



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:26 AM UTC

PDB ID : 5FQD / pdb_00005fqd
Title : Structural basis of Lenalidomide induced CK1a degradation by the crl4crbn ubiquitin ligase
Authors : Petzold, G.; Fischer, E.S.; Thoma, N.H.
Deposited on : 2015-12-09
Resolution : 2.45 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

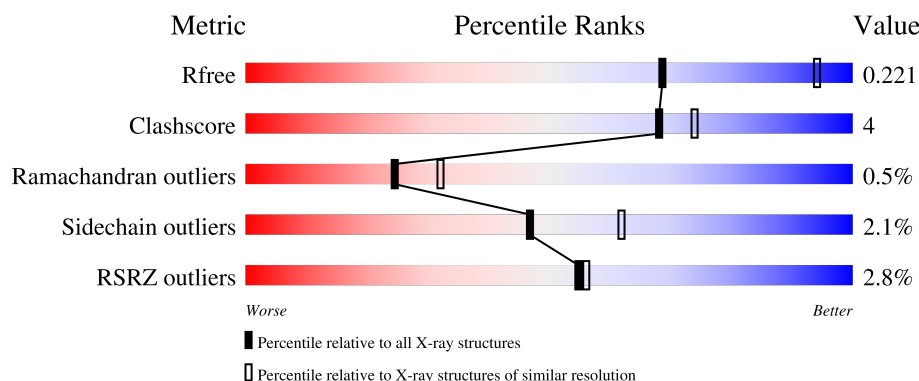
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	 3% 81% 11% • 8%
1	D	856	 % 80% 11% • 8%
2	B	426	 2% 77% 11% • 11%
2	E	426	 5% 74% 11% • 14%
3	C	341	 3% 76% 9% • 14%

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Mol	Chain	Length	Quality of chain
3	F	341	% 78% 8% • 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23544 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	789	Total	C	N	O	S	0	0	0
			6128	3892	1024	1178	34			
1	D	790	Total	C	N	O	S	0	0	0
			6196	3935	1042	1184	35			

There are 52 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	396	GLY	-	linker	UNP Q16531
A	397	ASN	-	linker	UNP Q16531
A	398	GLY	-	linker	UNP Q16531
A	399	ASN	-	linker	UNP Q16531
A	400	SER	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	401	GLY	-	linker	UNP Q16531
D	-19	MET	-	expression tag	UNP Q16531
D	-18	HIS	-	expression tag	UNP Q16531
D	-17	HIS	-	expression tag	UNP Q16531
D	-16	HIS	-	expression tag	UNP Q16531
D	-15	HIS	-	expression tag	UNP Q16531
D	-14	HIS	-	expression tag	UNP Q16531
D	-13	HIS	-	expression tag	UNP Q16531
D	-12	VAL	-	expression tag	UNP Q16531
D	-11	ASP	-	expression tag	UNP Q16531
D	-10	GLU	-	expression tag	UNP Q16531
D	-9	GLU	-	expression tag	UNP Q16531
D	-8	ASN	-	expression tag	UNP Q16531
D	-7	LEU	-	expression tag	UNP Q16531
D	-6	TYR	-	expression tag	UNP Q16531
D	-5	PHE	-	expression tag	UNP Q16531
D	-4	GLN	-	expression tag	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	396	GLY	-	linker	UNP Q16531
D	397	ASN	-	linker	UNP Q16531
D	398	GLY	-	linker	UNP Q16531
D	399	ASN	-	linker	UNP Q16531
D	400	SER	-	linker	UNP Q16531
D	401	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called PROTEIN CEREBLON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	381	Total	C	N	O	S	0	0	0
			3068	1954	521	569	24			
2	E	367	Total	C	N	O	S	0	0	0
			2949	1881	499	545	24			

There are 48 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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	38	GLY	-	expression tag	UNP Q96SW2
E	39	GLY	-	expression tag	UNP Q96SW2
E	40	ARG	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called CASEIN KINASE I ISOFORM ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	294	Total	C	N	O	S	0	0	0
			2423	1561	423	424	15			
3	F	294	Total	C	N	O	S	0	0	0
			2435	1568	424	428	15			

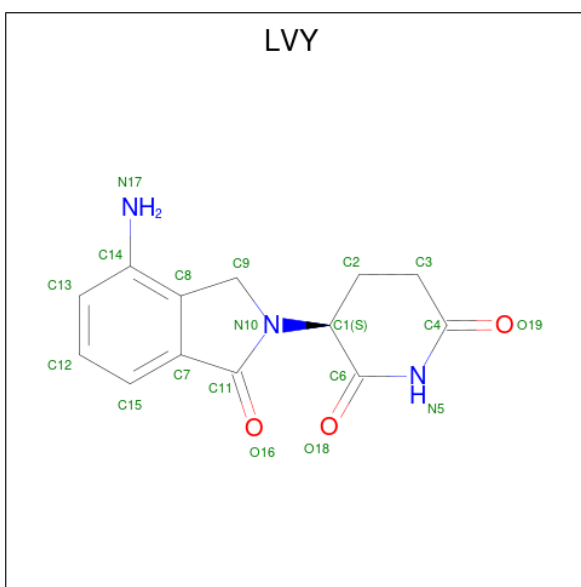
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P48729
C	-2	GLY	-	expression tag	UNP P48729
C	-1	GLY	-	expression tag	UNP P48729
C	0	ARG	-	expression tag	UNP P48729
F	-3	GLY	-	expression tag	UNP P48729
F	-2	GLY	-	expression tag	UNP P48729
F	-1	GLY	-	expression tag	UNP P48729
F	0	ARG	-	expression tag	UNP P48729

- 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	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is S-Lenalidomide (CCD ID: LVY) (formula: C₁₃H₁₃N₃O₃).



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

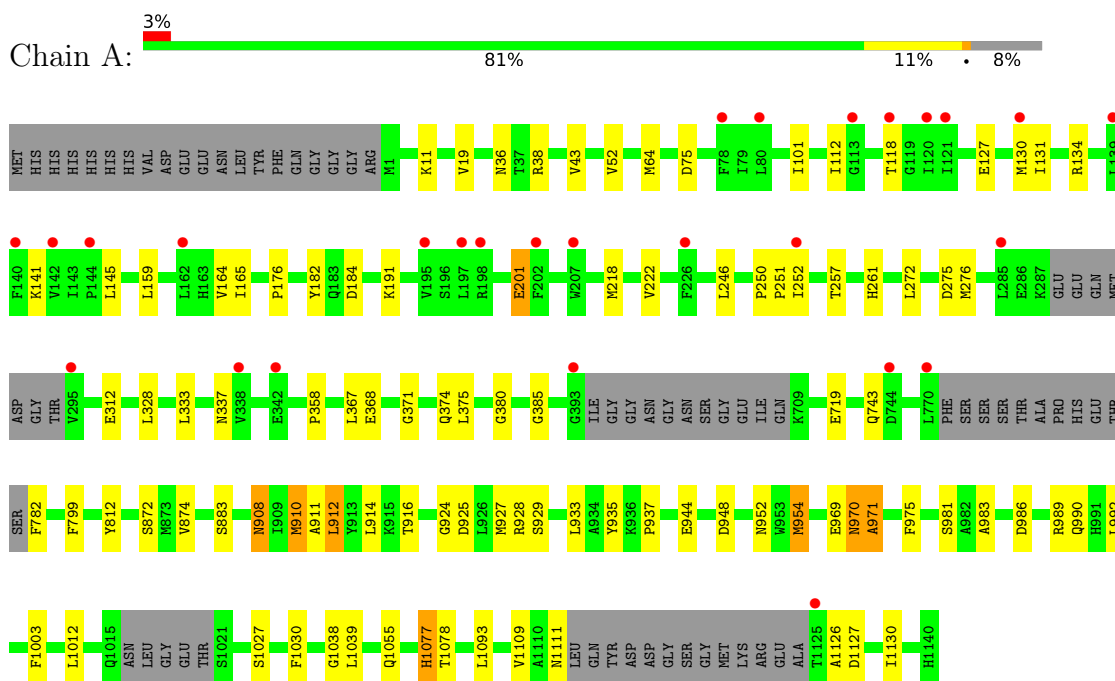
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	52	Total	O	0	0
			52	52		
6	C	48	Total	O	0	0
			48	48		
6	D	93	Total	O	0	0
			93	93		
6	E	10	Total	O	0	0
			10	10		
6	F	48	Total	O	0	0
			48	48		

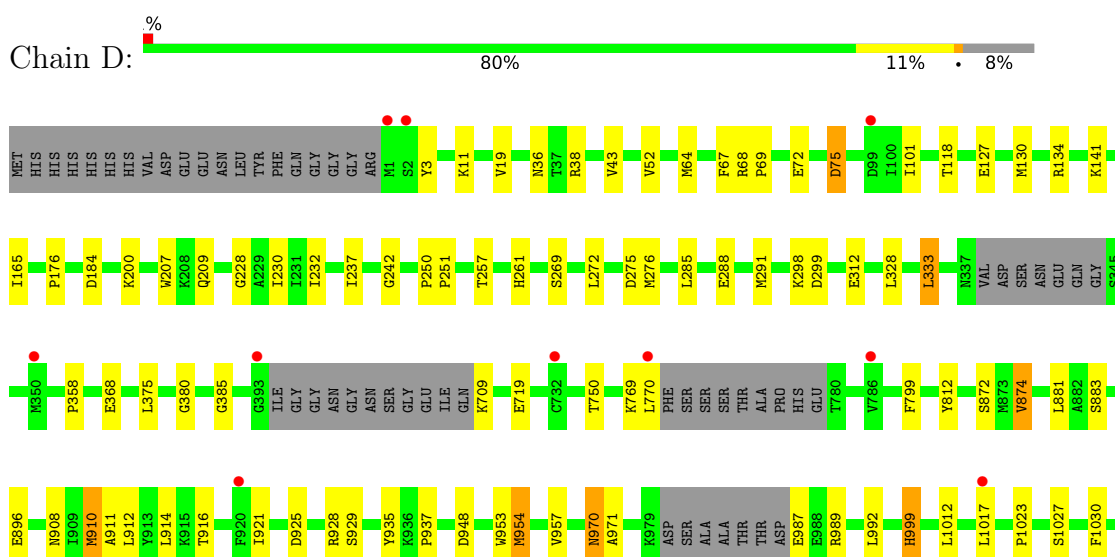
3 Residue-property plots [i](#)

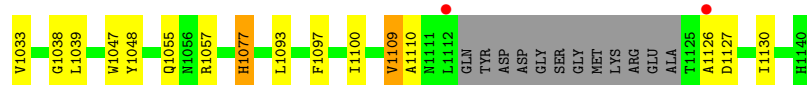
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

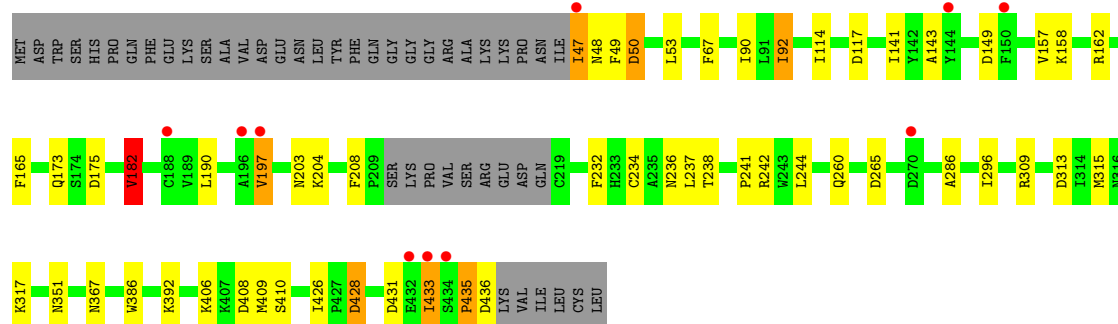
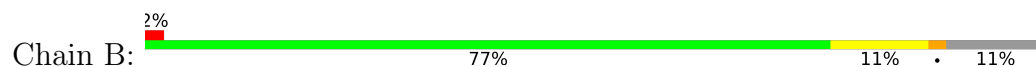


• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1

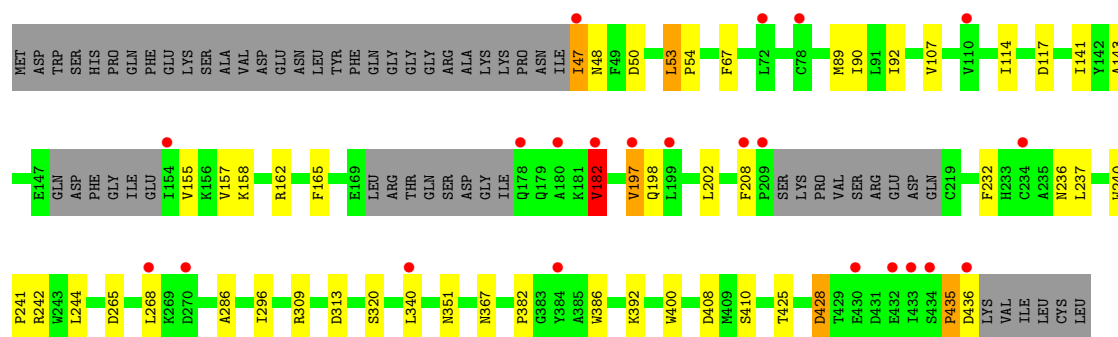
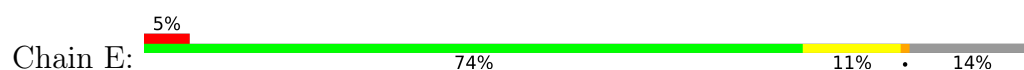




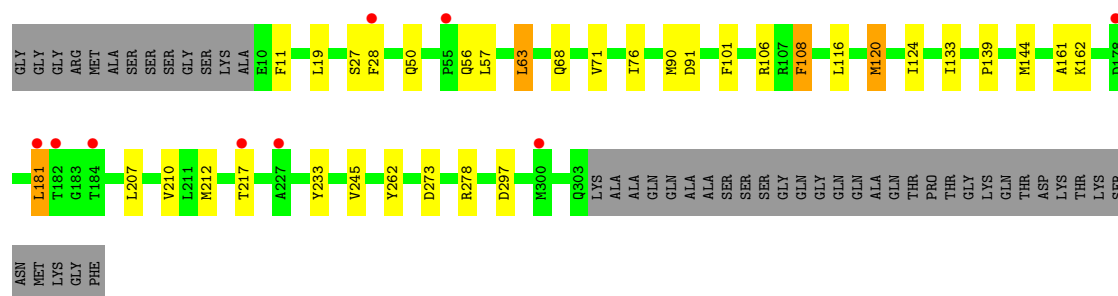
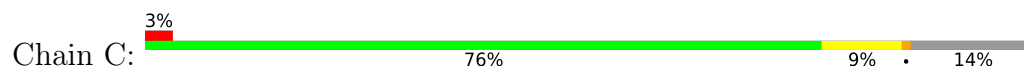
• Molecule 2: PROTEIN CEREBLON



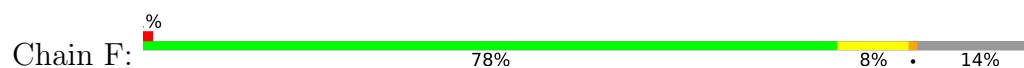
• Molecule 2: PROTEIN CEREBLON

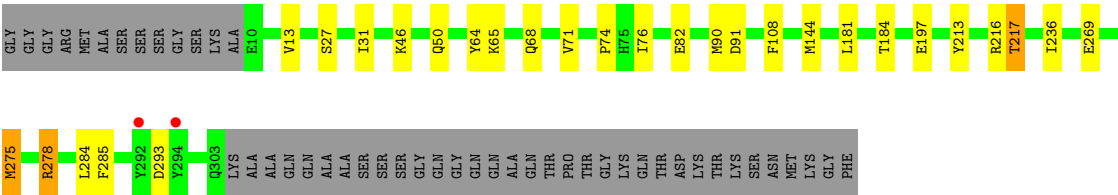


• Molecule 3: CASEIN KINASE I ISOFORM ALPHA



• Molecule 3: CASEIN KINASE I ISOFORM ALPHA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.97Å 109.93Å 112.40Å 106.02° 93.19° 101.63°	Depositor
Resolution (Å)	65.30 – 2.45 65.30 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.3 (65.30-2.45) 97.3 (65.30-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.181 , 0.210 0.193 , 0.221	Depositor DCC
R_{free} test set	6991 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23544	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.81	1/6237 (0.0%)	1.23	23/8449 (0.3%)
1	D	0.85	1/6305 (0.0%)	1.23	16/8526 (0.2%)
2	B	0.88	0/3141	1.29	13/4264 (0.3%)
2	E	0.84	0/3018	1.29	17/4097 (0.4%)
3	C	0.93	3/2480 (0.1%)	1.39	12/3336 (0.4%)
3	F	0.92	3/2492 (0.1%)	1.37	19/3350 (0.6%)
All	All	0.86	8/23673 (0.0%)	1.28	100/32022 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	120	MET	SD-CE	-9.36	1.56	1.79
1	D	954	MET	SD-CE	-8.24	1.58	1.79
3	C	144	MET	SD-CE	-7.08	1.61	1.79
3	C	212	MET	SD-CE	6.87	1.96	1.79
1	A	954	MET	SD-CE	-6.74	1.62	1.79
3	F	275	MET	SD-CE	6.67	1.96	1.79
3	F	144	MET	SD-CE	-6.22	1.64	1.79
3	F	217	THR	CA-C	5.83	1.60	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	970	ASN	CA-C-N	9.93	140.51	121.54
1	D	970	ASN	C-N-CA	9.93	140.51	121.54
3	F	50	GLN	N-CA-C	-9.10	95.82	110.20
3	C	50	GLN	N-CA-C	-8.62	96.05	109.76
1	A	925	ASP	CA-CB-CG	8.60	121.20	112.60
2	B	435	PRO	CA-C-N	8.10	136.28	121.70
2	B	435	PRO	C-N-CA	8.10	136.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	970	ASN	CA-C-N	8.01	136.84	121.54
1	A	970	ASN	C-N-CA	8.01	136.84	121.54
2	E	435	PRO	CA-C-N	7.72	135.59	121.70
2	E	435	PRO	C-N-CA	7.72	135.59	121.70
3	C	27	SER	CA-C-N	7.12	130.13	120.44
3	C	27	SER	C-N-CA	7.12	130.13	120.44
3	F	27	SER	CA-C-N	6.80	129.69	120.44
3	F	27	SER	C-N-CA	6.80	129.69	120.44
1	A	75	ASP	CA-CB-CG	6.76	119.36	112.60
1	D	925	ASP	CA-CB-CG	6.73	119.33	112.60
3	F	91	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	184	ASP	CA-CB-CG	6.54	119.14	112.60
3	F	108	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	337	ASN	CA-C-N	6.33	128.76	120.60
1	A	337	ASN	C-N-CA	6.33	128.76	120.60
1	D	1077	HIS	CA-C-N	6.30	132.20	121.87
1	D	1077	HIS	C-N-CA	6.30	132.20	121.87
1	D	184	ASP	CA-CB-CG	6.20	118.80	112.60
2	E	351	ASN	CA-CB-CG	6.19	118.79	112.60
2	E	268	LEU	CA-C-N	6.06	128.41	120.28
2	E	268	LEU	C-N-CA	6.06	128.41	120.28
1	D	799	PHE	CA-CB-CG	-5.98	107.82	113.80
3	C	91	ASP	CA-CB-CG	5.94	118.54	112.60
1	D	75	ASP	CA-CB-CG	5.92	118.53	112.60
3	C	108	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	799	PHE	CA-CB-CG	-5.87	107.93	113.80
2	B	351	ASN	CA-CB-CG	5.77	118.37	112.60
3	F	278	ARG	CA-C-N	5.75	127.99	120.28
3	F	278	ARG	C-N-CA	5.75	127.99	120.28
3	C	262	TYR	CA-C-N	5.67	128.35	120.29
3	C	262	TYR	C-N-CA	5.67	128.35	120.29
2	E	48	ASN	CA-CB-CG	5.66	118.26	112.60
2	E	265	ASP	CA-CB-CG	5.66	118.26	112.60
3	F	181	LEU	CA-C-N	5.65	130.79	123.00
3	F	181	LEU	C-N-CA	5.65	130.79	123.00
2	B	265	ASP	CA-CB-CG	5.59	118.19	112.60
2	B	182	VAL	N-CA-CB	-5.59	101.59	111.93
3	C	278	ARG	CA-C-N	5.57	127.75	120.28
3	C	278	ARG	C-N-CA	5.57	127.75	120.28
1	D	999	HIS	CA-C-N	5.53	127.97	120.44
1	D	999	HIS	C-N-CA	5.53	127.97	120.44
2	E	117	ASP	CA-CB-CG	5.52	118.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	49	PHE	CA-C-N	5.49	132.03	121.54
2	B	49	PHE	C-N-CA	5.49	132.03	121.54
1	A	969	GLU	CA-C-N	5.49	130.12	121.56
1	A	969	GLU	C-N-CA	5.49	130.12	121.56
1	A	1077	HIS	CA-C-N	5.46	130.83	121.87
1	A	1077	HIS	C-N-CA	5.46	130.83	121.87
2	E	182	VAL	N-CA-CB	-5.46	101.84	111.93
3	F	269	GLU	CB-CG-CD	5.45	121.87	112.60
3	F	285	PHE	CA-C-N	5.43	127.83	120.44
3	F	285	PHE	C-N-CA	5.43	127.83	120.44
2	B	117	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	1111	ASN	CA-CB-CG	5.41	118.01	112.60
3	F	284	LEU	CA-C-N	5.38	127.75	120.38
3	F	284	LEU	C-N-CA	5.38	127.75	120.38
2	B	428	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	312	GLU	N-CA-C	-5.31	105.06	112.45
2	B	48	ASN	CA-C-N	5.31	128.17	120.79
2	B	48	ASN	C-N-CA	5.31	128.17	120.79
1	A	983	ALA	CA-C-N	5.29	127.90	120.28
1	A	983	ALA	C-N-CA	5.29	127.90	120.28
3	F	184	THR	CA-C-N	5.29	127.36	120.28
3	F	184	THR	C-N-CA	5.29	127.36	120.28
3	C	273	ASP	CA-CB-CG	5.26	117.86	112.60
2	E	428	ASP	CA-CB-CG	5.25	117.85	112.60
2	E	309	ARG	CA-C-N	5.25	127.31	120.28
2	E	309	ARG	C-N-CA	5.25	127.31	120.28
1	A	312	GLU	N-CA-C	-5.24	105.16	112.45
1	A	368	GLU	CA-C-N	5.24	129.06	120.63
1	A	368	GLU	C-N-CA	5.24	129.06	120.63
1	D	333	LEU	N-CA-C	-5.23	99.89	108.41
2	E	340	LEU	N-CA-C	-5.20	106.33	113.30
1	A	333	LEU	N-CA-C	-5.18	99.96	108.41
2	B	309	ARG	CA-C-N	5.18	127.22	120.28
2	B	309	ARG	C-N-CA	5.18	127.22	120.28
1	A	1078	THR	N-CA-C	-5.17	101.25	108.96
3	C	181	LEU	CA-C-N	5.16	130.12	123.00
3	C	181	LEU	C-N-CA	5.16	130.12	123.00
1	D	275	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	908	ASN	N-CA-C	-5.13	106.52	112.89
2	E	197	VAL	CA-C-N	5.10	131.28	121.54
2	E	197	VAL	C-N-CA	5.10	131.28	121.54
1	A	201	GLU	CB-CG-CD	5.10	121.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	929	SER	N-CA-C	-5.08	101.68	109.76
2	E	54	PRO	CA-C-N	5.08	127.59	120.28
2	E	54	PRO	C-N-CA	5.08	127.59	120.28
3	F	236	ILE	CA-C-N	5.07	127.03	120.44
3	F	236	ILE	C-N-CA	5.07	127.03	120.44
1	D	896	GLU	CA-C-N	5.04	130.10	122.68
1	D	896	GLU	C-N-CA	5.04	130.10	122.68
3	F	293	ASP	CA-CB-CG	5.00	117.60	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	6128	0	6031	49	0
1	D	6196	0	6168	56	0
2	B	3068	0	3036	30	0
2	E	2949	0	2915	25	0
3	C	2423	0	2420	15	0
3	F	2435	0	2442	10	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	B	19	0	13	1	0
5	E	19	0	13	3	0
6	A	54	0	0	0	0
6	B	52	0	0	2	0
6	C	48	0	0	2	0
6	D	93	0	0	0	0
6	E	10	0	0	0	0
6	F	48	0	0	1	0
All	All	23544	0	23038	168	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 (168) 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:874:VAL:HG11	1:A:916:THR:HG22	1.38	1.02
2:E:313:ASP:OD2	2:E:435:PRO:HD2	1.72	0.88
3:C:11:PHE:HD2	3:C:19:LEU:HD22	1.39	0.87
2:B:313:ASP:OD2	2:B:435:PRO:HD2	1.74	0.86
1:D:971:ALA:HB3	1:D:1077:HIS:O	1.79	0.82
3:C:116:LEU:HB3	3:C:120:MET:HE2	1.66	0.78
1:A:874:VAL:HG11	1:A:916:THR:CG2	2.14	0.76
3:C:106:ARG:HB2	6:C:2012:HOH:O	1.87	0.74
1:A:201:GLU:HG3	1:D:200:LYS:HE2	1.69	0.74
1:D:954:MET:HE2	1:D:957:VAL:HB	1.70	0.74
1:A:118:THR:HG21	1:A:165:ILE:O	1.90	0.72
1:D:118:THR:HG21	1:D:165:ILE:O	1.90	0.71
1:A:954:MET:HE3	1:A:975:PHE:HZ	1.57	0.70
2:B:173:GLN:HB2	6:B:2020:HOH:O	1.90	0.69
1:A:971:ALA:HB3	1:A:1077:HIS:O	1.95	0.66
1:D:11:LYS:HD3	1:D:38:ARG:HD2	1.77	0.66
1:A:954:MET:HE3	1:A:975:PHE:CZ	2.32	0.65
2:B:53:LEU:HD23	6:B:2003:HOH:O	1.97	0.65
1:D:69:PRO:HD2	1:D:72:GLU:HG3	1.80	0.64
3:F:275:MET:HE2	3:F:278:ARG:HH21	1.64	0.62
3:C:63:LEU:HD21	3:C:161:ALA:HB3	1.82	0.62
1:A:812:TYR:CZ	2:B:241:PRO:HB3	2.35	0.61
3:C:124:ILE:HD12	3:C:207:LEU:HD22	1.81	0.60
1:D:257:THR:HB	1:D:276:MET:HE3	1.84	0.59
2:E:165:PHE:HB2	2:E:182:VAL:HG13	1.83	0.59
2:B:197:VAL:HG11	2:B:238:THR:CG2	2.33	0.59
1:D:812:TYR:CZ	2:E:241:PRO:HB3	2.37	0.59
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.84	0.59
1:A:130:MET:HE3	1:A:176:PRO:HG2	1.86	0.58
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	1.85	0.58
2:B:317:LYS:NZ	2:B:433:ILE:HG23	2.17	0.58
1:A:257:THR:HB	1:A:276:MET:HE3	1.86	0.57
1:D:1027:SER:OG	1:D:1039:LEU:HD11	2.04	0.57
1:A:908:ASN:O	2:B:435:PRO:HA	2.05	0.57
1:D:130:MET:HE3	1:D:176:PRO:HG2	1.87	0.56
1:D:43:VAL:HG23	1:D:52:VAL:HG21	1.88	0.56
1:D:1109:VAL:HG11	1:D:1126:ALA:HA	1.87	0.56
1:A:910:MET:HE1	2:B:244:LEU:HD11	1.88	0.56
1:A:367:LEU:HB2	1:A:374:GLN:HE21	1.71	0.56
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.06	0.55
1:D:948:ASP:HB2	1:D:992:LEU:HB2	1.88	0.55
2:E:47:ILE:N	2:E:410:SER:HG	2.04	0.55
1:A:948:ASP:HB2	1:A:992:LEU:HB2	1.88	0.55
3:F:90:MET:HE2	6:F:2011:HOH:O	2.06	0.55
1:D:328:LEU:HD21	2:E:237:LEU:HD21	1.89	0.55
1:A:118:THR:O	2:B:203:ASN:HB3	2.07	0.54
2:B:367:ASN:HA	2:B:392:LYS:HD2	1.90	0.54
2:E:367:ASN:HA	2:E:392:LYS:HD2	1.91	0.53
1:D:910:MET:HE1	2:E:244:LEU:HD11	1.89	0.53
1:D:207:TRP:CH2	1:D:228:GLY:HA2	2.44	0.53
1:D:908:ASN:O	2:E:435:PRO:HA	2.10	0.52
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.92	0.52
1:D:874:VAL:HG23	1:D:881:LEU:HB3	1.92	0.51
1:D:916:THR:HG22	1:D:921:ILE:HG13	1.91	0.51
3:C:181:LEU:HD23	3:C:233:TYR:CE2	2.44	0.51
1:A:118:THR:HB	1:A:134:ARG:HH22	1.75	0.51
3:F:213:TYR:O	3:F:216:ARG:O	2.29	0.51
1:D:954:MET:CE	1:D:957:VAL:HB	2.40	0.50
3:F:76:ILE:HD13	3:F:90:MET:HB3	1.92	0.50
3:C:76:ILE:HD13	3:C:90:MET:HB3	1.93	0.50
2:B:50:ASP:HB3	2:B:53:LEU:HD12	1.93	0.50
1:A:986:ASP:HA	1:A:989:ARG:HG2	1.94	0.50
2:E:320:SER:HB3	2:E:425:THR:HB	1.94	0.50
1:D:1127:ASP:HA	1:D:1130:ILE:HD12	1.94	0.50
1:D:118:THR:HB	1:D:134:ARG:HH22	1.76	0.49
2:E:90:ILE:HD13	2:E:296:ILE:HG13	1.93	0.49
3:C:139:PRO:HG3	3:C:210:VAL:HG13	1.95	0.49
2:B:386:TRP:CZ2	5:B:1438:LVY:H92	2.48	0.49
3:F:13:VAL:HA	3:F:82:GLU:HG3	1.94	0.49
1:D:769:LYS:HB3	1:D:770:LEU:HD23	1.94	0.49
1:A:385:GLY:HA3	1:A:719:GLU:O	2.13	0.48
1:D:883:SER:HB2	1:D:911:ALA:HB3	1.95	0.48
2:B:114:ILE:HD11	2:B:141:ILE:HG21	1.95	0.48
2:B:47:ILE:N	2:B:410:SER:HG	2.12	0.48
1:A:1127:ASP:HA	1:A:1130:ILE:HD12	1.95	0.48
2:B:90:ILE:HD13	2:B:296:ILE:HG13	1.96	0.48
2:B:197:VAL:O	2:B:234:CYS:HB3	2.14	0.48
1:D:872:SER:HB3	1:D:914:LEU:HB2	1.96	0.48
2:E:386:TRP:CZ2	5:E:1438:LVY:H92	2.49	0.48
3:F:65:LYS:O	3:F:68:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:PRO:HD2	1:D:380:GLY:HA2	1.96	0.47
1:D:385:GLY:HA3	1:D:719:GLU:O	2.14	0.47
2:E:400:TRP:NE1	5:E:1438:LVY:H22C	2.30	0.47
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.95	0.47
1:A:11:LYS:HD3	1:A:38:ARG:HD2	1.96	0.47
1:D:1023:PRO:HB3	1:D:1047:TRP:CZ2	2.50	0.47
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.97	0.46
1:A:910:MET:HE2	1:A:910:MET:HB3	1.78	0.46
3:C:108:PHE:HA	3:C:297:ASP:OD2	2.15	0.46
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.97	0.46
1:A:874:VAL:CG1	1:A:916:THR:CG2	2.90	0.46
2:E:143:ALA:HB3	2:E:158:LYS:HB2	1.97	0.46
1:A:924:GLY:HA2	1:A:929:SER:O	2.16	0.46
1:D:207:TRP:HH2	1:D:228:GLY:HA2	1.79	0.46
1:D:987:GLU:HG3	1:D:989:ARG:HG3	1.98	0.46
1:A:328:LEU:HD21	2:B:237:LEU:HD21	1.97	0.46
2:B:92:ILE:HD13	2:B:286:ALA:HA	1.97	0.45
1:D:19:VAL:HG22	1:D:64:MET:HE3	1.98	0.45
1:D:3:TYR:HB3	1:D:1048:TYR:HB2	1.98	0.45
1:D:910:MET:CE	1:D:912:LEU:HD13	2.47	0.45
1:D:1057:ARG:HH12	1:D:1110:ALA:HB3	1.82	0.45
1:D:971:ALA:O	1:D:999:HIS:CE1	2.70	0.45
1:D:1097:PHE:O	1:D:1100:ILE:HG12	2.17	0.45
1:A:19:VAL:HG22	1:A:64:MET:HE3	1.97	0.45
1:A:872:SER:HB3	1:A:914:LEU:HB2	1.99	0.44
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.99	0.44
2:B:232:PHE:O	2:B:242:ARG:HG2	2.18	0.44
1:A:367:LEU:HB2	1:A:374:GLN:NE2	2.31	0.44
1:D:910:MET:HE2	1:D:910:MET:HB3	1.79	0.44
2:E:232:PHE:O	2:E:242:ARG:HG2	2.18	0.44
3:F:275:MET:CE	3:F:278:ARG:HH21	2.30	0.44
3:C:101:PHE:CE2	3:C:106:ARG:HG3	2.52	0.44
2:E:114:ILE:HD11	2:E:141:ILE:HG21	2.00	0.44
2:E:386:TRP:CG	5:E:1438:LVY:H31C	2.52	0.44
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.53	0.43
1:A:935:TYR:O	1:A:937:PRO:HD3	2.18	0.43
1:D:935:TYR:O	1:D:937:PRO:HD3	2.19	0.43
1:D:953:TRP:HB2	1:D:970:ASN:HB2	2.01	0.43
1:D:1055:GLN:HG2	1:D:1093:LEU:HD23	2.01	0.43
1:A:1003:PHE:CE2	2:B:197:VAL:HG22	2.54	0.43
3:C:133:ILE:HD11	3:C:162:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:PRO:HA	1:D:251:PRO:HD3	1.95	0.43
2:E:92:ILE:HD13	2:E:286:ALA:HA	2.00	0.43
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.54	0.43
2:E:53:LEU:HD22	2:E:382:PRO:HG2	2.01	0.43
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.00	0.43
1:A:159:LEU:HD21	1:A:164:VAL:HG21	2.00	0.42
1:D:68:ARG:HB2	1:D:75:ASP:OD1	2.19	0.42
3:F:64:TYR:HE1	3:F:74:PRO:HD2	1.85	0.42
2:B:406:LYS:HB2	2:B:409:MET:HE3	2.01	0.42
3:C:63:LEU:CD2	3:C:161:ALA:HB3	2.48	0.42
1:A:912:LEU:HD11	2:B:244:LEU:HD21	2.02	0.42
1:D:67:PHE:CE2	1:D:69:PRO:HG3	2.54	0.42
2:E:165:PHE:CB	2:E:182:VAL:HG13	2.48	0.42
3:C:217:THR:HA	6:C:2013:HOH:O	2.19	0.42
3:C:28:PHE:HB3	3:C:56:GLN:HG2	2.02	0.42
1:D:276:MET:HE2	2:E:202:LEU:HD22	2.01	0.42
1:D:912:LEU:HG	2:E:240:TRP:CZ2	2.55	0.42
1:A:131:ILE:HD11	1:A:145:LEU:HD21	2.02	0.41
1:D:261:HIS:HA	1:D:272:LEU:O	2.19	0.41
1:D:912:LEU:HD12	1:D:912:LEU:HA	1.82	0.41
1:A:986:ASP:O	1:A:990:GLN:HG2	2.20	0.41
2:E:107:VAL:HG22	2:E:155:VAL:HG12	2.02	0.41
1:A:182:TYR:HE1	1:A:191:LYS:HB2	1.85	0.41
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.95	0.41
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.95	0.41
2:B:165:PHE:CB	2:B:182:VAL:HG13	2.48	0.41
2:E:67:PHE:HZ	2:E:114:ILE:HG23	1.86	0.41
1:D:358:PRO:HA	1:D:1033:VAL:O	2.21	0.41
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	2.02	0.41
1:A:261:HIS:HA	1:A:272:LEU:O	2.21	0.41
1:A:952:ASN:OD1	1:A:970:ASN:HB3	2.20	0.41
2:B:317:LYS:HZ3	2:B:433:ILE:HG23	1.86	0.41
3:C:63:LEU:HD21	3:C:161:ALA:CB	2.49	0.41
3:F:31:ILE:HG12	3:F:46:LYS:HG2	2.02	0.41
3:F:216:ARG:O	3:F:217:THR:C	2.63	0.41
1:A:927:MET:HE3	2:B:190:LEU:CD1	2.50	0.41
1:D:232:ILE:HG12	1:D:237:ILE:HG12	2.01	0.41
1:D:812:TYR:OH	2:E:241:PRO:HB3	2.21	0.41
2:E:89:MET:HE2	2:E:89:MET:HB3	1.99	0.41
1:A:218:MET:HE2	2:B:204:LYS:HE3	2.03	0.41
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:LEU:HD23	1:A:944:GLU:HA	2.03	0.40
2:B:260:GLN:HG2	2:B:315:MET:SD	2.61	0.40
1:D:230:ILE:HD11	1:D:285:LEU:HD21	2.03	0.40
2:B:67:PHE:HZ	2:B:114:ILE:HG23	1.87	0.40
1:A:743:GLN:HB3	1:A:782:PHE:HB3	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	777/856 (91%)	744 (96%)	29 (4%)	4 (0%)	24	32
1	D	778/856 (91%)	744 (96%)	30 (4%)	4 (0%)	24	32
2	B	377/426 (88%)	364 (97%)	10 (3%)	3 (1%)	16	20
2	E	359/426 (84%)	347 (97%)	9 (2%)	3 (1%)	16	20
3	C	292/341 (86%)	282 (97%)	10 (3%)	0	100	100
3	F	292/341 (86%)	279 (96%)	13 (4%)	0	100	100
All	All	2875/3246 (89%)	2760 (96%)	101 (4%)	14 (0%)	24	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	50	ASP
2	E	50	ASP
1	D	368	GLU
1	D	1017	LEU
1	A	371	GLY
2	E	198	GLN
2	B	428	ASP

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Mol	Chain	Res	Type
2	B	431	ASP
1	D	36	ASN
1	D	1109	VAL
2	E	428	ASP
1	A	36	ASN
1	A	971	ALA
1	A	981	SER

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	671/744 (90%)	661 (98%)	10 (2%)	57	70
1	D	686/744 (92%)	674 (98%)	12 (2%)	53	67
2	B	344/385 (89%)	330 (96%)	14 (4%)	27	40
2	E	330/385 (86%)	320 (97%)	10 (3%)	36	51
3	C	256/293 (87%)	251 (98%)	5 (2%)	48	63
3	F	260/293 (89%)	258 (99%)	2 (1%)	73	83
All	All	2547/2844 (90%)	2494 (98%)	53 (2%)	47	62

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	112	ILE
1	A	127	GLU
1	A	141	LYS
1	A	222	VAL
1	A	246	LEU
1	A	252	ILE
1	A	910	MET
1	A	912	LEU
1	A	928	ARG
2	B	47	ILE

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Mol	Chain	Res	Type
2	B	92	ILE
2	B	149	ASP
2	B	157	VAL
2	B	162	ARG
2	B	175	ASP
2	B	182	VAL
2	B	197	VAL
2	B	208	PHE
2	B	236	ASN
2	B	408	ASP
2	B	426	ILE
2	B	433	ILE
2	B	436	ASP
3	C	57	LEU
3	C	63	LEU
3	C	68	GLN
3	C	71	VAL
3	C	245	VAL
1	D	101	ILE
1	D	127	GLU
1	D	141	LYS
1	D	209	GLN
1	D	269	SER
1	D	291	MET
1	D	299	ASP
1	D	709	LYS
1	D	750	THR
1	D	874	VAL
1	D	910	MET
1	D	928	ARG
2	E	47	ILE
2	E	53	LEU
2	E	157	VAL
2	E	162	ARG
2	E	182	VAL
2	E	197	VAL
2	E	208	PHE
2	E	236	ASN
2	E	408	ASP
2	E	436	ASP
3	F	71	VAL
3	F	197	GLU

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	4	ASN
1	A	234	GLN
1	A	711	HIS
1	A	759	GLN
1	A	1106	GLN
2	B	68	HIS
2	B	127	ASN
2	B	129	GLN
2	B	173	GLN
2	B	228	GLN
2	B	297	GLN
3	C	198	GLN
1	D	241	ASN
1	D	711	HIS
1	D	727	GLN
1	D	759	GLN
1	D	970	ASN
1	D	1059	ASN
1	D	1111	ASN
2	E	127	ASN
2	E	198	GLN
2	E	228	GLN
2	E	297	GLN
3	F	198	GLN
3	F	290	HIS

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	LVY	B	1438	-	21,21,21	1.32	3 (14%)	29,31,31	2.51	13 (44%)
5	LVY	E	1438	-	21,21,21	1.46	3 (14%)	29,31,31	2.23	12 (41%)

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	LVY	B	1438	-	-	0/4/29/29	0/3/3/3
5	LVY	E	1438	-	-	0/4/29/29	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1438	LVY	C14-C8	4.03	1.42	1.40
5	B	1438	LVY	C9-C8	2.99	1.54	1.50
5	E	1438	LVY	C9-C8	2.85	1.53	1.50
5	B	1438	LVY	C12-C13	2.38	1.43	1.38
5	B	1438	LVY	C12-C15	2.15	1.42	1.38
5	E	1438	LVY	C1-N10	2.01	1.48	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1438	LVY	C7-C11-N10	6.19	110.36	106.42
5	E	1438	LVY	C7-C11-N10	4.73	109.43	106.42
5	B	1438	LVY	C8-C7-C11	-4.48	104.76	108.62
5	B	1438	LVY	C3-C4-N5	4.27	121.23	116.69
5	B	1438	LVY	O16-C11-N10	4.25	128.71	125.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1438	LVY	O16-C11-C7	-4.00	120.91	128.66
5	E	1438	LVY	C6-C1-N10	-3.98	106.64	110.32
5	B	1438	LVY	C9-N10-C11	-3.86	111.52	113.15
5	E	1438	LVY	C2-C1-N10	-3.40	110.32	114.03
5	E	1438	LVY	C1-C6-N5	3.38	121.17	116.24
5	E	1438	LVY	C3-C2-C1	3.26	115.65	109.77
5	B	1438	LVY	C9-C8-C7	3.20	111.82	109.82
5	E	1438	LVY	C8-C9-N10	3.00	102.69	101.79
5	E	1438	LVY	C3-C4-N5	2.99	119.86	116.69
5	E	1438	LVY	O16-C11-C7	-2.97	122.90	128.66
5	E	1438	LVY	C9-N10-C11	-2.90	111.93	113.15
5	E	1438	LVY	C9-N10-C1	2.88	126.42	123.68
5	E	1438	LVY	O16-C11-N10	2.85	127.60	125.34
5	B	1438	LVY	C9-N10-C1	2.66	126.22	123.68
5	B	1438	LVY	C3-C2-C1	2.66	114.57	109.77
5	E	1438	LVY	C8-C7-C11	-2.33	106.61	108.62
5	B	1438	LVY	C2-C1-N10	-2.29	111.53	114.03
5	B	1438	LVY	C8-C14-N17	-2.29	118.23	121.10
5	B	1438	LVY	C1-C6-N5	2.28	119.56	116.24
5	B	1438	LVY	C2-C3-C4	-2.09	109.54	113.87

There are no chirality outliers.

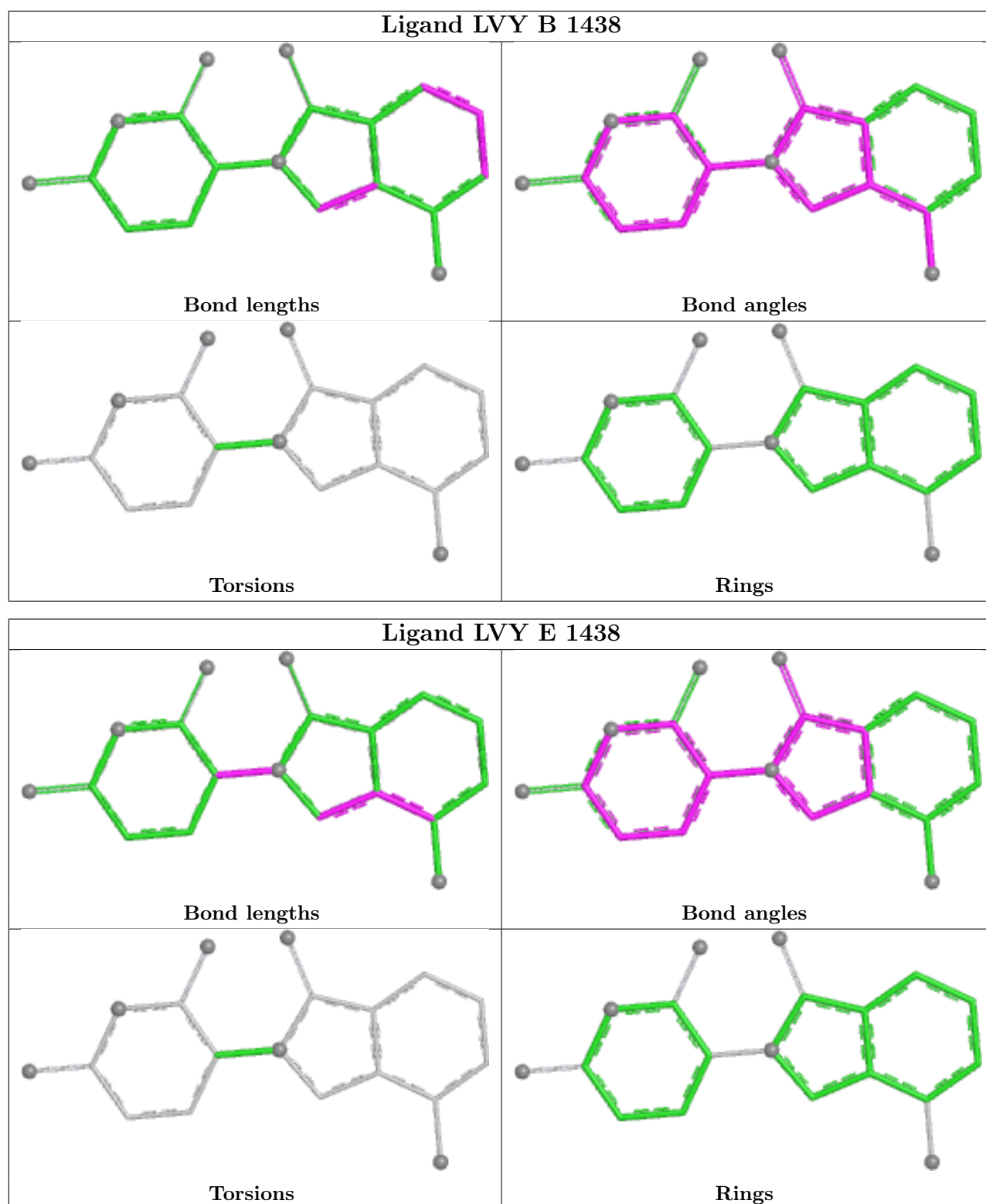
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1438	LVY	1	0
5	E	1438	LVY	3	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

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	789/856 (92%)	0.39	27 (3%)	48 48	53, 106, 181, 202	0
1	D	790/856 (92%)	0.05	12 (1%)	72 74	50, 82, 131, 172	0
2	B	381/426 (89%)	0.20	10 (2%)	57 58	54, 78, 134, 159	0
2	E	367/426 (86%)	0.62	22 (5%)	27 24	57, 114, 206, 218	0
3	C	294/341 (86%)	0.12	9 (3%)	51 52	56, 77, 126, 165	1 (0%)
3	F	294/341 (86%)	-0.02	2 (0%)	84 86	52, 75, 117, 162	2 (0%)
All	All	2915/3246 (89%)	0.23	82 (2%)	55 56	50, 88, 172, 218	3 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	197	VAL	5.2
2	E	47	ILE	4.6
1	A	770	LEU	4.6
1	A	1125	THR	4.4
1	D	770	LEU	4.1
1	A	140	PHE	4.1
1	D	1112	LEU	4.0
1	D	99	ASP	3.9
1	A	393	GLY	3.9
1	A	295	VAL	3.5
3	C	28	PHE	3.5
2	B	432	GLU	3.5
3	C	178	ASP	3.4
1	A	130	MET	3.3
2	E	197	VAL	3.3
3	C	184	THR	3.3
1	A	338	VAL	3.1
1	A	198	ARG	3.0
3	C	182	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	144	PRO	2.9
1	D	1	MET	2.9
1	A	142	VAL	2.9
2	E	180	ALA	2.9
3	C	227	ALA	2.8
2	B	196	ALA	2.8
2	E	436	ASP	2.8
2	E	340	LEU	2.7
2	E	432	GLU	2.7
1	A	744	ASP	2.6
1	A	78	PHE	2.6
2	E	433	ILE	2.6
1	A	195	VAL	2.6
1	A	207	TRP	2.5
2	E	209	PRO	2.5
1	A	113	GLY	2.5
2	E	199	LEU	2.5
1	A	120	ILE	2.4
2	B	150	PHE	2.4
2	E	434	SER	2.4
1	D	393	GLY	2.4
3	F	294	TYR	2.4
1	D	786	VAL	2.4
2	B	47	ILE	2.4
2	E	72	LEU	2.4
1	A	197	LEU	2.3
2	B	433	ILE	2.3
2	B	144	TYR	2.3
1	A	162	LEU	2.2
1	A	252	ILE	2.2
2	E	234	CYS	2.2
1	A	121	ILE	2.2
2	B	434	SER	2.2
2	E	178	GLN	2.2
1	A	226	PHE	2.2
1	D	732	CYS	2.2
2	E	78	CYS	2.2
1	D	2	SER	2.2
2	E	208	PHE	2.2
2	E	182	VAL	2.1
3	C	300	MET	2.1
1	A	285	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	384	TYR	2.1
1	D	350	MET	2.1
2	E	270	ASP	2.1
1	A	118	THR	2.1
2	B	188	CYS	2.1
2	B	270	ASP	2.1
2	E	268	LEU	2.1
1	A	342	GLU	2.1
3	C	217	THR	2.1
2	E	154	ILE	2.1
1	A	202	PHE	2.0
2	E	110	VAL	2.0
1	D	1126	ALA	2.0
1	A	80	LEU	2.0
1	A	139	LEU	2.0
1	D	1017	LEU	2.0
2	E	430	GLU	2.0
3	F	292	TYR	2.0
1	D	920	PHE	2.0
3	C	181	LEU	2.0
3	C	55	PRO	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
5	LVY	E	1438	19/19	0.90	0.09	81,92,113,114	0
5	LVY	B	1438	19/19	0.97	0.06	48,55,58,61	0

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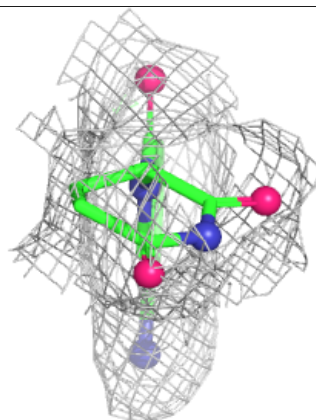
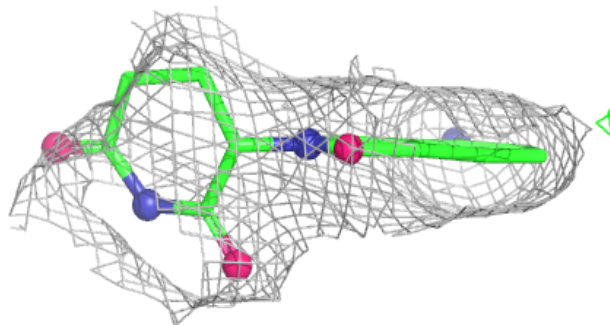
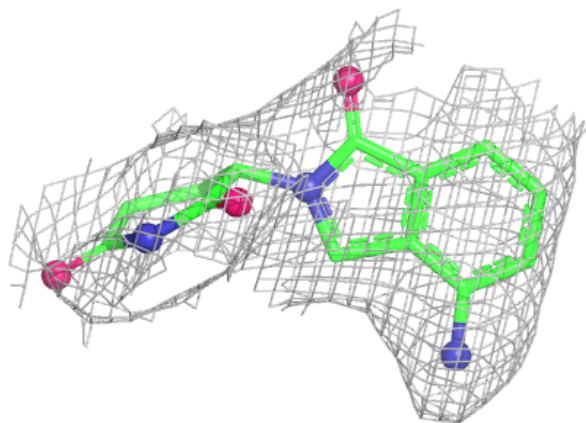
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	B	1437	1/1	0.99	0.07	94,94,94,94	0
4	ZN	E	1437	1/1	0.99	0.07	101,101,101,101	0

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.

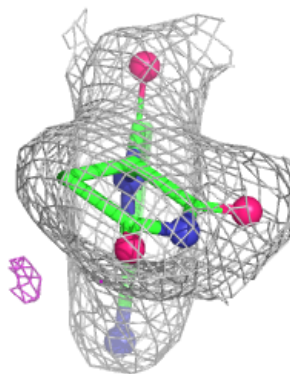
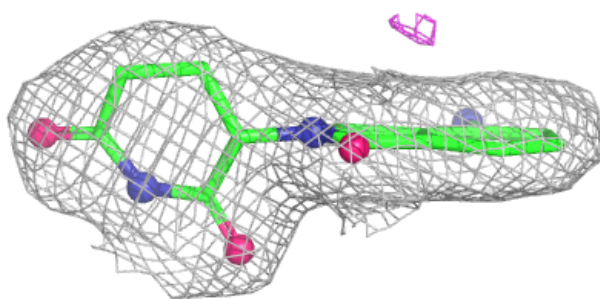
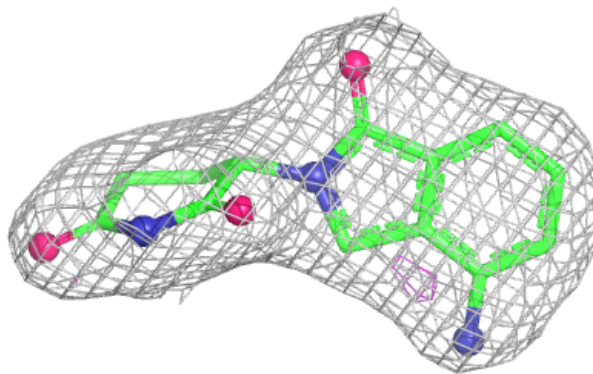
Electron density around LVY E 1438:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LVY B 1438:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.