



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 PM UTC

PDB ID : 9Q22 / pdb_00009q22
Title : Crystal structure of ternary complex Helios-ZF2:I-19:CRBN:DDB1
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Deposited on : 2025-08-14
Resolution : 3.41 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

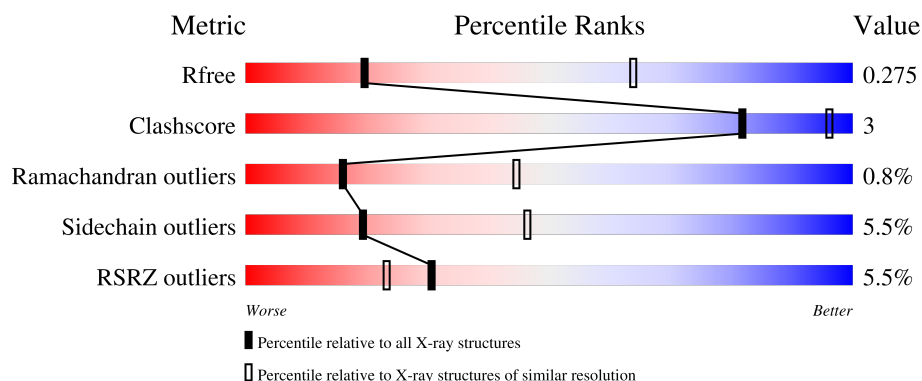
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	4% 82% 10% 7%
2	B	426	7% 79% 10% 10%
3	C	31	74% 13% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18612 atoms, of which 9181 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 40 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	382	PHE	-	linker	UNP Q16531
A	383	LYS	-	linker	UNP Q16531
A	384	GLU	-	linker	UNP Q16531
A	385	GLY	-	linker	UNP Q16531
A	386	SER	-	linker	UNP Q16531
A	387	LEU	-	linker	UNP Q16531
A	388	ARG	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	389	ILE	-	linker	UNP Q16531
A	390	ILE	-	linker	UNP Q16531
A	391	ARG	-	linker	UNP Q16531
A	392	ASN	-	linker	UNP Q16531
A	393	GLY	-	linker	UNP Q16531
A	698	ILE	-	linker	UNP Q16531
A	699	GLY	-	linker	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	2950	0	0
			5993	1935	2950	513	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

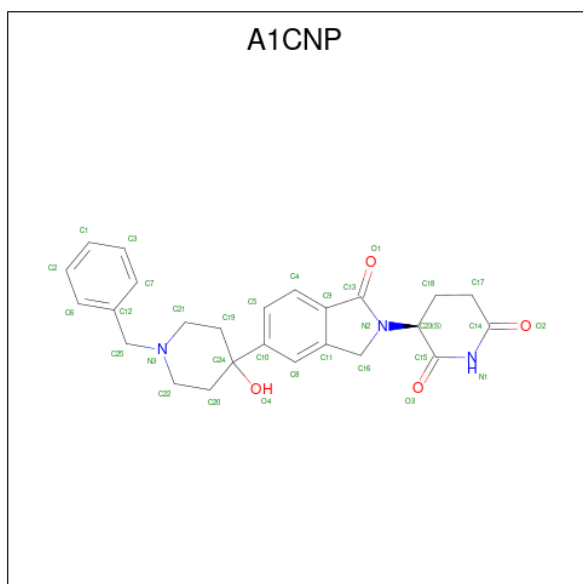
- Molecule 3 is a protein called Zinc finger protein Helios.

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
C	134	SER	-	expression tag	UNP Q9UKS7

- Molecule 4 is (3S)-3-[5-(1-benzyl-4-hydroxypiperidin-4-yl)-1-oxo-1,3-dihydro-2H-isoindol-2-yl]piperidine-2,6-dione (CCD ID: A1CNP) (formula: C₂₅H₂₇N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	27	0
			59	25	27	3	4		

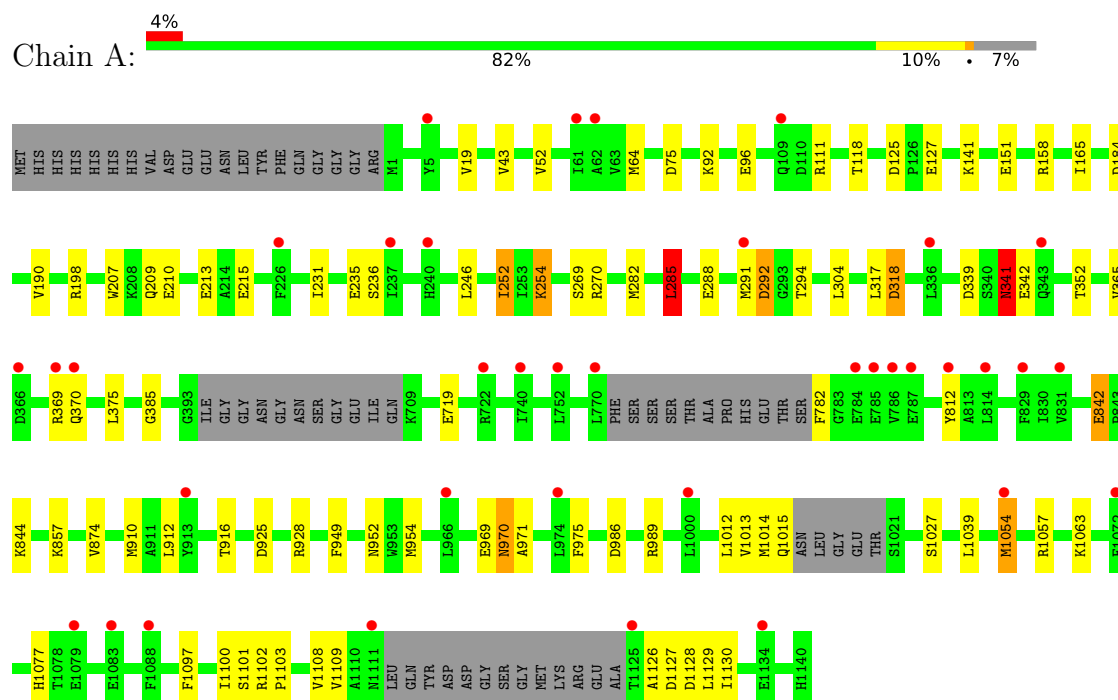
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

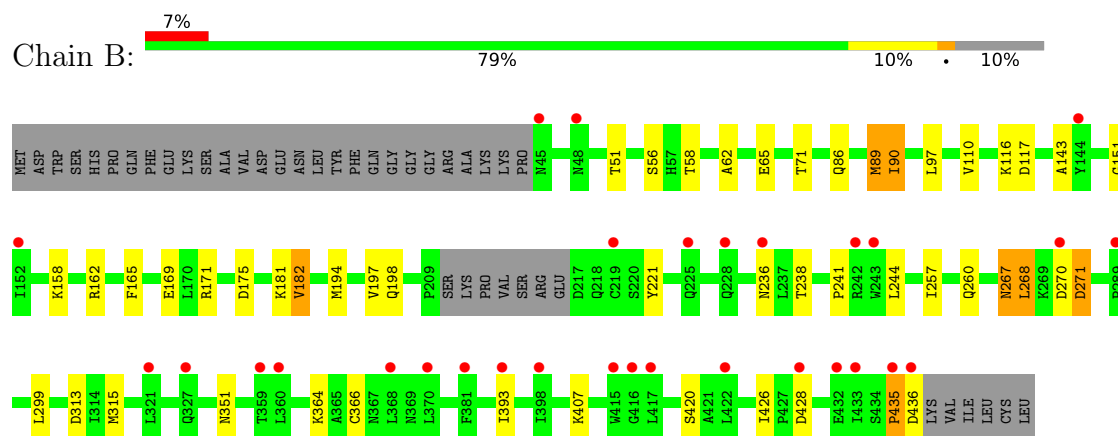
3 Residue-property plots [i](#)

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	260.24Å 260.24Å 123.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	130.12 – 3.41 130.12 – 3.41	Depositor EDS
% Data completeness (in resolution range)	64.0 (130.12-3.41) 64.0 (130.12-3.41)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
R, R_{free}	0.220 , 0.252 0.232 , 0.275	Depositor DCC
R_{free} test set	1083 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å ²)	123.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 142.4	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	0.91	EDS
Total number of atoms	18612	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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, A1CNP

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	0.77	0/6242	1.04	16/8462 (0.2%)
2	B	0.83	0/3115	1.08	10/4239 (0.2%)
3	C	0.77	0/227	1.08	1/302 (0.3%)
All	All	0.79	0/9584	1.05	27/13003 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	292	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	341	ASN	CA-CB-CG	7.08	119.68	112.60
2	B	271	ASP	CA-CB-CG	7.08	119.68	112.60
1	A	925	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	970	ASN	CA-C-N	6.02	131.21	122.36
1	A	970	ASN	C-N-CA	6.02	131.21	122.36
1	A	782	PHE	CA-CB-CG	5.81	119.61	113.80
2	B	267	ASN	CA-C-N	5.75	128.87	120.71
2	B	267	ASN	C-N-CA	5.75	128.87	120.71
2	B	268	LEU	N-CA-C	5.64	118.41	110.23
1	A	207	TRP	N-CA-C	5.55	117.50	109.07
2	B	351	ASN	CA-CB-CG	5.53	118.13	112.60
3	C	143	ASN	CA-CB-CG	5.51	118.11	112.60
2	B	435	PRO	CA-C-N	5.46	131.53	121.70
2	B	435	PRO	C-N-CA	5.46	131.53	121.70
1	A	285	LEU	N-CA-CB	5.36	119.21	110.37
1	A	75	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	969	GLU	CA-C-N	5.28	129.17	121.31
1	A	969	GLU	C-N-CA	5.28	129.17	121.31
1	A	236	SER	N-CA-C	5.11	117.89	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	TRP	CA-C-N	5.10	131.28	121.54
1	A	207	TRP	C-N-CA	5.10	131.28	121.54
1	A	949	PHE	CA-CB-CG	5.09	118.89	113.80
2	B	270	ASP	CA-CB-CG	5.05	117.65	112.60
2	B	181	LYS	N-CA-C	-5.03	101.55	109.25
2	B	90	ILE	CB-CA-C	5.03	117.42	111.59

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	35	0
2	B	3043	2950	2950	14	0
3	C	222	214	214	1	0
4	B	32	27	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	9431	9181	9157	47	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 3.

All (47) 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:190:VAL:O	1:A:209:GLN:HA	1.73	0.89
2:B:313:ASP:OD2	2:B:435:PRO:HD2	1.89	0.73
1:A:125:ASP:OD2	1:A:127:GLU:HG2	1.90	0.68
1:A:971:ALA:HB3	1:A:1077:HIS:O	1.96	0.65
1:A:118:THR:HG21	1:A:165:ILE:O	1.96	0.64
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.85	0.58
1:A:910:MET:HE1	2:B:244:LEU:HD11	1.85	0.58
2:B:89:MET:HE2	2:B:97:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.88	0.56
1:A:118:THR:O	1:A:118:THR:HG22	2.06	0.55
2:B:194:MET:HA	2:B:194:MET:HE2	1.89	0.55
1:A:874:VAL:HG11	1:A:916:THR:HG22	1.91	0.53
1:A:954:MET:HE3	1:A:975:PHE:CZ	2.45	0.52
2:B:197:VAL:HG11	2:B:238:THR:CG2	2.38	0.52
1:A:1127:ASP:HA	1:A:1130:ILE:HD12	1.92	0.52
3:C:154:ASN:O	3:C:157:ARG:HG2	2.09	0.51
1:A:812:TYR:CZ	2:B:241:PRO:HB3	2.47	0.49
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.13	0.48
1:A:285:LEU:H	1:A:285:LEU:HD13	1.79	0.48
1:A:986:ASP:OD1	1:A:989:ARG:HD3	2.15	0.47
1:A:1013:VAL:O	1:A:1015:GLN:OE1	2.32	0.47
1:A:270:ARG:CB	1:A:282:MET:HE3	2.45	0.47
1:A:954:MET:HE3	1:A:975:PHE:HZ	1.78	0.47
1:A:1109:VAL:HG12	1:A:1129:LEU:HD22	1.97	0.47
1:A:952:ASN:OD1	1:A:970:ASN:HB3	2.14	0.46
2:B:56:SER:HB2	2:B:58:THR:HG23	1.96	0.46
1:A:19:VAL:HG22	1:A:64:MET:HE3	1.99	0.45
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.18	0.44
1:A:341:ASN:ND2	1:A:342:GLU:H	2.16	0.44
2:B:197:VAL:HG11	2:B:238:THR:HG22	1.98	0.44
1:A:235:GLU:O	1:A:254:LYS:HE3	2.18	0.43
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	1.99	0.43
1:A:1054:MET:SD	1:A:1129:LEU:HD21	2.59	0.43
1:A:285:LEU:HD13	1:A:285:LEU:N	2.33	0.43
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.01	0.42
2:B:143:ALA:HB3	2:B:158:LYS:HB2	2.00	0.42
1:A:252:ILE:HD11	1:A:304:LEU:HD22	2.02	0.42
1:A:1101:SER:OG	1:A:1103:PRO:HD2	2.20	0.42
1:A:842:GLU:HB3	1:A:844:LYS:NZ	2.34	0.42
1:A:385:GLY:HA3	1:A:719:GLU:O	2.20	0.42
1:A:317:LEU:O	1:A:318:ASP:HB2	2.20	0.41
2:B:71:THR:HG21	2:B:117:ASP:OD1	2.20	0.41
1:A:1057:ARG:HD3	1:A:1108:VAL:O	2.21	0.40
2:B:257:ILE:HG23	2:B:315:MET:HE1	2.03	0.40
1:A:213:GLU:OE2	1:A:215:GLU:HB2	2.20	0.40
2:B:393:ILE:HD12	2:B:393:ILE:N	2.37	0.40
1:A:912:LEU:HD11	2:B:244:LEU:HD21	2.03	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	786/856 (92%)	746 (95%)	36 (5%)	4 (0%)	24	54
2	B	381/426 (89%)	358 (94%)	18 (5%)	5 (1%)	9	33
3	C	26/31 (84%)	22 (85%)	4 (15%)	0	100	100
All	All	1193/1313 (91%)	1126 (94%)	58 (5%)	9 (1%)	16	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLN
1	A	339	ASP
2	B	198	GLN
2	B	428	ASP
2	B	62	ALA
2	B	151	GLY
1	A	369	ARG
2	B	116	LYS
1	A	318	ASP

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%)	635 (96%)	29 (4%)	25	51
2	B	334/385 (87%)	310 (93%)	24 (7%)	13	39
3	C	24/26 (92%)	21 (88%)	3 (12%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1022/1155 (88%)	966 (94%)	56 (6%)	19	46

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	96	GLU
1	A	111	ARG
1	A	141	LYS
1	A	151	GLU
1	A	158	ARG
1	A	198	ARG
1	A	210	GLU
1	A	231	ILE
1	A	246	LEU
1	A	252	ILE
1	A	254	LYS
1	A	269	SER
1	A	285	LEU
1	A	288	GLU
1	A	291	MET
1	A	292	ASP
1	A	294	THR
1	A	341	ASN
1	A	352	THR
1	A	365	VAL
1	A	842	GLU
1	A	857	LYS
1	A	928	ARG
1	A	1014	MET
1	A	1054	MET
1	A	1063	LYS
1	A	1102	ARG
1	A	1128	ASP
2	B	51	THR
2	B	65	GLU
2	B	86	GLN
2	B	89	MET
2	B	90	ILE
2	B	110	VAL
2	B	162	ARG
2	B	169	GLU

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Mol	Chain	Res	Type
2	B	171	ARG
2	B	175	ASP
2	B	182	VAL
2	B	221	TYR
2	B	236	ASN
2	B	260	GLN
2	B	267	ASN
2	B	268	LEU
2	B	271	ASP
2	B	299	LEU
2	B	364	LYS
2	B	366	CYS
2	B	407	LYS
2	B	420	SER
2	B	426	ILE
2	B	436	ASP
3	C	143	ASN
3	C	148	SER
3	C	161	LEU

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	4	ASN
1	A	203	ASN
1	A	234	GLN
1	A	341	ASN
1	A	711	HIS
1	A	991	HIS
1	A	1034	ASN
2	B	86	GLN
2	B	127	ASN
2	B	129	GLN
2	B	173	GLN
2	B	225	GLN
2	B	233	HIS
2	B	325	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	$\# Z > 2$
4	A1CNP	B	4000	-	36,36,36	0.25	0	53,53,53	0.48	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
4	A1CNP	B	4000	-	-	0/14/51/51	0/5/5/5

There are no bond length outliers.

There are no bond angle outliers.

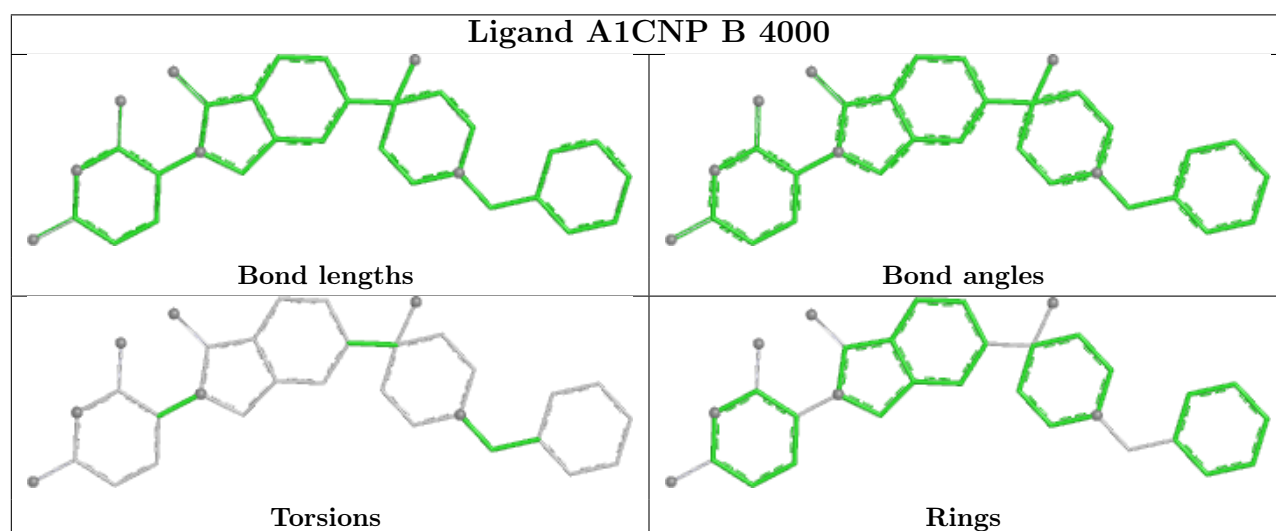
There are no chirality outliers.

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

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	796/856 (92%)	0.17	37 (4%) 37 27	45, 74, 106, 131	0
2	B	385/426 (90%)	0.40	30 (7%) 19 16	46, 76, 117, 140	0
3	C	28/31 (90%)	-0.21	0 100 100	60, 79, 93, 108	0
All	All	1209/1313 (92%)	0.23	67 (5%) 30 23	45, 75, 110, 140	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	786	VAL	6.5
1	A	1079	GLU	5.0
1	A	787	GLU	4.3
2	B	381	PHE	4.3
1	A	829	PHE	4.2
1	A	831	VAL	4.0
2	B	393	ILE	3.9
1	A	336	LEU	3.7
1	A	62	ALA	3.6
1	A	770	LEU	3.5
2	B	243	TRP	3.5
2	B	225	GLN	3.5
1	A	240	HIS	3.5
2	B	415	TRP	3.4
1	A	1000	LEU	3.3
2	B	436	ASP	3.1
2	B	228	GLN	3.0
2	B	433	ILE	3.0
2	B	144	TYR	3.0
2	B	152	ILE	2.9
1	A	369	ARG	2.9
1	A	61	ILE	2.9
1	A	1111	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	752	LEU	2.8
2	B	359	THR	2.8
1	A	784	GLU	2.8
2	B	360	LEU	2.7
1	A	1054	MET	2.7
2	B	270	ASP	2.7
1	A	740	ILE	2.7
1	A	291	MET	2.7
1	A	966	LEU	2.7
2	B	289	PRO	2.6
1	A	1083	GLU	2.6
2	B	398	ILE	2.6
1	A	812	TYR	2.6
1	A	913	TYR	2.6
2	B	368	LEU	2.6
2	B	370	LEU	2.5
2	B	327	GLN	2.5
1	A	370	GLN	2.5
1	A	722	ARG	2.4
1	A	785	GLU	2.4
2	B	432	GLU	2.4
1	A	974	LEU	2.4
2	B	242	ARG	2.3
2	B	45	ASN	2.3
2	B	417	LEU	2.3
1	A	366	ASP	2.3
1	A	814	LEU	2.3
2	B	321	LEU	2.3
2	B	236	ASN	2.3
1	A	226	PHE	2.2
1	A	109	GLN	2.2
1	A	1134	GLU	2.2
2	B	435	PRO	2.2
1	A	5	TYR	2.2
2	B	48	ASN	2.2
1	A	237	ILE	2.1
2	B	416	GLY	2.1
1	A	1088	PHE	2.1
1	A	1125	THR	2.0
2	B	428	ASP	2.0
2	B	219	CYS	2.0
1	A	343	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1072	PHE	2.0
2	B	422	LEU	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](#)

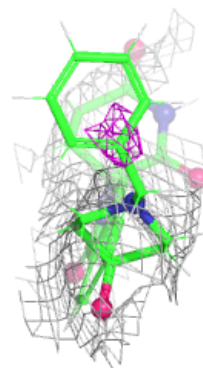
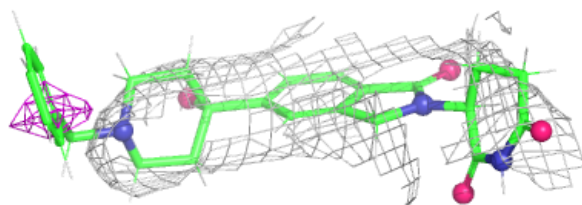
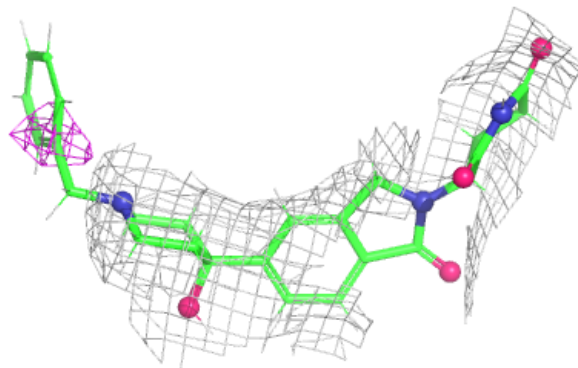
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A1CNP	B	4000	32/32	0.95	0.09	138,145,190,194	27
5	ZN	B	4001	1/1	1.00	0.03	127,127,127,127	0
5	ZN	C	201	1/1	1.00	0.05	121,121,121,121	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 A1CNP B 4000:

$2mF_o-DF_c$ (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.