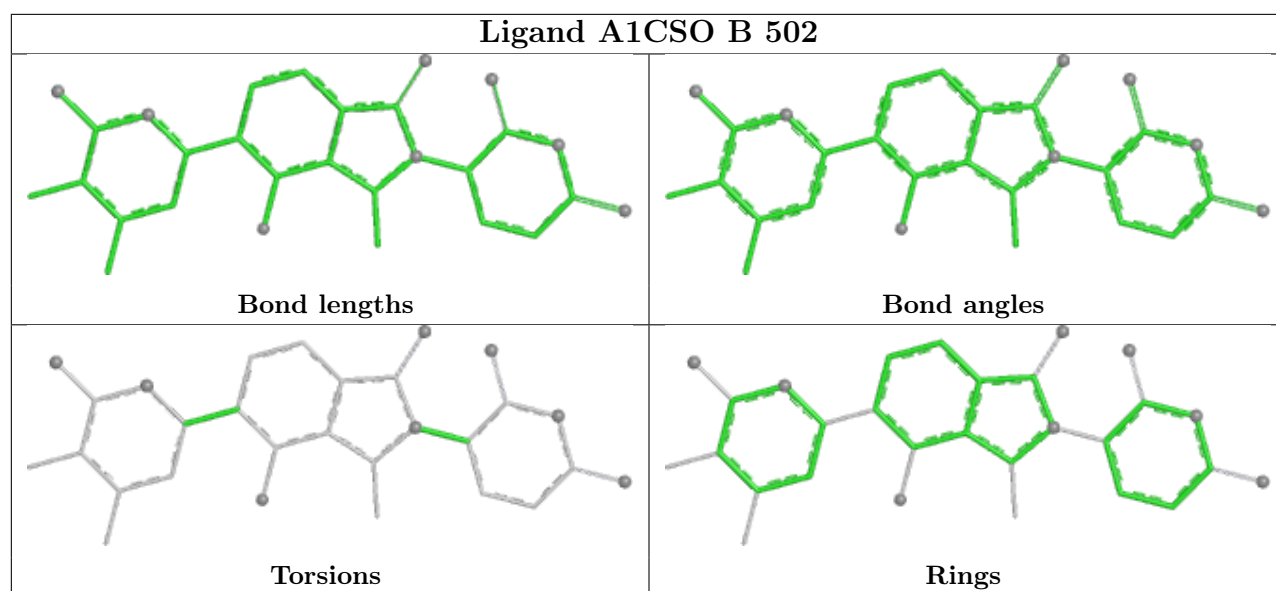
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	796/856 (92%)	-0.26	5 (0%) 85 63	58, 87, 118, 146	0
2	B	385/426 (90%)	-0.10	2 (0%) 87 66	60, 90, 133, 157	0
3	C	28/31 (90%)	-0.32	0 100 100	72, 94, 107, 124	0
All	All	1209/1313 (92%)	-0.21	7 (0%) 85 63	58, 88, 123, 157	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	786	VAL	2.8
1	A	240	HIS	2.6
1	A	831	VAL	2.6
2	B	219	CYS	2.4
1	A	1098	LEU	2.2
2	B	436	ASP	2.2
1	A	5	TYR	2.2

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.

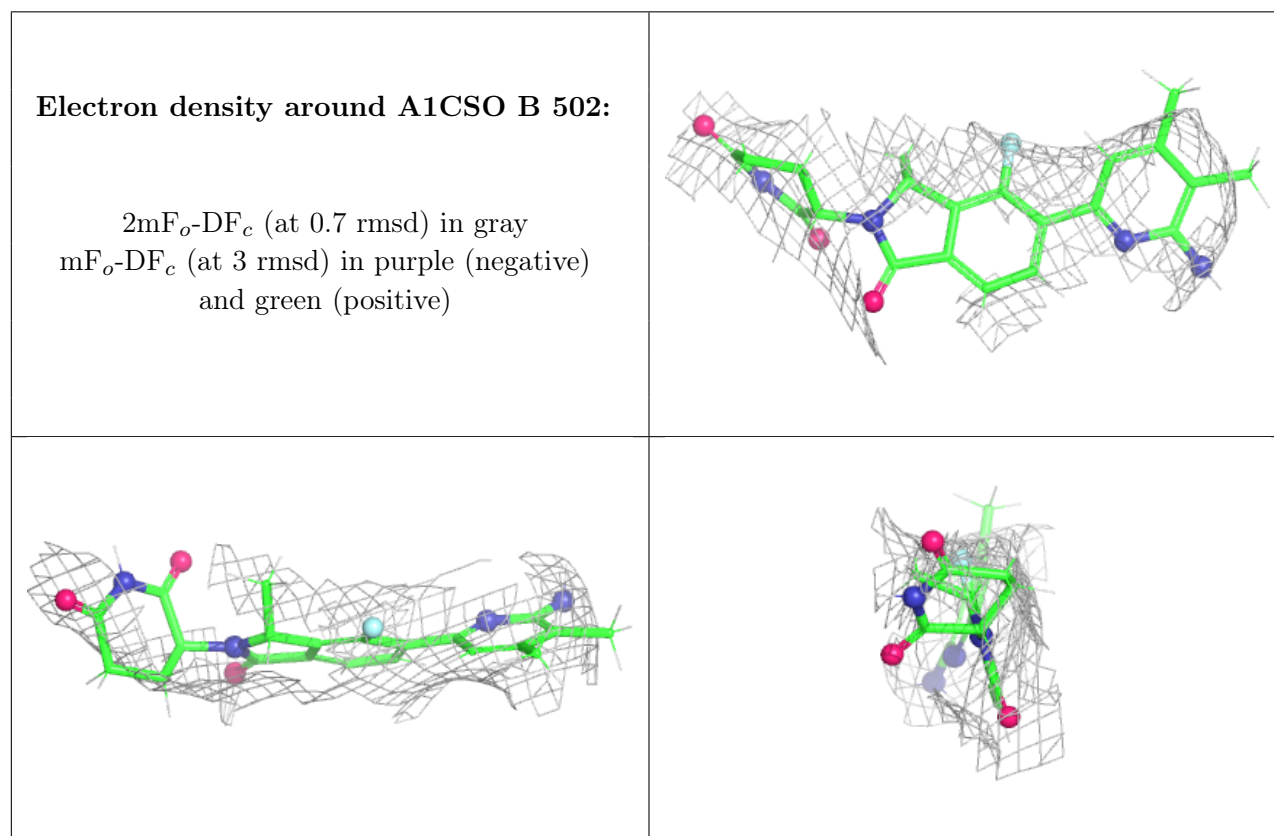
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
5	A1CSO	B	502	29/29	0.95	0.07	150,151,195,196	50
4	ZN	C	201	1/1	1.00	0.05	144,144,144,144	0
4	ZN	B	501	1/1	1.00	0.05	150,150,150,150	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 [i](#)

There are no such residues in this entry.