



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:45 AM UTC

PDB ID : 9SFM / pdb_00009sfm
Title : Crystal structure of Cereblon-DDB1 in complex with SB-405483 and Lenalido-
mide
Authors : Chung, C.
Deposited on : 2025-08-19
Resolution : 2.39 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

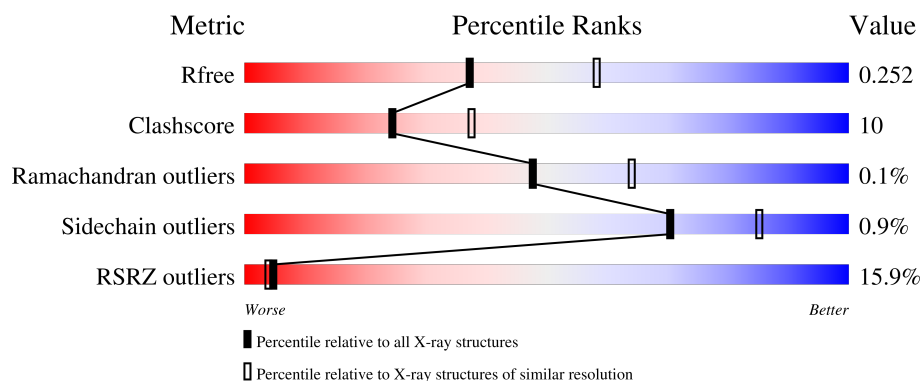
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	1148	15% 78% 19% ..
2	B	382	16% 73% 24% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12372 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	1124	Total	C	N	O	S	0	4	0
			8798	5578	1490	1681	49			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1141	TRP	-	expression tag	UNP Q16531
A	1142	SER	-	expression tag	UNP Q16531
A	1143	HIS	-	expression tag	UNP Q16531
A	1144	PRO	-	expression tag	UNP Q16531
A	1145	GLN	-	expression tag	UNP Q16531
A	1146	PHE	-	expression tag	UNP Q16531
A	1147	GLU	-	expression tag	UNP Q16531
A	1148	LYS	-	expression tag	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	376	Total	C	N	O	S	0	3	0
			3053	1949	523	557	24			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

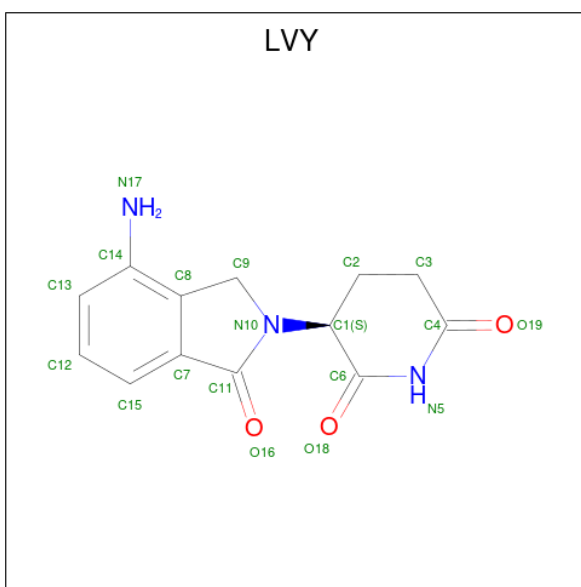


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

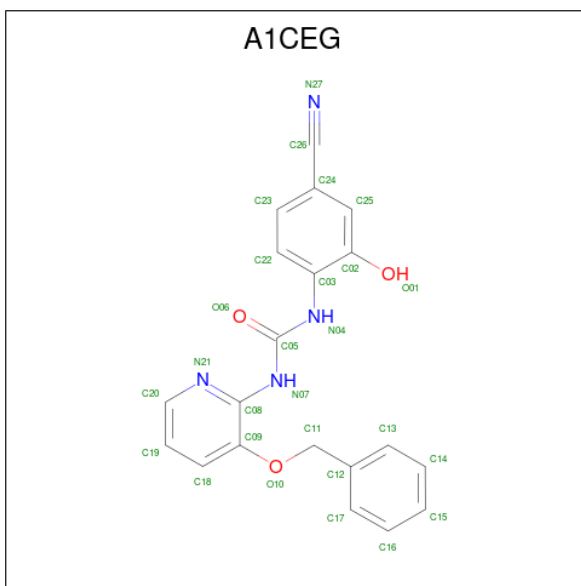
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- 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		

- Molecule 6 is N-[3-(benzyloxy)pyridin-2-yl]-N'-(4-cyano-2-hydroxyphenyl)urea (CCD ID: A1CEG) (formula: $C_{20}H_{16}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			27	20	4	3		

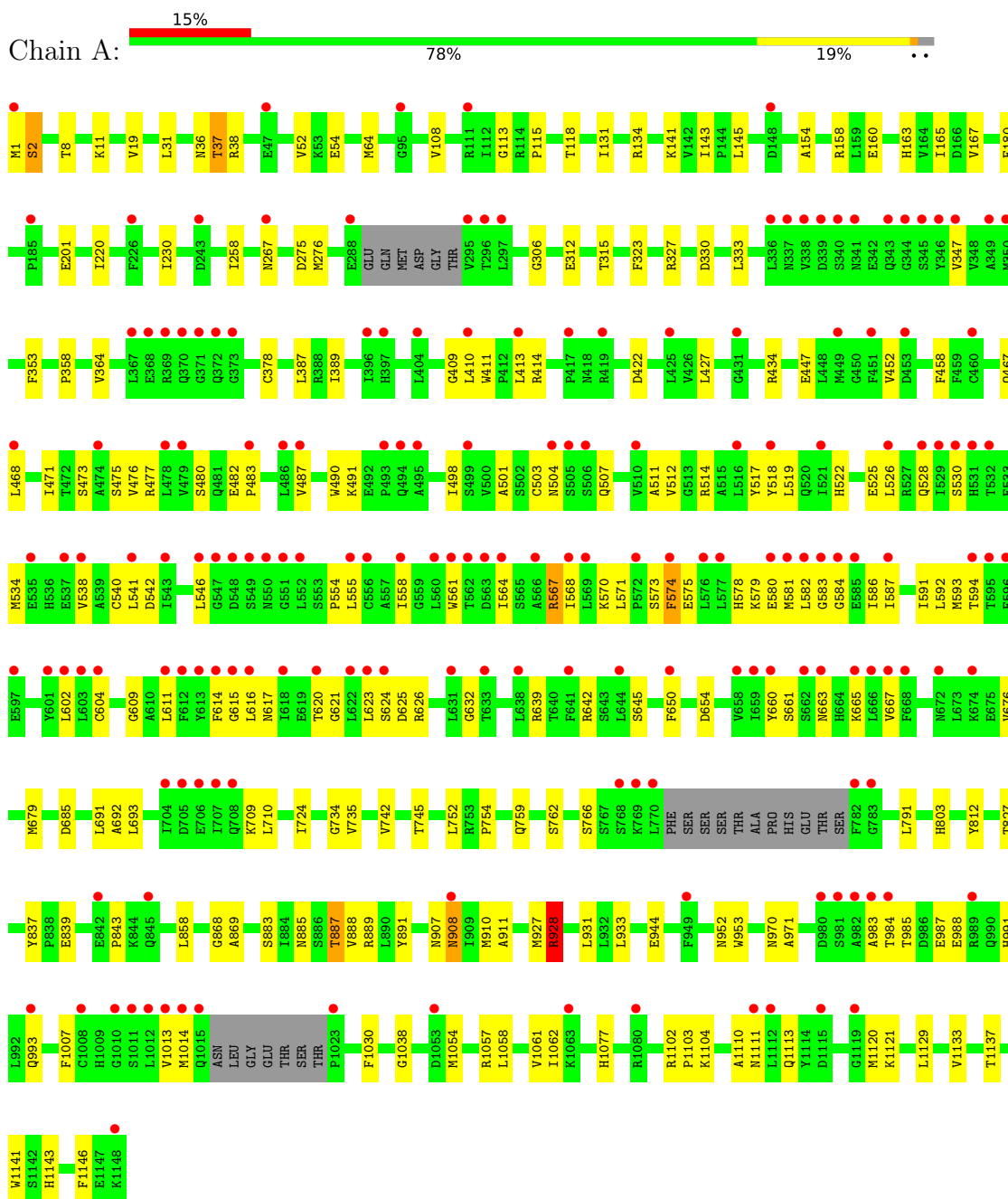
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	371	Total 371	O 371	0	0
7	B	79	Total 79	O 79	0	0

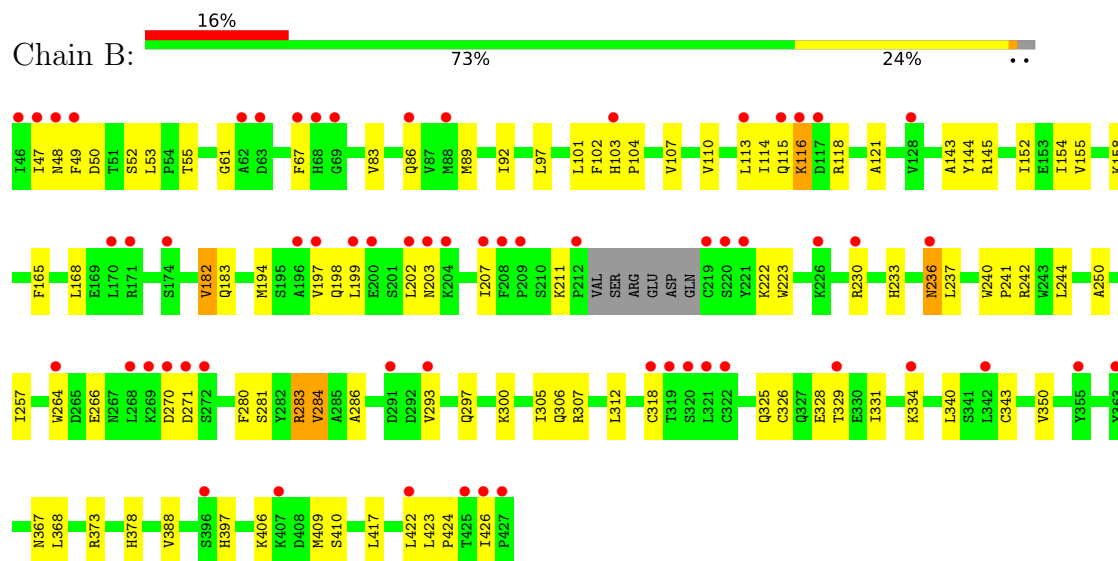
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.16Å 129.52Å 198.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.40 – 2.39 99.40 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (99.40-2.39) 100.0 (99.40-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.195 , 0.244 0.216 , 0.252	Depositor DCC
R_{free} test set	3697 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.0	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	0.94	EDS
Total number of atoms	12372	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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, LVY, EDO, A1CEG

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	0/8961	0.97	2/12139 (0.0%)
2	B	0.94	0/3127	1.21	0/4244
All	All	0.79	0/12088	1.04	2/16383 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	2
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	984	THR	N-CA-C	-5.80	106.85	114.04
1	A	574	PHE	CA-CB-CG	5.38	119.18	113.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	THR	Mainchain
1	A	434	ARG	Sidechain
1	A	567	ARG	Sidechain
1	A	928	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	242	ARG	Sidechain
2	B	283	ARG	Sidechain

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	8798	0	8738	170	1
2	B	3053	0	3038	73	1
3	A	20	0	30	1	0
3	B	4	0	6	1	0
4	B	1	0	0	0	0
5	B	19	0	13	0	0
6	B	27	0	0	1	0
7	A	371	0	0	5	1
7	B	79	0	0	1	1
All	All	12372	0	11825	236	2

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 10.

All (236) 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:650:PHE:HB3	1:A:679:MET:HE2	1.49	0.91
1:A:570:LYS:HB2	1:A:573:SER:HB2	1.54	0.87
1:A:498:ILE:HA	1:A:512:VAL:HG12	1.60	0.82
2:B:86:GLN:NE2	2:B:103[B]:HIS:HD2	1.78	0.81
2:B:86:GLN:NE2	2:B:103[B]:HIS:CD2	2.50	0.79
1:A:639:ARG:HB3	1:A:679:MET:HE1	1.62	0.79
1:A:602:LEU:HB2	1:A:616:LEU:HD23	1.65	0.79
2:B:199:LEU:HD12	2:B:202:LEU:HD12	1.66	0.78
1:A:868:GLY:HA3	1:A:885:ASN:HD21	1.48	0.77
1:A:927:MET:HE2	2:B:306:GLN:HG3	1.69	0.73
1:A:504:ASN:HD21	1:A:507:GLN:HG3	1.52	0.73
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:HB	2:B:410:SER:HB3	1.73	0.68
1:A:742:VAL:HG23	1:A:752:LEU:HD21	1.74	0.68
1:A:480:SER:HB2	1:A:483:PRO:HD2	1.76	0.68
2:B:197:VAL:HA	7:B:607:HOH:O	1.95	0.67
2:B:86:GLN:HE22	2:B:103[B]:HIS:CD2	2.13	0.67
1:A:364:VAL:HG11	1:A:1013:VAL:HG11	1.76	0.66
1:A:908:ASN:H	1:A:908:ASN:ND2	1.92	0.66
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.76	0.65
1:A:118:THR:HB	1:A:134:ARG:HH22	1.62	0.64
1:A:158:ARG:HH12	1:A:160:GLU:HG2	1.63	0.64
2:B:102:PHE:HD2	2:B:154:ILE:HD12	1.63	0.63
1:A:827:THR:H	3:A:1204:EDO:H21	1.63	0.63
1:A:327:ARG:HH11	2:B:199:LEU:HD23	1.62	0.63
1:A:868:GLY:HA3	1:A:885:ASN:ND2	2.14	0.62
1:A:991:HIS:HE1	1:A:993:GLN:HE22	1.47	0.62
2:B:326:CYS:HB2	2:B:328:GLU:HG2	1.81	0.61
6:B:504:A1CEG:N21	6:B:504:A1CEG:N04	2.48	0.61
1:A:11:LYS:HB3	1:A:38[B]:ARG:HD2	1.81	0.61
2:B:102:PHE:CD2	2:B:154:ILE:HD12	2.36	0.61
1:A:639:ARG:HB3	1:A:679:MET:CE	2.30	0.60
1:A:578:HIS:CE1	1:A:623:LEU:H	2.19	0.60
2:B:318:CYS:O	2:B:334:LYS:HD3	2.01	0.60
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.84	0.60
2:B:423:LEU:HD12	2:B:424:PRO:HD2	1.83	0.60
2:B:280:PHE:O	2:B:284:VAL:HG12	2.02	0.59
1:A:991:HIS:HE1	1:A:993:GLN:NE2	2.00	0.59
1:A:471:ILE:HG23	1:A:476:VAL:HG22	1.85	0.59
1:A:511:ALA:HB2	1:A:541:LEU:HD11	1.85	0.59
1:A:1013:VAL:HG23	1:A:1014:MET:HG3	1.83	0.59
2:B:203:ASN:HD21	3:B:502:EDO:H21	1.67	0.59
2:B:240:TRP:HB3	2:B:244:LEU:HD23	1.85	0.59
1:A:118:THR:HG21	1:A:165:ILE:O	2.04	0.58
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.86	0.58
1:A:985:THR:HB	1:A:988:GLU:HG3	1.86	0.57
1:A:928:ARG:HB2	1:A:952:ASN:O	2.04	0.57
2:B:67:PHE:HE1	2:B:144:TYR:HB3	1.69	0.57
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.39	0.57
1:A:650:PHE:HB3	1:A:679:MET:CE	2.29	0.57
1:A:511:ALA:HB1	1:A:538:VAL:HG21	1.87	0.56
2:B:211:LYS:HB3	2:B:223:TRP:CE2	2.41	0.56
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:HG22	2:B:121:ALA:HB3	1.87	0.56
1:A:709:LYS:HB2	7:A:1417:HOH:O	2.06	0.55
1:A:908:ASN:ND2	1:A:908:ASN:N	2.54	0.55
1:A:358:PRO:HG3	2:B:237:LEU:HD23	1.89	0.55
1:A:691:LEU:HD13	1:A:693:LEU:HD21	1.89	0.55
2:B:50:ASP:HB3	2:B:53:LEU:HG	1.87	0.55
1:A:742:VAL:CG2	1:A:752:LEU:HD21	2.37	0.55
1:A:685:ASP:OD1	1:A:685:ASP:N	2.40	0.54
1:A:617:ASN:O	1:A:621:GLY:N	2.41	0.54
1:A:971:ALA:HB3	1:A:1077:HIS:O	2.08	0.54
2:B:92:ILE:HD12	2:B:286:ALA:HA	1.90	0.54
2:B:331:ILE:HD12	2:B:368:LEU:HD21	1.88	0.54
2:B:61:GLY:HA3	2:B:145:ARG:HH22	1.73	0.54
1:A:8:THR:HG22	1:A:1143:HIS:HE1	1.73	0.53
1:A:592:LEU:HG	1:A:594:THR:HG23	1.90	0.53
2:B:202:LEU:HD11	2:B:233:HIS:ND1	2.23	0.53
1:A:327:ARG:NH1	2:B:199:LEU:HD23	2.21	0.53
1:A:564:ILE:HD11	1:A:583:GLY:N	2.23	0.53
1:A:201:GLU:HG3	7:A:1415:HOH:O	2.07	0.53
1:A:663:ASN:HB2	1:A:665:LYS:HE3	1.90	0.53
2:B:230:ARG:HE	2:B:230:ARG:HA	1.72	0.53
2:B:89:MET:SD	2:B:97:LEU:HD13	2.49	0.53
1:A:609:GLY:HA3	1:A:632:GLY:O	2.09	0.53
1:A:507:GLN:HB2	1:A:518:TYR:HE1	1.73	0.53
1:A:315:THR:CG2	1:A:323:PHE:HB3	2.39	0.52
1:A:561:TRP:CD1	1:A:587:ILE:HG12	2.44	0.52
2:B:115:GLN:O	2:B:116:LYS:HB2	2.08	0.52
1:A:452:VAL:HB	1:A:477:ARG:NH1	2.24	0.52
1:A:452:VAL:HB	1:A:477:ARG:HH11	1.74	0.52
2:B:165:PHE:CB	2:B:182:VAL:HG13	2.40	0.52
1:A:511:ALA:CB	1:A:538:VAL:HG21	2.40	0.52
1:A:564:ILE:O	1:A:582:LEU:HB3	2.10	0.52
1:A:36:ASN:ND2	1:A:37:THR:HG23	2.24	0.51
1:A:754:PRO:HB2	1:A:759:GLN:OE1	2.10	0.51
1:A:888:VAL:HG23	1:A:907:ASN:HD21	1.76	0.51
1:A:564:ILE:HG21	1:A:586:ILE:O	2.10	0.51
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.93	0.51
1:A:570:LYS:CB	1:A:573:SER:HB2	2.35	0.51
2:B:230:ARG:HA	2:B:230:ARG:NE	2.26	0.50
1:A:490:TRP:CG	1:A:519:LEU:HD21	2.46	0.50
2:B:113:LEU:HG	2:B:118:ARG:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ASN:HB3	1:A:620:THR:OG1	2.11	0.50
1:A:1014:MET:HG2	1:A:1141:TRP:CE2	2.47	0.50
1:A:1061:VAL:HG13	1:A:1104:LYS:HD2	1.94	0.50
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.93	0.50
2:B:236:ASN:H	2:B:236:ASN:HD22	1.60	0.49
1:A:163:HIS:HB3	2:B:207:ILE:HD13	1.94	0.49
1:A:409:GLY:HA3	1:A:411:TRP:CH2	2.48	0.49
1:A:554:PRO:O	1:A:571:LEU:N	2.45	0.49
1:A:642:ARG:HH22	1:A:645:SER:HA	1.78	0.49
1:A:108:VAL:O	1:A:141:LYS:HE3	2.13	0.49
1:A:315:THR:HG23	1:A:323:PHE:HB3	1.94	0.49
1:A:1057:ARG:HH22	1:A:1111:ASN:HB2	1.78	0.49
1:A:1113:GLN:HG3	1:A:1121:LYS:HB3	1.95	0.49
1:A:503:CYS:SG	1:A:504:ASN:N	2.86	0.48
1:A:458:PHE:HE2	1:A:473:SER:HB3	1.77	0.48
2:B:266:GLU:CD	2:B:266:GLU:H	2.21	0.48
1:A:661:SER:HA	1:A:665:LYS:O	2.13	0.48
1:A:676:VAL:HG11	1:A:693:LEU:HD12	1.95	0.48
1:A:991:HIS:CE1	1:A:993:GLN:HE22	2.31	0.48
1:A:364:VAL:HG11	1:A:1013:VAL:CG1	2.44	0.48
1:A:1014:MET:HG2	1:A:1141:TRP:NE1	2.29	0.48
1:A:887:THR:HG21	1:A:889:ARG:HH21	1.78	0.48
1:A:615:GLY:HA3	1:A:624:SER:HB3	1.94	0.48
1:A:908:ASN:N	1:A:908:ASN:HD22	2.12	0.48
1:A:564:ILE:HD11	1:A:583:GLY:H	1.79	0.47
1:A:812:TYR:CZ	2:B:241:PRO:HB3	2.49	0.47
1:A:11:LYS:NZ	7:A:1319:HOH:O	2.45	0.47
1:A:158:ARG:NH1	1:A:160:GLU:HG2	2.29	0.47
1:A:514:ARG:HD3	1:A:534:MET:O	2.13	0.47
1:A:1057:ARG:NH1	1:A:1110:ALA:O	2.40	0.47
1:A:542:ASP:OD2	1:A:592:LEU:HD12	2.15	0.47
1:A:306:GLY:HA3	1:A:347:VAL:HG12	1.97	0.47
1:A:709:LYS:HG2	1:A:710:LEU:N	2.29	0.47
1:A:839:GLU:CD	1:A:839:GLU:H	2.23	0.47
2:B:152:ILE:HG22	2:B:154:ILE:HD11	1.95	0.47
1:A:54:GLU:HB2	1:A:1146:PHE:CD2	2.51	0.46
1:A:160:GLU:HG3	7:A:1567:HOH:O	2.16	0.46
1:A:414:ARG:HG2	1:A:422:ASP:HA	1.98	0.46
1:A:1054:MET:SD	1:A:1129:LEU:HD12	2.56	0.46
1:A:933:LEU:HD23	1:A:944:GLU:HA	1.96	0.46
1:A:267:ASN:HD22	1:A:267:ASN:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLN:NE2	1:A:487:VAL:HG21	2.30	0.46
2:B:270:ASP:OD1	2:B:271:ASP:N	2.48	0.46
1:A:389:ILE:HD12	1:A:389:ILE:N	2.31	0.45
1:A:1102:ARG:HB3	1:A:1103:PRO:HD3	1.97	0.45
2:B:281:SER:HB2	2:B:307:ARG:HD2	1.98	0.45
1:A:471:ILE:CD1	1:A:476:VAL:HG13	2.46	0.45
1:A:570:LYS:O	1:A:574:PHE:N	2.44	0.45
1:A:512:VAL:HG22	1:A:517:TYR:HE1	1.82	0.45
1:A:220:ILE:HB	1:A:230:ILE:HB	1.98	0.45
1:A:333:LEU:HG	1:A:353:PHE:CE2	2.52	0.45
1:A:541:LEU:HD21	1:A:558:ILE:HD13	1.98	0.45
2:B:250:ALA:HB2	2:B:305:ILE:CD1	2.46	0.45
2:B:107:VAL:HG13	2:B:155:VAL:HG23	1.98	0.45
2:B:388:VAL:HG13	2:B:397:HIS:CD2	2.51	0.45
1:A:1058:LEU:HD22	1:A:1062:ILE:HD11	1.98	0.44
1:A:542:ASP:OD2	1:A:592:LEU:HA	2.17	0.44
1:A:587:ILE:N	1:A:587:ILE:HD12	2.33	0.44
2:B:194:MET:O	2:B:198:GLN:N	2.50	0.44
1:A:910:MET:HE3	1:A:910:MET:HB2	1.81	0.44
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.99	0.44
1:A:604:CYS:O	1:A:611:LEU:HD12	2.17	0.44
1:A:113:GLY:O	1:A:115:PRO:HD3	2.17	0.44
1:A:518:TYR:C	1:A:519:LEU:HD12	2.43	0.44
1:A:573:SER:O	1:A:575:GLU:HG3	2.17	0.44
1:A:581:MET:HB2	1:A:626:ARG:HH11	1.83	0.44
1:A:413:LEU:HD11	1:A:468:LEU:HD13	1.99	0.44
1:A:654:ASP:OD1	1:A:654:ASP:N	2.50	0.44
2:B:67:PHE:CE1	2:B:144:TYR:HB3	2.52	0.44
2:B:329:THR:HG23	2:B:367:ASN:CB	2.47	0.44
1:A:330:ASP:OD2	7:A:1301:HOH:O	2.21	0.43
2:B:194:MET:HA	2:B:194:MET:HE2	1.99	0.43
1:A:931:LEU:HD11	1:A:944:GLU:HG3	1.98	0.43
1:A:614:PHE:HA	1:A:625:ASP:O	2.19	0.43
1:A:983:ALA:HB1	1:A:988:GLU:HB2	2.00	0.43
1:A:1:MET:HG2	1:A:2:SER:N	2.34	0.43
1:A:614:PHE:CD1	1:A:626:ARG:HA	2.53	0.43
2:B:350:VAL:O	2:B:378:HIS:HE1	2.01	0.43
2:B:48:ASN:HB2	2:B:409:MET:HA	1.99	0.43
1:A:490:TRP:HB2	1:A:526:LEU:HD23	2.00	0.43
1:A:165:ILE:CD1	2:B:207:ILE:HB	2.49	0.43
1:A:985:THR:HG22	1:A:987:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.19	0.43
2:B:283:ARG:HD2	2:B:343:CYS:O	2.19	0.43
1:A:471:ILE:HG21	1:A:501:ALA:HB1	2.01	0.43
1:A:593:MET:HG2	1:A:602:LEU:HD13	2.01	0.43
1:A:791:LEU:HD23	1:A:858:LEU:HD21	2.01	0.43
2:B:86:GLN:HE21	2:B:103[B]:HIS:HD2	1.60	0.43
1:A:276:MET:HE1	2:B:230:ARG:HH12	1.84	0.42
1:A:167:VAL:HB	1:A:180:PHE:HB3	2.02	0.42
2:B:110:VAL:O	2:B:114:ILE:HG12	2.19	0.42
2:B:406:LYS:HD2	2:B:409:MET:HE3	2.00	0.42
1:A:378:CYS:SG	1:A:724:ILE:HB	2.59	0.42
1:A:762:SER:O	1:A:803:HIS:HA	2.20	0.42
1:A:540:CYS:HB2	1:A:591:ILE:HG22	2.02	0.42
1:A:333:LEU:HG	1:A:353:PHE:HE2	1.84	0.42
1:A:530:SER:HB3	1:A:574:PHE:CD2	2.54	0.42
1:A:889:ARG:HD2	1:A:891:TYR:OH	2.19	0.42
2:B:199:LEU:HB2	2:B:202:LEU:HB2	2.00	0.42
1:A:564:ILE:HD11	1:A:584:GLY:H	1.84	0.42
1:A:1007:PHE:CD1	1:A:1030:PHE:HB3	2.55	0.42
2:B:257:ILE:HG12	2:B:312:LEU:HG	2.01	0.42
2:B:426:ILE:HD12	2:B:426:ILE:N	2.35	0.42
1:A:616:LEU:C	1:A:616:LEU:HD12	2.45	0.42
2:B:52:SER:O	2:B:55:THR:HG22	2.19	0.42
2:B:101:LEU:CD1	2:B:110:VAL:HG21	2.50	0.41
2:B:103[A]:HIS:ND1	2:B:104:PRO:HD2	2.35	0.41
1:A:504:ASN:ND2	1:A:507:GLN:HG3	2.28	0.41
1:A:258:ILE:HD13	1:A:275:ASP:HB3	2.02	0.41
1:A:546:LEU:HD11	1:A:593:MET:O	2.20	0.41
1:A:1:MET:HG2	1:A:2:SER:H	1.85	0.41
1:A:1120:MET:HE3	1:A:1120:MET:HB2	1.54	0.41
2:B:293:VAL:O	2:B:297:GLN:HG3	2.21	0.41
1:A:475:SER:HB3	1:A:491:LYS:HD2	2.02	0.41
1:A:582:LEU:HD12	1:A:582:LEU:O	2.21	0.41
1:A:843:PRO:HG2	1:A:869:ALA:HB2	2.02	0.41
2:B:198:GLN:NE2	2:B:202:LEU:HB3	2.35	0.41
1:A:131:ILE:HD11	1:A:145:LEU:HD21	2.03	0.41
1:A:410:LEU:HD23	1:A:427:LEU:HG	2.03	0.41
1:A:858:LEU:HD12	1:A:858:LEU:HA	1.90	0.41
1:A:31:LEU:CD1	1:A:315:THR:HG21	2.51	0.41
1:A:679:MET:HA	1:A:692:ALA:O	2.21	0.41
1:A:312:GLU:HB2	1:A:327:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HD23	1:A:568:ILE:HG21	2.03	0.41
2:B:49:PHE:CE2	2:B:340:LEU:HG	2.56	0.41
2:B:297:GLN:HA	2:B:300:LYS:HE2	2.03	0.41
1:A:541:LEU:CD2	1:A:558:ILE:HD13	2.51	0.40
1:A:567:ARG:HG2	1:A:579:LYS:HG2	2.03	0.40
1:A:580:GLU:OE1	1:A:623:LEU:HB3	2.21	0.40
1:A:581:MET:HE2	1:A:581:MET:HB3	1.92	0.40
1:A:837:TYR:HB3	1:A:839:GLU:OE2	2.21	0.40
2:B:417:LEU:HB3	2:B:422:LEU:HD11	2.03	0.40
1:A:724:ILE:HA	1:A:734:GLY:O	2.21	0.40
2:B:250:ALA:HB2	2:B:305:ILE:HD13	2.03	0.40
2:B:264:TRP:CZ2	2:B:334:LYS:HD2	2.56	0.40
1:A:19:VAL:HG22	1:A:64:MET:HE3	2.03	0.40
2:B:61:GLY:HA3	2:B:145:ARG:NH2	2.36	0.40
1:A:623:LEU:HD22	1:A:626:ARG:HD3	2.03	0.40
2:B:89:MET:HE3	2:B:89:MET:HB2	1.91	0.40
2:B:168:LEU:HD11	2:B:183:GLN:HB2	2.03	0.40
1:A:522:HIS:HB2	1:A:525:GLU:HB2	2.02	0.40
2:B:329:THR:HG22	2:B:331:ILE:HD13	2.03	0.40

All (2) 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)
1:A:447:GLU:OE2	2:B:373:ARG:CD[3_544]	1.76	0.44
7:A:1641:HOH:O	7:B:651:HOH:O[4_554]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	1120/1148 (98%)	1089 (97%)	31 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	375/382 (98%)	369 (98%)	4 (1%)	2 (0%)	24	37
All	All	1495/1530 (98%)	1458 (98%)	35 (2%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	LYS
2	B	325	GLN

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	975/1007 (97%)	967 (99%)	8 (1%)	73	86
2	B	341/346 (99%)	337 (99%)	4 (1%)	63	81
All	All	1316/1353 (97%)	1304 (99%)	12 (1%)	70	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	52	VAL
1	A	528	GLN
1	A	745	THR
1	A	766	SER
1	A	887	THR
1	A	908	ASN
1	A	928	ARG
2	B	182	VAL
2	B	222	LYS
2	B	236	ASN
2	B	284	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	156	ASN
1	A	163	HIS
1	A	183	GLN
1	A	392	ASN
1	A	578	HIS
1	A	672	ASN
1	A	711	HIS
1	A	790	ASN
1	A	885	ASN
1	A	907	ASN
1	A	908	ASN
1	A	964	ASN
1	A	978	GLN
1	A	991	HIS
2	B	86	GLN
2	B	100	GLN
2	B	112	ASN
2	B	129	GLN
2	B	178	GLN
2	B	179	GLN
2	B	203	ASN
2	B	236	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
6	A1CEG	B	504	-	29,29,29	0.64	0	35,38,38	1.15	5 (14%)
3	EDO	B	502	-	3,3,3	0.51	0	2,2,2	0.33	0
3	EDO	A	1204	-	3,3,3	0.43	0	2,2,2	0.69	0
3	EDO	A	1201	-	3,3,3	0.38	0	2,2,2	0.84	0
5	LVY	B	503	-	21,21,21	1.03	1 (4%)	29,31,31	4.15	12 (41%)
3	EDO	A	1202	-	3,3,3	0.52	0	2,2,2	0.32	0
3	EDO	A	1205	-	3,3,3	0.68	0	2,2,2	0.12	0
3	EDO	A	1203	-	3,3,3	0.47	0	2,2,2	0.50	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
6	A1CEG	B	504	-	-	2/15/15/15	0/3/3/3
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	1204	-	-	0/1/1/1	-
3	EDO	A	1201	-	-	1/1/1/1	-
5	LVY	B	503	-	-	0/4/29/29	0/3/3/3
3	EDO	A	1202	-	-	1/1/1/1	-
3	EDO	A	1205	-	-	1/1/1/1	-
3	EDO	A	1203	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	LVY	C14-C8	-2.48	1.39	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	LVY	C8-C9-N10	12.78	105.65	101.79
5	B	503	LVY	C9-N10-C11	-11.19	108.43	113.15
5	B	503	LVY	C7-C11-N10	8.18	111.62	106.42
5	B	503	LVY	C3-C4-N5	4.93	121.93	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	LVY	C9-N10-C1	4.85	128.30	123.68
5	B	503	LVY	C9-C8-C7	-4.38	107.07	109.82
5	B	503	LVY	C4-N5-C6	-3.70	121.81	126.69
5	B	503	LVY	C2-C1-N10	-3.30	110.42	114.03
6	B	504	A1CEG	O06-C05-N07	-3.02	118.27	123.64
6	B	504	A1CEG	N07-C05-N04	2.94	118.13	112.44
5	B	503	LVY	C1-C6-N5	2.89	120.46	116.24
5	B	503	LVY	C6-C1-N10	2.62	112.75	110.32
5	B	503	LVY	C2-C3-C4	-2.45	108.80	113.87
5	B	503	LVY	O16-C11-N10	-2.37	123.45	125.34
6	B	504	A1CEG	C11-O10-C09	2.31	122.33	117.76
6	B	504	A1CEG	N07-C08-N21	2.13	123.06	117.54
6	B	504	A1CEG	C20-N21-C08	2.08	120.78	116.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	EDO	O1-C1-C2-O2
3	A	1203	EDO	O1-C1-C2-O2
3	A	1205	EDO	O1-C1-C2-O2
3	A	1201	EDO	O1-C1-C2-O2
6	B	504	A1CEG	C18-C09-O10-C11
6	B	504	A1CEG	C08-C09-O10-C11

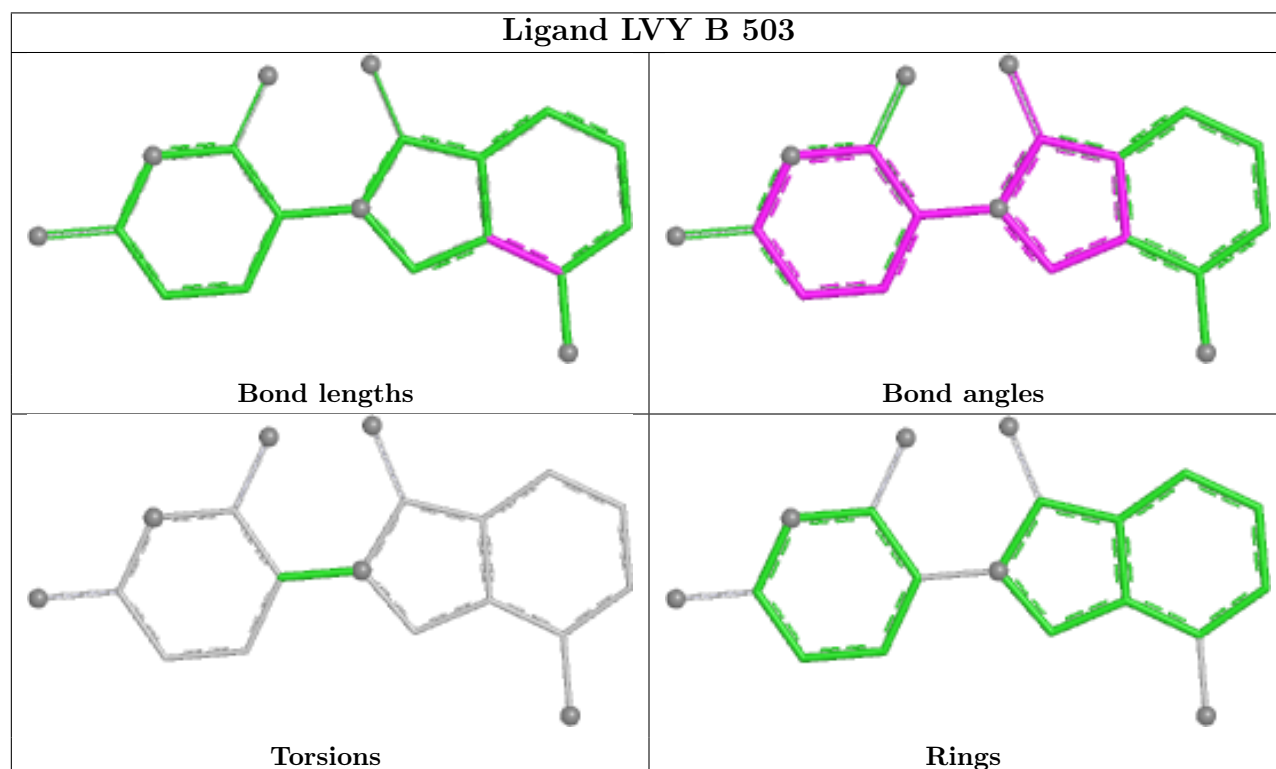
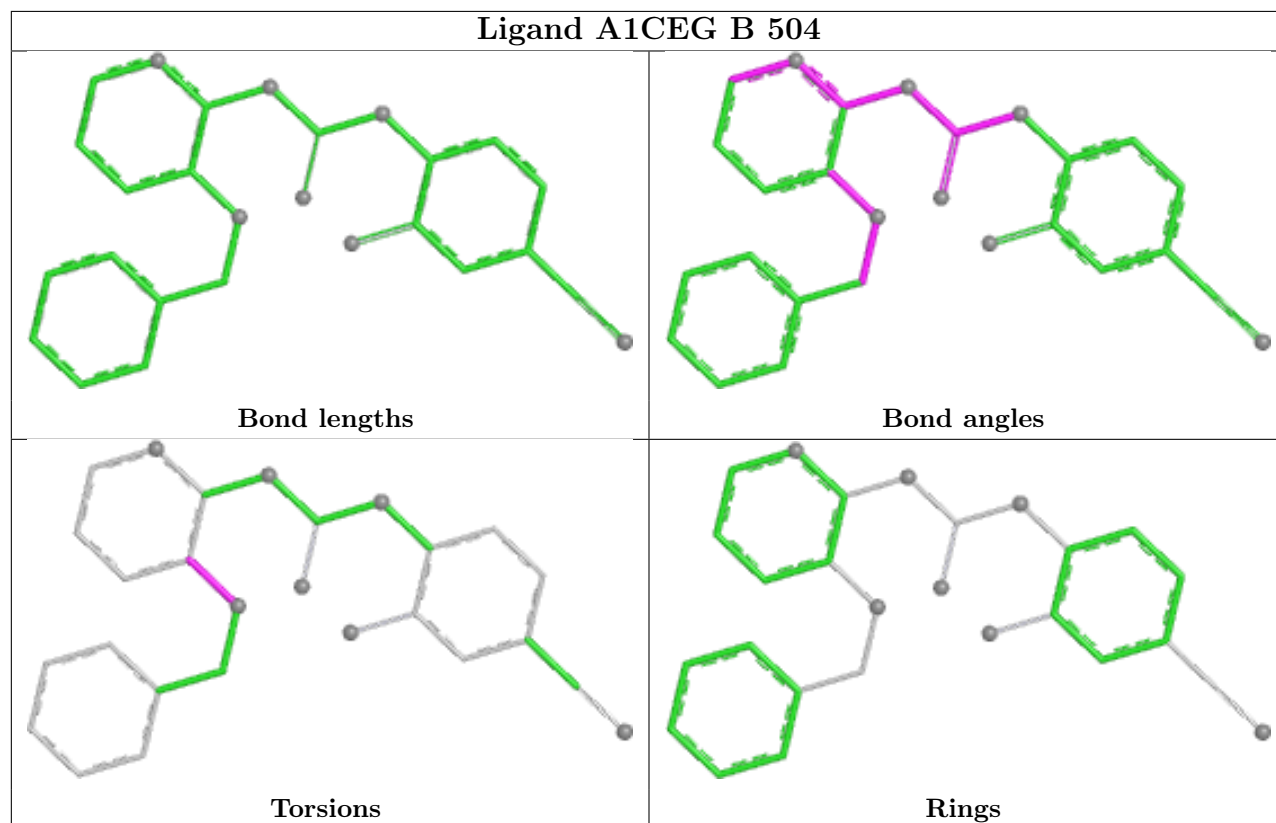
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	504	A1CEG	1	0
3	B	502	EDO	1	0
3	A	1204	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1124/1148 (97%)	0.74	177 (15%) 5 4	21, 56, 126, 184	4 (0%)
2	B	376/382 (98%)	1.15	61 (16%) 4 4	29, 64, 122, 176	3 (0%)
All	All	1500/1530 (98%)	0.84	238 (15%) 5 4	21, 58, 126, 184	7 (0%)

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	TYR	6.0
2	B	212	PRO	5.5
1	A	574	PHE	5.4
1	A	295	VAL	5.4
2	B	426	ILE	5.3
1	A	561	TRP	5.2
1	A	582	LEU	5.1
1	A	460	CYS	5.0
2	B	197	VAL	5.0
2	B	219	CYS	4.9
2	B	220	SER	4.6
2	B	355[A]	TYR	4.5
1	A	367	LEU	4.5
1	A	707	ILE	4.5
1	A	516	LEU	4.2
2	B	236	ASN	4.1
2	B	103[A]	HIS	4.1
1	A	548	ASP	4.1
1	A	372	GLN	4.1
1	A	338	VAL	4.1
2	B	170	LEU	4.0
1	A	1012	LEU	4.0
1	A	1023	PRO	3.9
1	A	543	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	770	LEU	3.8
1	A	982	ALA	3.8
1	A	371	GLY	3.8
1	A	576	LEU	3.8
2	B	319	THR	3.7
1	A	1013	VAL	3.7
1	A	618	ILE	3.6
1	A	550	ASN	3.6
2	B	425	THR	3.6
1	A	404	LEU	3.5
1	A	337	ASN	3.5
1	A	644	LEU	3.5
1	A	585	GLU	3.4
1	A	551	GLY	3.4
2	B	47	ILE	3.4
1	A	495	ALA	3.4
1	A	580	GLU	3.4
2	B	88	MET	3.3
1	A	601	TYR	3.3
1	A	667	VAL	3.3
1	A	339	ASP	3.3
1	A	566	ALA	3.2
1	A	572	PRO	3.2
1	A	370	GLN	3.2
1	A	340	SER	3.2
2	B	208	PHE	3.2
1	A	518	TYR	3.2
2	B	427	PRO	3.2
1	A	660	TYR	3.1
1	A	148	ASP	3.1
1	A	486	LEU	3.1
1	A	396	ILE	3.0
1	A	584	GLY	3.0
1	A	474	ALA	3.0
2	B	268	LEU	3.0
1	A	368	GLU	3.0
1	A	529	ILE	3.0
1	A	984	THR	3.0
1	A	1111	ASN	3.0
1	A	614	PHE	3.0
1	A	526	LEU	3.0
2	B	221	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	768	SER	3.0
1	A	949	PHE	2.9
1	A	521	ILE	2.9
1	A	568	ILE	2.9
1	A	537	GLU	2.9
1	A	782	PHE	2.9
1	A	297	LEU	2.9
1	A	397[A]	HIS	2.9
1	A	663	ASN	2.9
1	A	705	ASP	2.9
1	A	226	PHE	2.9
1	A	631	LEU	2.9
1	A	641	PHE	2.9
1	A	558	ILE	2.9
2	B	320	SER	2.9
2	B	68	HIS	2.9
1	A	468	LEU	2.9
1	A	1015	GLN	2.9
2	B	86	GLN	2.8
1	A	413	LEU	2.8
1	A	531	HIS	2.8
1	A	345	SER	2.8
1	A	560	LEU	2.8
1	A	1014	MET	2.8
1	A	296	THR	2.7
2	B	318	CYS	2.7
2	B	322	CYS	2.7
1	A	1	MET	2.7
1	A	603	LEU	2.7
1	A	616	LEU	2.7
1	A	658	VAL	2.7
1	A	981	SER	2.7
1	A	47	GLU	2.7
2	B	269	LYS	2.7
1	A	555	LEU	2.7
2	B	202	LEU	2.7
1	A	650	PHE	2.7
2	B	67	PHE	2.7
2	B	293	VAL	2.7
2	B	200	GLU	2.7
2	B	204	LYS	2.7
1	A	615	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	499	SER	2.7
1	A	577	LEU	2.7
1	A	623	LEU	2.7
1	A	538	VAL	2.6
2	B	271	ASP	2.6
1	A	983	ALA	2.6
1	A	341	ASN	2.6
1	A	532	THR	2.6
1	A	908	ASN	2.6
1	A	347	VAL	2.6
1	A	487	VAL	2.6
1	A	336	LEU	2.5
1	A	706	GLU	2.5
1	A	980	ASP	2.5
1	A	587	ILE	2.5
1	A	1011	SER	2.5
1	A	613	TYR	2.5
2	B	363	TYR	2.5
1	A	569	LEU	2.5
1	A	665	LYS	2.5
1	A	622	LEU	2.5
2	B	407	LYS	2.5
1	A	581	MET	2.5
1	A	349	ALA	2.5
1	A	594	THR	2.4
1	A	530	SER	2.4
1	A	596	PHE	2.4
2	B	264	TRP	2.4
1	A	638	LEU	2.4
2	B	270	ASP	2.4
2	B	272	SER	2.4
2	B	46	ILE	2.4
1	A	602	LEU	2.4
1	A	666	LEU	2.4
1	A	708	GLN	2.4
2	B	171	ARG	2.4
1	A	493	PRO	2.4
2	B	62	ALA	2.4
1	A	510	VAL	2.4
1	A	583	GLY	2.4
1	A	769	LYS	2.4
1	A	546	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	111	ARG	2.4
2	B	230	ARG	2.4
1	A	185	PRO	2.3
1	A	1010	GLY	2.3
2	B	329	THR	2.3
1	A	556	CYS	2.3
2	B	342	LEU	2.3
1	A	267	ASN	2.3
1	A	672	ASN	2.3
1	A	417	PRO	2.3
1	A	547	GLY	2.3
1	A	449	MET	2.3
1	A	562	THR	2.3
2	B	174	SER	2.3
1	A	1112	LEU	2.3
1	A	344	GLY	2.3
1	A	783	GLY	2.3
1	A	1080	ARG	2.3
1	A	451	PHE	2.3
1	A	552	LEU	2.3
1	A	604	CYS	2.3
2	B	117	ASP	2.3
1	A	483	PRO	2.3
2	B	196	ALA	2.3
1	A	597	GLU	2.3
2	B	115	GLN	2.3
2	B	199	LEU	2.2
1	A	453	ASP	2.2
2	B	203	ASN	2.2
1	A	369	ARG	2.2
1	A	431	GLY	2.2
1	A	1063	LYS	2.2
1	A	425	LEU	2.2
1	A	478	LEU	2.2
2	B	128	VAL	2.2
1	A	504	ASN	2.2
2	B	291	ASP	2.2
1	A	989	ARG	2.2
1	A	95	GLY	2.2
1	A	350	MET	2.2
1	A	845[A]	GLN	2.2
2	B	396	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	541	LEU	2.2
1	A	479	VAL	2.2
2	B	226	LYS	2.2
2	B	69	GLY	2.2
1	A	505	SER	2.2
1	A	419	ARG	2.1
2	B	63	ASP	2.1
2	B	49	PHE	2.1
1	A	620	THR	2.1
1	A	659	ILE	2.1
1	A	704	ILE	2.1
2	B	321	LEU	2.1
1	A	243	ASP	2.1
1	A	1053	ASP	2.1
1	A	528	GLN	2.1
1	A	612	PHE	2.1
1	A	668	PHE	2.1
1	A	1119	GLY	2.1
1	A	662	SER	2.1
1	A	1148	LYS	2.1
1	A	288	GLU	2.1
1	A	842	GLU	2.1
2	B	422	LEU	2.1
1	A	563	ASP	2.1
1	A	549	SER	2.1
1	A	595	THR	2.1
1	A	674	LYS	2.1
1	A	410	LEU	2.1
1	A	564	ILE	2.1
1	A	1115	ASP	2.1
2	B	207	ILE	2.1
1	A	506	SER	2.0
1	A	993	GLN	2.0
1	A	611	LEU	2.0
2	B	209	PRO	2.0
1	A	373	GLY	2.0
2	B	116	LYS	2.0
2	B	334	LYS	2.0
1	A	535	GLU	2.0
1	A	624	SER	2.0
1	A	633	THR	2.0
1	A	343	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	494	GLN	2.0
1	A	1008	CYS	2.0
2	B	48	ASN	2.0
2	B	113	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](#)

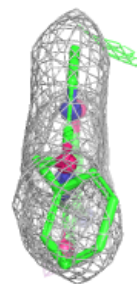
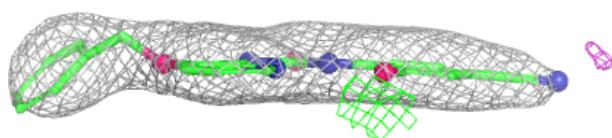
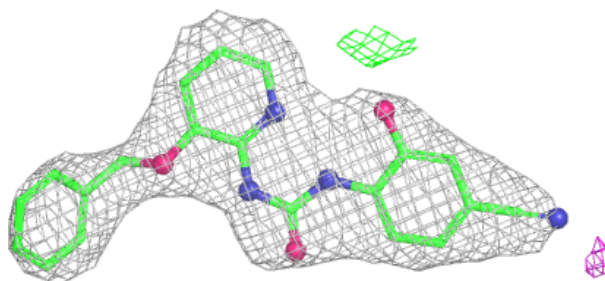
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	502	4/4	0.78	0.17	68,78,78,79	0
3	EDO	A	1204	4/4	0.82	0.15	57,58,69,70	0
3	EDO	A	1205	4/4	0.87	0.18	62,69,70,82	0
3	EDO	A	1201	4/4	0.90	0.13	42,42,43,61	0
3	EDO	A	1202	4/4	0.93	0.11	47,48,48,65	0
6	A1CEG	B	504	27/27	0.93	0.11	62,69,86,87	0
5	LVY	B	503	19/19	0.96	0.07	39,50,56,63	0
3	EDO	A	1203	4/4	0.97	0.10	43,43,44,50	0
4	ZN	B	501	1/1	0.98	0.04	56,56,56,56	0

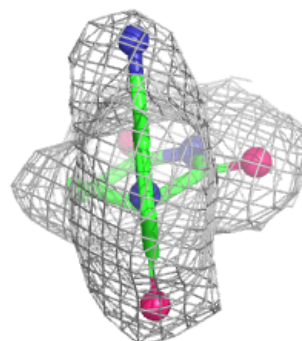
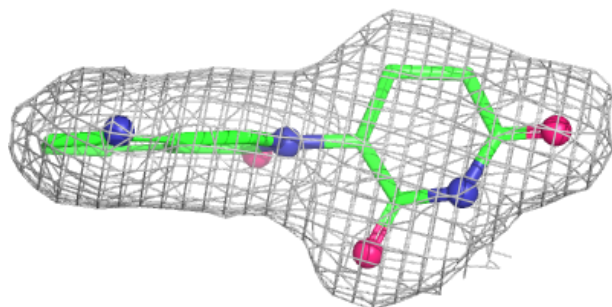
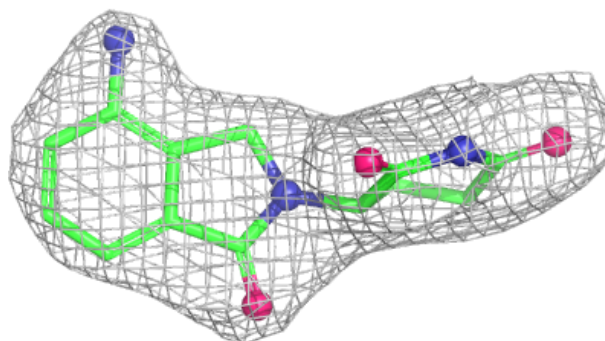
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1CEG B 504:

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

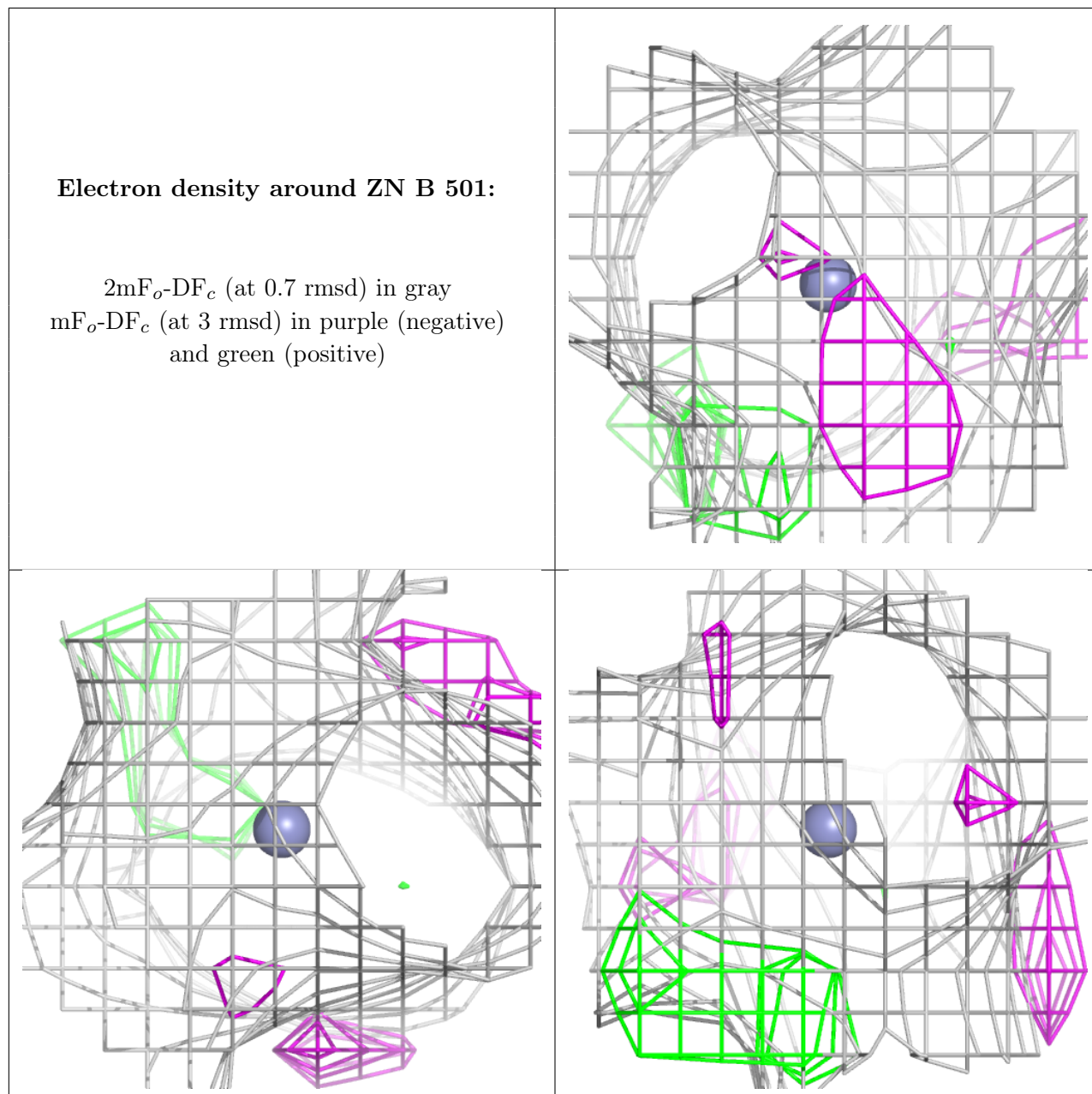
**Electron density around LVY B 503:**

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



Electron density around ZN B 501:

$2mF_o - DF_c$ (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.