



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:48 PM UTC

PDB ID : 4CI2 / pdb_00004ci2
Title : Structure of the DDB1-CRBN E3 ubiquitin ligase bound to lenalidomide
Authors : Fischer, E.S.; Boehm, K.; Thoma, N.H.
Deposited on : 2013-12-05
Resolution : 2.95 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

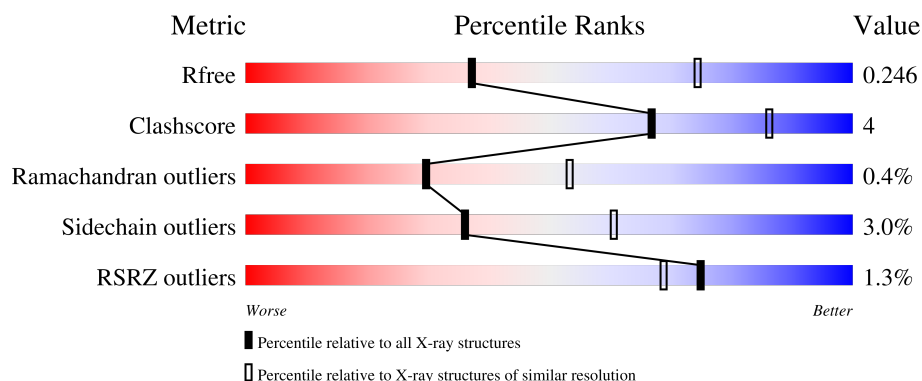
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

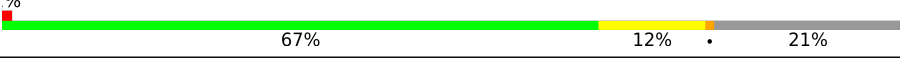
The reported resolution of this entry is 2.95 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	1158	
2	B	469	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11439 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 DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1091	Total	C	N	O	S	0	0	0
			8434	5361	1420	1608	45			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	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	HIS	-	expression tag	UNP Q16531
A	-11	HIS	-	expression tag	UNP Q16531
A	-10	ARG	-	expression tag	UNP Q16531
A	-9	ARG	-	expression tag	UNP Q16531
A	-8	LEU	-	expression tag	UNP Q16531
A	-7	VAL	-	expression tag	UNP Q16531
A	-6	PRO	-	expression tag	UNP Q16531
A	-5	ARG	-	expression tag	UNP Q16531
A	-4	GLY	-	expression tag	UNP Q16531
A	-3	SER	-	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

- Molecule 2 is a protein called PROTEIN CEREBLON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	370	Total	C	N	O	S	0	0	0
			2977	1891	522	542	22			

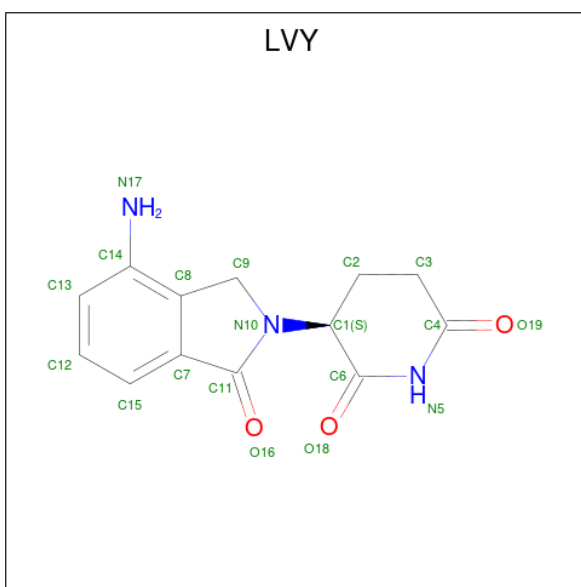
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP P0CF65
B	-22	ASP	-	expression tag	UNP P0CF65
B	-21	TRP	-	expression tag	UNP P0CF65
B	-20	SER	-	expression tag	UNP P0CF65
B	-19	HIS	-	expression tag	UNP P0CF65
B	-18	PRO	-	expression tag	UNP P0CF65
B	-17	GLN	-	expression tag	UNP P0CF65
B	-16	PHE	-	expression tag	UNP P0CF65
B	-15	GLU	-	expression tag	UNP P0CF65
B	-14	LYS	-	expression tag	UNP P0CF65
B	-13	SER	-	expression tag	UNP P0CF65
B	-12	ALA	-	expression tag	UNP P0CF65
B	-11	VAL	-	expression tag	UNP P0CF65
B	-10	ASP	-	expression tag	UNP P0CF65
B	-9	GLU	-	expression tag	UNP P0CF65
B	-8	ASN	-	expression tag	UNP P0CF65
B	-7	LEU	-	expression tag	UNP P0CF65
B	-6	TYR	-	expression tag	UNP P0CF65
B	-5	PHE	-	expression tag	UNP P0CF65
B	-4	GLN	-	expression tag	UNP P0CF65
B	-3	GLY	-	expression tag	UNP P0CF65
B	-2	GLY	-	expression tag	UNP P0CF65
B	-1	GLY	-	expression tag	UNP P0CF65
B	0	ARG	-	expression tag	UNP P0CF65

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0

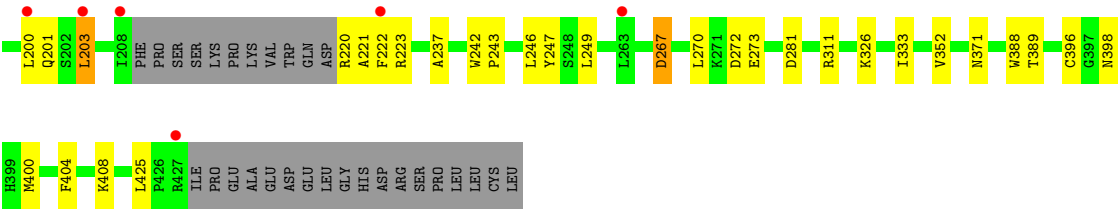
- Molecule 4 is S-Lenalidomide (CCD ID: LVY) (formula: C₁₃H₁₃N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			19	13	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.11Å 172.11Å 139.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 2.95 29.71 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.71-2.95) 99.7 (29.71-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.193 , 0.234 0.207 , 0.246	Depositor DCC
R_{free} test set	2528 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11439	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: LVY, ZN

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	0.80	1/8589 (0.0%)	1.25	25/11653 (0.2%)
2	B	0.82	0/3051	1.32	20/4141 (0.5%)
All	All	0.80	1/11640 (0.0%)	1.27	45/15794 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	954	MET	SD-CE	-6.81	1.62	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	LYS	CA-C-N	7.78	131.04	120.38
2	B	117	LYS	C-N-CA	7.78	131.04	120.38
1	A	925	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	970	ASN	CA-C-N	6.80	134.53	121.54
1	A	970	ASN	C-N-CA	6.80	134.53	121.54
1	A	312	GLU	N-CA-C	-6.26	104.69	112.90
1	A	275	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	1134	GLU	CA-C-N	6.01	128.62	120.38
1	A	1134	GLU	C-N-CA	6.01	128.62	120.38
2	B	49	ASN	CA-CB-CG	5.99	118.59	112.60
2	B	200	LEU	N-CA-C	-5.96	101.38	109.54
1	A	633	THR	N-CA-C	-5.90	106.42	113.97
1	A	851	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	202	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	332	GLN	CA-C-N	5.71	131.05	123.00
1	A	332	GLN	C-N-CA	5.71	131.05	123.00
1	A	116	SER	CA-C-N	5.70	128.19	120.44
1	A	116	SER	C-N-CA	5.70	128.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	920	PHE	CA-CB-CG	5.68	119.48	113.80
2	B	201	GLN	N-CA-C	5.62	115.53	108.45
2	B	281	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	55	PRO	CA-C-N	5.45	128.34	120.38
2	B	55	PRO	C-N-CA	5.45	128.34	120.38
2	B	371	ASN	CA-CB-CG	5.28	117.88	112.60
2	B	203	LEU	CA-C-N	5.25	127.31	120.28
2	B	203	LEU	C-N-CA	5.25	127.31	120.28
1	A	23	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	110	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	182	LYS	N-CA-C	-5.22	100.58	108.67
1	A	1070	HIS	CA-C-N	5.18	127.94	120.38
1	A	1070	HIS	C-N-CA	5.18	127.94	120.38
2	B	220	ARG	CA-C-N	5.17	131.41	121.54
2	B	220	ARG	C-N-CA	5.17	131.41	121.54
2	B	408	LYS	CA-C-N	5.16	127.92	120.38
2	B	408	LYS	C-N-CA	5.16	127.92	120.38
1	A	1107	GLU	CA-C-N	5.12	127.02	120.56
1	A	1107	GLU	C-N-CA	5.12	127.02	120.56
1	A	1030	PHE	CA-CB-CG	5.10	118.90	113.80
2	B	222	PHE	CA-CB-CG	5.09	118.89	113.80
2	B	267	ASP	CA-C-N	5.06	127.48	120.29
2	B	267	ASP	C-N-CA	5.06	127.48	120.29
2	B	237	ALA	N-CA-C	-5.06	106.37	112.54
1	A	207	TRP	CA-C-N	5.05	128.24	120.82
1	A	207	TRP	C-N-CA	5.05	128.24	120.82
1	A	744	ASP	CA-CB-CG	5.02	117.62	112.60

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	8434	0	8337	68	0
2	B	2977	0	2918	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	B	19	0	13	0	0
5	A	6	0	0	0	0
5	B	2	0	0	0	0
All	All	11439	0	11268	84	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 4.

All (84) 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:144:ALA:HB3	2:B:159:LYS:HB2	1.60	0.83
1:A:954:MET:HE2	1:A:975:PHE:HZ	1.51	0.75
1:A:765:VAL:HG12	1:A:806:GLN:HB3	1.71	0.72
1:A:255:GLN:HB2	1:A:279:ARG:HH22	1.57	0.69
1:A:910:MET:HE3	2:B:311:ARG:HH22	1.64	0.62
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.82	0.62
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.82	0.61
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.82	0.60
1:A:889:ARG:HH11	1:A:904:ASN:HD21	1.48	0.60
1:A:928:ARG:HA	1:A:954:MET:HE3	1.83	0.60
1:A:826:ASN:HB3	1:A:852:GLN:HE22	1.67	0.58
2:B:83:PRO:HB2	2:B:110:MET:HE2	1.85	0.58
1:A:971:ALA:HB3	1:A:1077:HIS:O	2.05	0.56
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.05	0.56
1:A:180:PHE:HE1	1:A:193:TYR:HD2	1.53	0.56
1:A:324:VAL:HB	1:A:332:GLN:HB2	1.88	0.54
1:A:1039:LEU:HD22	1:A:1139:ILE:HD12	1.90	0.54
1:A:1080:ARG:HG3	1:A:1081:LYS:H	1.73	0.54
1:A:49:LEU:HD22	1:A:333:LEU:HD11	1.91	0.53
2:B:100:LEU:HB2	2:B:158:VAL:HG22	1.91	0.53
2:B:267:ASP:HB3	2:B:270:LEU:HB2	1.91	0.53
1:A:432:GLN:HG2	1:A:434:ARG:HH21	1.74	0.52
2:B:167:LYS:HB2	2:B:186:LEU:HD21	1.91	0.52
1:A:14:ALA:HB1	1:A:327:ARG:HG3	1.92	0.52
1:A:812:TYR:CZ	2:B:243:PRO:HB3	2.48	0.49
1:A:578:HIS:NE2	1:A:580:GLU:HG2	2.28	0.49
1:A:340:SER:HB3	1:A:346:TYR:CE2	2.48	0.49
1:A:45:THR:C	1:A:47:GLU:H	2.20	0.48
1:A:449:MET:HE3	1:A:450:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ASN:OD1	1:A:970:ASN:HB3	2.13	0.48
2:B:76:ASP:HB3	2:B:187:PRO:HG3	1.95	0.48
2:B:65:MET:HG2	2:B:146:ARG:HB2	1.96	0.48
2:B:388:TRP:HB3	2:B:404:PHE:CE1	2.48	0.47
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.96	0.47
2:B:246:LEU:HD12	2:B:249:LEU:HD12	1.95	0.47
1:A:269:SER:HA	1:A:285:LEU:HB2	1.96	0.47
1:A:272:LEU:HD21	1:A:336:LEU:HD11	1.96	0.47
1:A:1109:VAL:HG21	1:A:1126:ALA:HB2	1.97	0.47
2:B:120:THR:HG22	2:B:141:GLU:HG3	1.97	0.47
1:A:261:HIS:HA	1:A:272:LEU:O	2.15	0.47
1:A:864:LYS:HE2	1:A:891:TYR:HE1	1.80	0.47
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.98	0.46
1:A:1105:MET:SD	1:A:1130:ILE:HD11	2.56	0.46
2:B:194:THR:HG21	2:B:247:TYR:HD1	1.81	0.46
1:A:564:ILE:HG22	1:A:582:LEU:HB2	1.97	0.46
2:B:396:CYS:SG	2:B:398:ASN:HB2	2.55	0.46
2:B:242:TRP:HB3	2:B:246:LEU:HD23	1.97	0.46
1:A:1109:VAL:HG12	1:A:1129:LEU:HD22	1.98	0.45
1:A:32:LEU:HD13	1:A:66:LEU:HD11	1.98	0.45
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.98	0.45
1:A:40:GLU:HB3	1:A:42:TYR:CE2	2.51	0.45
1:A:18:CYS:HG	1:A:313:CYS:HG	1.64	0.45
1:A:403:ASP:HA	1:A:698:THR:HG22	1.98	0.44
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.98	0.44
1:A:385:GLY:HA3	1:A:719:GLU:O	2.17	0.44
1:A:1024:THR:HG22	1:A:1043:LEU:HD23	2.00	0.44
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	2.00	0.44
1:A:1076:PHE:O	1:A:1082:THR:HA	2.18	0.44
1:A:851:PHE:HB3	1:A:858:LEU:HD22	2.00	0.44
1:A:184:ASP:CG	1:A:189:HIS:HE2	2.26	0.43
1:A:516:LEU:HB2	1:A:532:THR:HG22	2.00	0.43
1:A:913:TYR:HB2	1:A:924:GLY:HA3	1.99	0.43
2:B:326:LYS:HG3	2:B:425:LEU:HD13	1.99	0.43
1:A:276:MET:HE2	2:B:203:LEU:HG	2.00	0.42
1:A:19:VAL:HG22	1:A:64:MET:HE3	2.00	0.42
1:A:762:SER:O	1:A:803:HIS:HA	2.19	0.41
1:A:895:THR:C	1:A:897:LYS:H	2.29	0.41
2:B:86:PRO:HG2	2:B:107:GLU:HG2	2.01	0.41
1:A:534:MET:HE2	1:A:558:ILE:HD13	2.02	0.41
1:A:586:ILE:HG13	1:A:608:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:HG12	1:A:349:ALA:HA	2.01	0.41
1:A:741:GLU:HG2	1:A:751:ALA:HA	2.02	0.41
2:B:333:ILE:HG12	2:B:400:MET:HE2	2.03	0.41
1:A:538:VAL:HG22	1:A:558:ILE:HD11	2.02	0.41
1:A:1104:LYS:HD3	1:A:1104:LYS:HA	1.87	0.41
1:A:607:GLY:HA2	1:A:635:PRO:HB3	2.02	0.41
1:A:40:GLU:HG2	1:A:54:GLU:HG3	2.02	0.41
1:A:168:LYS:HB3	1:A:221:ALA:HB2	2.03	0.41
1:A:907:ASN:C	1:A:909:ILE:H	2.29	0.41
1:A:596:PHE:HB3	1:A:661:SER:HB2	2.03	0.40
1:A:654:ASP:HA	1:A:675:GLU:HG3	2.02	0.40
1:A:586:ILE:HG21	1:A:608:ASP:H	1.86	0.40
1:A:793:ILE:HG21	1:A:853:TYR:CZ	2.56	0.40
1:A:282:MET:HB2	1:A:305:LEU:HD11	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	1077/1158 (93%)	1003 (93%)	69 (6%)	5 (0%)	24	49
2	B	366/469 (78%)	344 (94%)	21 (6%)	1 (0%)	36	59
All	All	1443/1627 (89%)	1347 (93%)	90 (6%)	6 (0%)	30	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	945	ILE
1	A	36	ASN
1	A	562	THR
2	B	221	ALA

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Mol	Chain	Res	Type
1	A	368	GLU
1	A	564	ILE

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	928/1014 (92%)	902 (97%)	26 (3%)	38	62
2	B	326/416 (78%)	315 (97%)	11 (3%)	32	58
All	All	1254/1430 (88%)	1217 (97%)	37 (3%)	36	60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	52	VAL
1	A	54	GLU
1	A	98	ILE
1	A	189	HIS
1	A	222	VAL
1	A	259	VAL
1	A	317	LEU
1	A	552	LEU
1	A	587	ILE
1	A	590	SER
1	A	614	PHE
1	A	661	SER
1	A	667	VAL
1	A	685	ASP
1	A	743	GLN
1	A	766	SER
1	A	785	GLU
1	A	786	VAL
1	A	919	ASP
1	A	920	PHE

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Mol	Chain	Res	Type
1	A	944	GLU
1	A	954	MET
1	A	987	GLU
1	A	1029	LEU
1	A	1137	THR
2	B	115	ILE
2	B	132	ARG
2	B	163	ARG
2	B	178	ILE
2	B	188	GLU
2	B	194	THR
2	B	223	ARG
2	B	272	ASP
2	B	273	GLU
2	B	352	VAL
2	B	389	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	203	ASN
1	A	211	ASN
1	A	241	ASN
1	A	261	HIS
1	A	332	GLN
1	A	465	HIS
1	A	481	GLN
1	A	522	HIS
1	A	648	ASN
1	A	664	HIS
1	A	672	ASN
1	A	677	ASN
1	A	797	HIS
1	A	852	GLN
1	A	877	ASN
1	A	904	ASN
1	A	999	HIS
1	A	1034	ASN
1	A	1059	ASN
2	B	116	GLN
2	B	164	GLN

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Mol	Chain	Res	Type
2	B	179	GLN
2	B	262	GLN
2	B	414	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 2 ligands modelled in this entry, 1 is 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	LVY	B	1429	-	21,21,21	0.93	1 (4%)	29,31,31	1.79	6 (20%)

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	LVY	B	1429	-	-	0/4/29/29	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1429	LVY	C12-C13	2.03	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1429	LVY	O16-C11-N10	5.46	129.67	125.34
4	B	1429	LVY	O16-C11-C7	-3.16	122.54	128.66
4	B	1429	LVY	C8-C7-C11	-2.88	106.14	108.62
4	B	1429	LVY	C3-C4-N5	2.57	119.42	116.69
4	B	1429	LVY	C2-C3-C4	-2.21	109.30	113.87
4	B	1429	LVY	C7-C11-N10	2.15	107.79	106.42

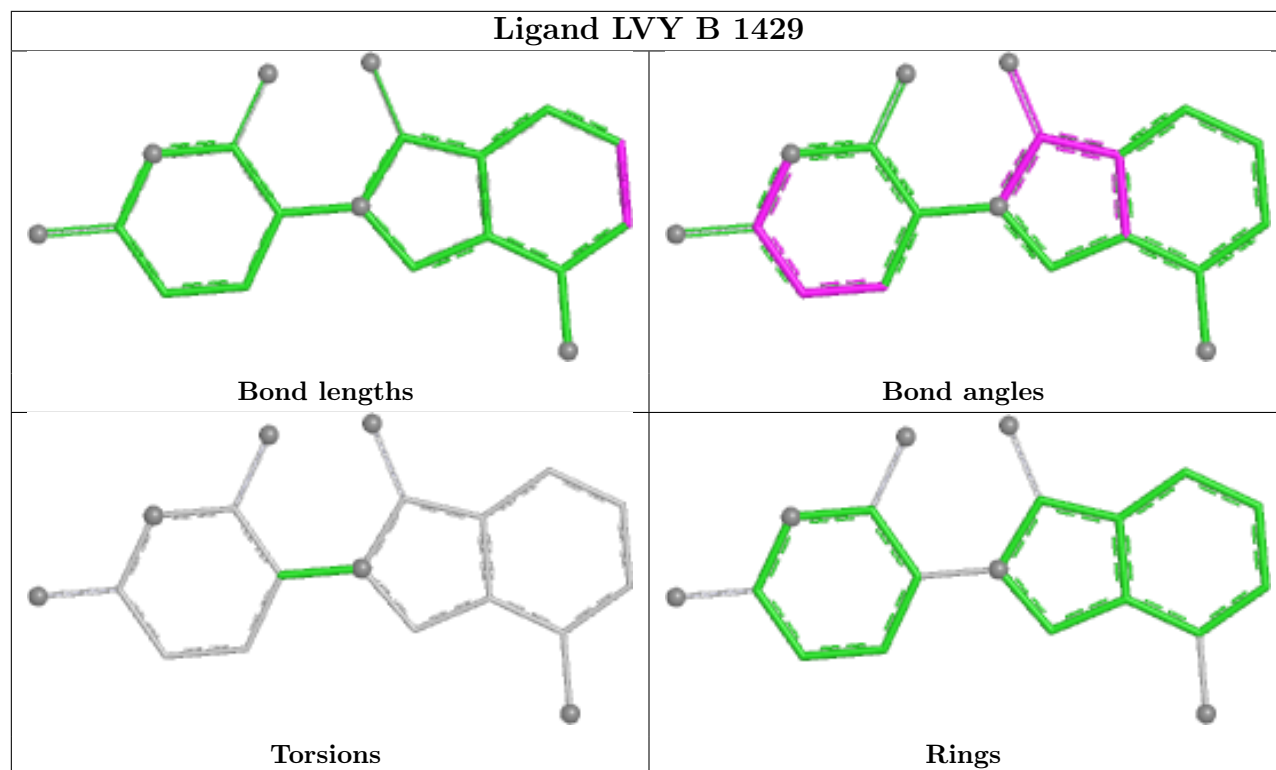
There are no chirality outliers.

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	1091/1158 (94%)	0.11	13 (1%) 76 71	52, 98, 140, 168	0
2	B	370/469 (78%)	-0.20	6 (1%) 70 63	44, 74, 121, 142	0
All	All	1461/1627 (89%)	0.03	19 (1%) 75 69	44, 93, 138, 168	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	208	ILE	4.4
2	B	200	LEU	3.3
1	A	221	ALA	2.8
2	B	222	PHE	2.6
1	A	771	PHE	2.4
1	A	551	GLY	2.3
1	A	246	LEU	2.2
1	A	224	GLU	2.2
1	A	169	PHE	2.2
2	B	203	LEU	2.1
1	A	318	ASP	2.1
2	B	263	LEU	2.1
2	B	427	ARG	2.1
1	A	770	LEU	2.1
1	A	145	LEU	2.0
1	A	984	THR	2.0
1	A	938	MET	2.0
1	A	965	PHE	2.0
1	A	979	LYS	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](#)

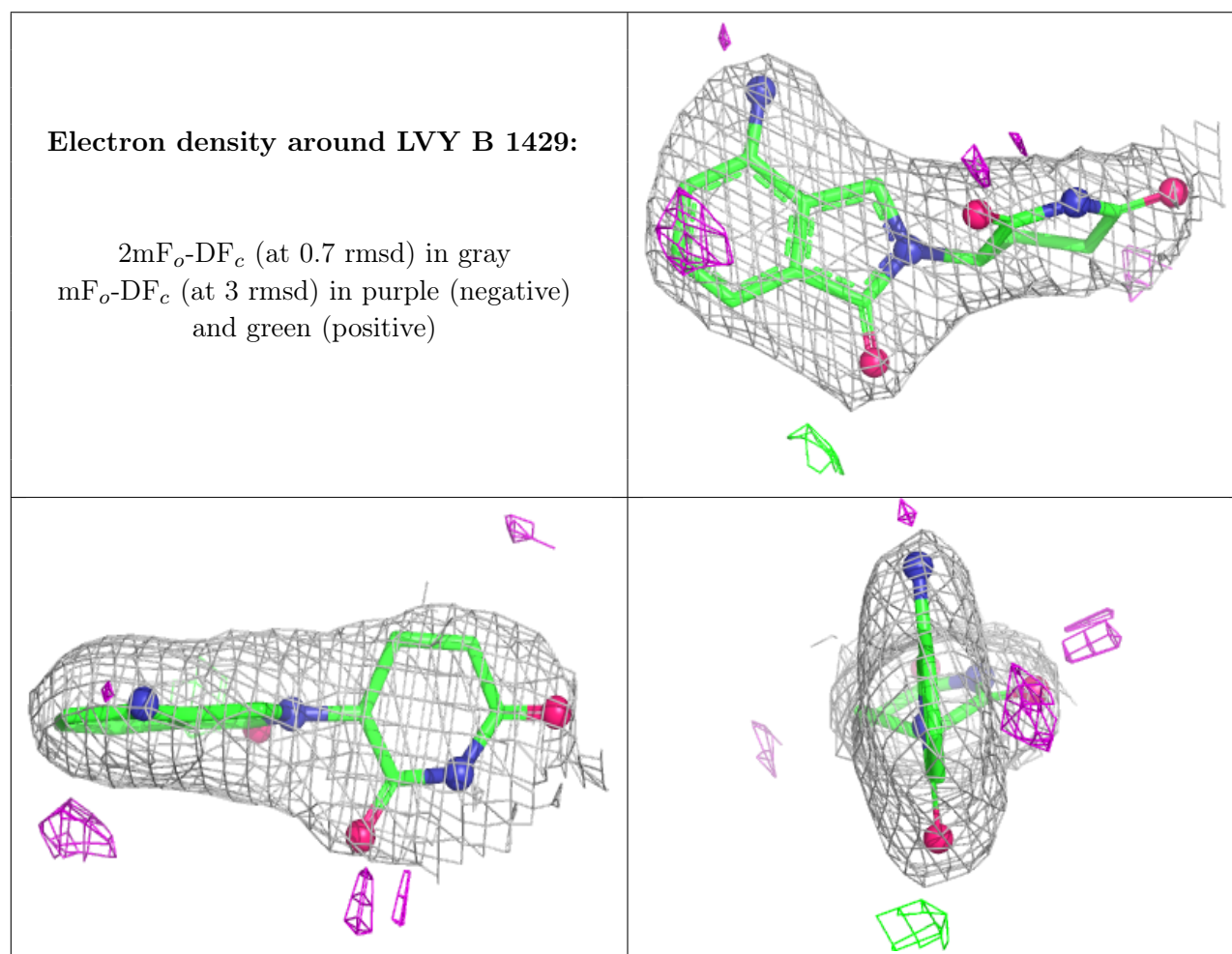
There are no oligosaccharides in this entry.

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	LVY	B	1429	19/19	0.97	0.07	43,54,61,61	0
3	ZN	B	1428	1/1	1.00	0.03	57,57,57,57	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.