



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2026 – 12:12 PM JST

PDB ID : 8HN9 / pdb_00008hn9
Title : Human SIRT3 Recognizing CCNE2K348la peptide
Authors : Wang, Y.; Ding, W.
Deposited on : 2022-12-07
Resolution : 3.70 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

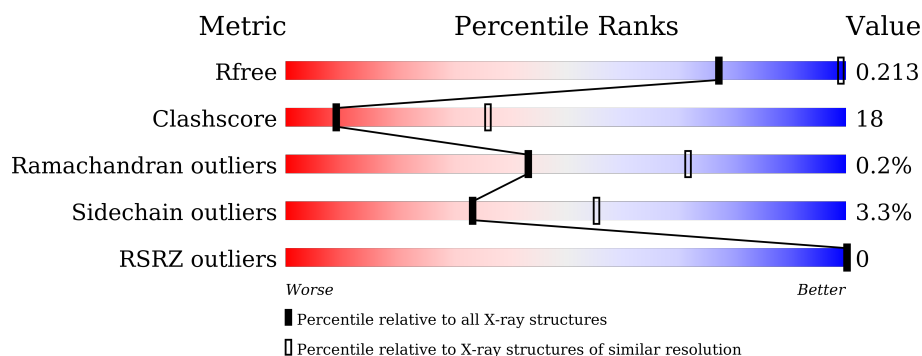
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	274	73% 24% .
1	B	274	71% 27% .
2	C	13	23% 54% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMD	C	201	-	-	X	-
4	IMD	C	202	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4417 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	1	0	0
			2143	1380	368	386	9			
1	B	274	Total	C	N	O	S	1	0	0
			2152	1386	370	387	9			

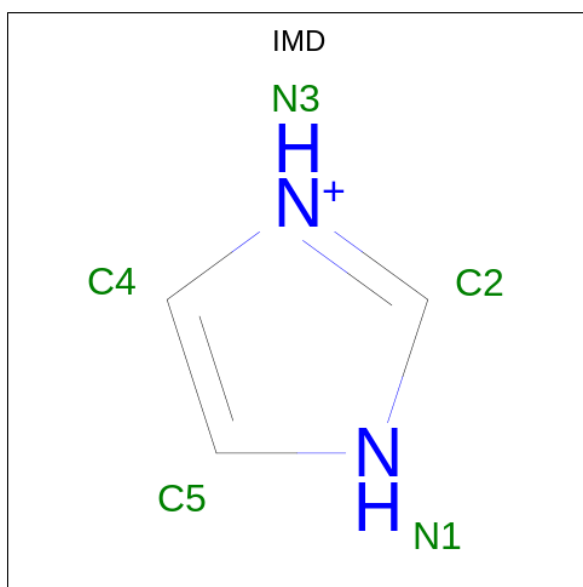
- Molecule 2 is a protein called CCNE2 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	S	0	0	0
			110	75	17	17	1			

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

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

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂) (labeled as "Ligand of Interest" by depositor).

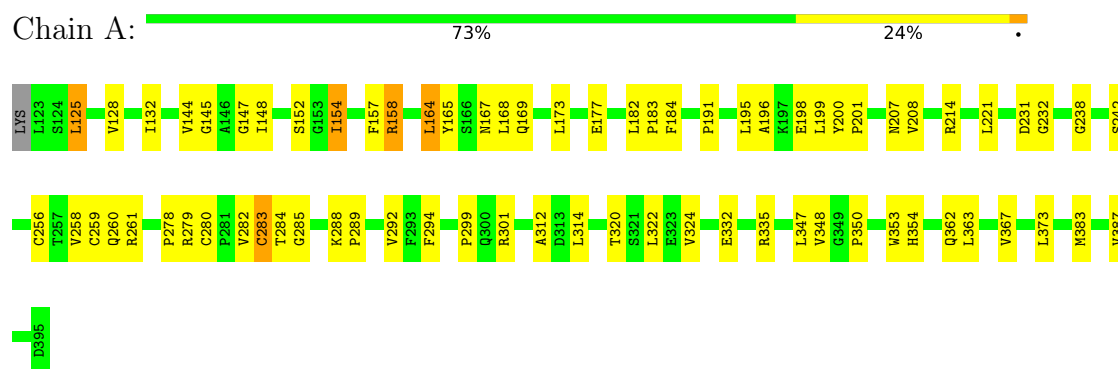


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	N	0	0
			5	3	2		
4	C	1	Total	C	N	0	0
			5	3	2		

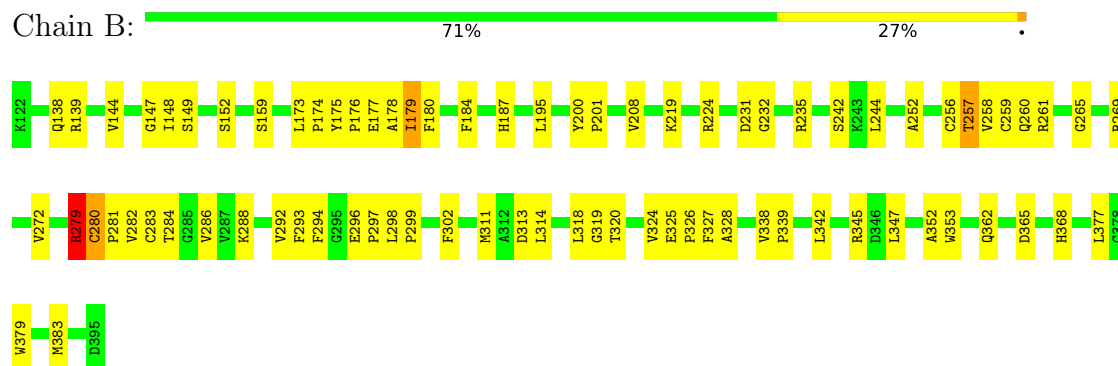
3 Residue-property plots

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: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 2: CCNE2 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	235.68Å 235.68Å 235.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.23 – 3.70 38.23 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.23-3.70) 99.5 (38.23-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.197 , 0.218 0.193 , 0.213	Depositor DCC
R_{free} test set	1235 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.408 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4417	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D8R, ZN, IMD

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	0.41	1/2198 (0.0%)	0.60	0/2996
1	B	0.39	0/2207	0.64	2/3007 (0.1%)
2	C	0.84	0/97	1.42	0/127
All	All	0.41	1/4502 (0.0%)	0.65	2/6130 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	PRO	C-O	-5.13	1.17	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	CA-C-N	-5.68	113.27	122.48
1	B	279	ARG	C-N-CA	-5.68	113.27	122.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2143	0	2153	73	0
1	B	2152	0	2168	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	110	0	116	25	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	C	10	0	10	11	0
All	All	4417	0	4447	163	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 18.

All (163) 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:256:CYS:SG	1:A:259:CYS:HB3	1.35	1.65
1:A:256:CYS:SG	1:A:259:CYS:CB	2.23	1.26
1:B:365:ASP:HB3	1:B:368:HIS:CD2	1.70	1.25
1:B:365:ASP:CB	1:B:368:HIS:HD2	1.64	1.09
2:C:10:D8R:O1	4:C:201:IMD:H2	1.53	1.07
1:A:324:VAL:HG21	2:C:3:VAL:HG22	1.35	1.04
1:A:324:VAL:CG2	2:C:3:VAL:HG22	1.91	1.01
1:B:280:CYS:SG	1:B:281:PRO:HD2	2.03	0.99
2:C:1:SER:N	2:C:2:PRO:HD3	1.78	0.98
1:B:365:ASP:HB3	1:B:368:HIS:HD2	0.83	0.98
1:A:256:CYS:SG	1:A:260:GLN:N	2.41	0.93
1:B:173:LEU:HD23	1:B:184:PHE:CZ	2.04	0.92
1:A:158:ARG:NH2	1:A:158:ARG:HB2	1.84	0.92
1:B:173:LEU:HD21	1:B:184:PHE:CE2	2.06	0.91
1:B:258:VAL:HB	1:B:283:CYS:SG	2.13	0.88
2:C:1:SER:H3	2:C:2:PRO:HD3	1.34	0.86
1:A:125:LEU:HD12	1:A:125:LEU:O	1.75	0.85
1:B:173:LEU:CD2	1:B:184:PHE:CE2	2.61	0.84
1:A:292:VAL:HG12	2:C:2:PRO:HG3	1.59	0.83
1:A:256:CYS:HG	1:A:259:CYS:CB	1.82	0.82
2:C:1:SER:N	2:C:2:PRO:CD	2.42	0.82
1:A:353:TRP:CE2	1:B:176:PRO:HG2	2.15	0.82
1:B:280:CYS:SG	1:B:281:PRO:CD	2.68	0.81
1:B:256:CYS:SG	1:B:259:CYS:HB2	2.21	0.80
1:A:200:TYR:CD1	1:A:201:PRO:HD2	2.17	0.79
1:B:180:PHE:O	1:B:293:PHE:CD2	2.36	0.79
1:A:256:CYS:SG	1:A:261:ARG:N	2.53	0.79
1:A:158:ARG:HB2	1:A:158:ARG:CZ	2.10	0.78
1:B:180:PHE:O	1:B:293:PHE:HD2	1.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HB3	1:A:294:PHE:HE2	1.49	0.77
2:C:10:D8R:O1	4:C:201:IMD:C2	2.32	0.77
1:B:365:ASP:CB	1:B:368:HIS:CD2	2.52	0.76
1:A:256:CYS:SG	1:A:259:CYS:C	2.70	0.74
1:A:256:CYS:SG	1:A:259:CYS:CA	2.76	0.74
1:A:144:VAL:HB	1:A:148:ILE:HD13	1.69	0.74
2:C:5:LEU:HD12	2:C:5:LEU:O	1.86	0.74
1:B:314:LEU:HD13	1:B:339:PRO:HG2	1.70	0.72
1:A:279:ARG:HH21	1:A:284:THR:CB	2.01	0.72
1:A:256:CYS:HG	1:A:259:CYS:HB3	0.90	0.71
1:A:288:LYS:HG2	1:A:289:PRO:O	1.90	0.71
1:A:353:TRP:CD2	1:B:176:PRO:CG	2.74	0.70
1:A:353:TRP:CD2	1:B:176:PRO:HG3	2.28	0.69
1:A:195:LEU:HD11	1:A:199:LEU:HD11	1.73	0.69
1:B:256:CYS:HG	1:B:259:CYS:HB2	1.57	0.69
1:A:354:HIS:NE2	1:B:173:LEU:O	2.25	0.69
1:A:279:ARG:HH21	1:A:284:THR:HB	1.57	0.68
1:B:173:LEU:HD22	1:B:178:ALA:HB3	1.77	0.67
1:B:324:VAL:HB	4:C:202:IMD:C2	2.23	0.67
1:B:179:ILE:HD11	1:B:195:LEU:CD2	2.23	0.67
1:A:292:VAL:CG1	2:C:2:PRO:HG3	2.24	0.67
1:B:173:LEU:CD2	1:B:184:PHE:CZ	2.77	0.66
1:A:125:LEU:HD12	1:A:125:LEU:C	2.20	0.66
2:C:1:SER:H2	2:C:2:PRO:HD3	1.60	0.66
1:A:279:ARG:NH2	1:A:284:THR:HB	2.10	0.66
1:A:324:VAL:HG22	2:C:3:VAL:HG22	1.78	0.66
1:B:258:VAL:CB	1:B:283:CYS:SG	2.85	0.65
1:B:201:PRO:O	1:B:269:ARG:NH2	2.30	0.64
1:A:164:LEU:HD11	1:A:198:GLU:CD	2.22	0.63
1:B:139:ARG:HE	1:B:311:MET:HG2	1.61	0.63
1:B:144:VAL:HG12	1:B:318:LEU:HB2	1.80	0.63
1:B:256:CYS:SG	1:B:260:GLN:N	2.72	0.63
1:A:353:TRP:CE3	1:B:176:PRO:HG3	2.34	0.63
1:B:279:ARG:NH1	1:B:279:ARG:HG3	2.14	0.62
1:B:325:GLU:HG2	1:B:328:ALA:HB3	1.82	0.62
1:B:179:ILE:HD11	1:B:195:LEU:HD23	1.82	0.61
1:A:125:LEU:HD11	1:A:373:LEU:HD13	1.83	0.61
1:A:312:ALA:O	1:A:335:ARG:NH1	2.34	0.60
1:A:347:LEU:HG	1:A:363:LEU:HD21	1.82	0.60
1:A:283:CYS:SG	1:A:285:GLY:N	2.75	0.60
2:C:1:SER:H2	2:C:2:PRO:CD	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:VAL:HG21	1:B:299:PRO:HD3	1.82	0.60
1:A:158:ARG:HD2	1:A:168:LEU:HD12	1.83	0.60
1:A:324:VAL:HG21	2:C:3:VAL:CG2	2.23	0.59
1:A:353:TRP:CD2	1:B:176:PRO:HG2	2.36	0.59
2:C:3:VAL:HG12	2:C:3:VAL:O	2.03	0.58
2:C:5:LEU:HD12	2:C:5:LEU:C	2.28	0.57
1:B:320:THR:HG21	1:B:327:PHE:HE2	1.70	0.57
1:B:325:GLU:HB3	1:B:326:PRO:HA	1.87	0.57
1:B:280:CYS:SG	1:B:281:PRO:N	2.78	0.56
1:B:302:PHE:CZ	1:B:326:PRO:HG2	2.41	0.56
1:B:149:SER:OG	1:B:231:ASP:OD2	2.23	0.56
1:A:158:ARG:CZ	1:A:158:ARG:CB	2.85	0.55
1:B:179:ILE:HD11	1:B:195:LEU:HD22	1.89	0.54
1:A:258:VAL:HB	1:A:283:CYS:SG	2.48	0.54
2:C:1:SER:H3	2:C:2:PRO:CD	2.09	0.54
1:A:173:LEU:HB2	1:B:353:TRP:HE1	1.71	0.54
1:B:320:THR:HG21	1:B:327:PHE:CE2	2.44	0.53
1:A:154:ILE:HG22	1:A:154:ILE:O	2.08	0.53
1:B:208:VAL:HG23	1:B:383:MET:HE2	1.91	0.53
1:A:195:LEU:HD11	1:A:199:LEU:CD1	2.37	0.53
1:B:179:ILE:CD1	1:B:195:LEU:HD22	2.39	0.53
1:B:283:CYS:O	1:B:284:THR:HG22	2.09	0.53
1:B:235:ARG:HG3	1:B:244:LEU:HD13	1.92	0.52
1:A:128:VAL:HG13	1:A:314:LEU:HD11	1.90	0.52
1:B:279:ARG:CG	1:B:279:ARG:HH11	2.23	0.52
1:B:298:LEU:HB2	2:C:12:PRO:HA	1.89	0.52
1:B:174:PRO:HB2	1:B:175:TYR:CD1	2.45	0.51
2:C:9:LYS:HA	4:C:202:IMD:N1	2.26	0.51
1:B:324:VAL:CG1	4:C:202:IMD:N3	2.74	0.51
1:A:158:ARG:HB2	1:A:158:ARG:HH21	1.71	0.50
1:A:208:VAL:HG11	1:A:367:VAL:HG13	1.93	0.50
1:A:231:ASP:OD1	1:A:232:GLY:N	2.45	0.50
1:B:279:ARG:NH1	1:B:279:ARG:CG	2.72	0.50
1:B:231:ASP:OD1	1:B:232:GLY:N	2.45	0.50
1:B:173:LEU:HD21	1:B:184:PHE:CD2	2.46	0.50
1:B:324:VAL:HG12	4:C:202:IMD:N3	2.27	0.49
1:B:138:GLN:N	1:B:313:ASP:OD2	2.45	0.49
1:A:177:GLU:HB3	1:A:294:PHE:CE2	2.40	0.49
1:A:165:TYR:CZ	1:B:353:TRP:HE3	2.31	0.49
1:A:132:ILE:HG23	1:A:221:LEU:HD13	1.95	0.48
2:C:8:PHE:HE2	4:C:201:IMD:C5	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TRP:CZ2	1:B:176:PRO:HG2	2.49	0.47
1:B:324:VAL:HG12	4:C:202:IMD:HN3	1.79	0.47
1:B:200:TYR:CE2	1:B:272:VAL:HG11	2.49	0.47
1:A:214:ARG:NH1	1:A:238:GLY:HA3	2.29	0.46
1:B:294:PHE:HZ	4:C:201:IMD:HN1	1.63	0.46
1:B:347:LEU:HD22	1:B:352:ALA:HB2	1.98	0.46
1:A:383:MET:O	1:A:387:VAL:HG23	2.16	0.46
1:B:173:LEU:HD22	1:B:178:ALA:CB	2.45	0.46
1:A:157:PHE:CD1	1:A:157:PHE:O	2.69	0.46
1:A:279:ARG:NH2	1:A:284:THR:CB	2.72	0.46
1:A:332:GLU:OE2	1:A:350:PRO:HB3	2.15	0.45
1:B:219:LYS:HE3	1:B:379:TRP:CE2	2.52	0.45
1:A:164:LEU:HD11	1:A:198:GLU:OE2	2.16	0.45
1:B:288:LYS:HD2	1:B:293:PHE:CE1	2.52	0.45
1:A:125:LEU:HD23	1:A:362:GLN:OE1	2.17	0.45
1:A:196:ALA:O	1:A:200:TYR:HB2	2.18	0.44
1:A:242:SER:HA	1:A:301:ARG:HH22	1.81	0.44
1:B:257:THR:OG1	1:B:286:VAL:O	2.36	0.44
1:B:293:PHE:HB2	1:B:296:GLU:HG3	1.99	0.44
1:B:379:TRP:O	1:B:383:MET:N	2.50	0.44
1:A:280:CYS:O	1:A:284:THR:HA	2.18	0.44
4:C:201:IMD:C5	4:C:202:IMD:H4	2.48	0.43
1:A:154:ILE:CD1	1:A:231:ASP:HB3	2.48	0.43
1:B:256:CYS:SG	1:B:261:ARG:HB2	2.59	0.43
1:A:259:CYS:SG	1:A:280:CYS:SG	3.17	0.43
1:A:292:VAL:HG21	1:A:299:PRO:HD3	2.01	0.43
1:B:184:PHE:O	1:B:187:HIS:HB3	2.18	0.43
1:B:175:TYR:HB2	1:B:176:PRO:HD2	2.02	0.42
1:B:252:ALA:O	1:B:265:GLY:N	2.50	0.42
2:C:6:LYS:HD2	2:C:6:LYS:N	2.34	0.42
1:B:259:CYS:SG	1:B:283:CYS:HB2	2.60	0.42
1:A:182:LEU:N	1:A:183:PRO:HD2	2.35	0.42
1:A:184:PHE:HE1	1:A:191:PRO:HG2	1.85	0.42
1:A:322:LEU:HD12	1:A:348:VAL:HG23	2.01	0.42
1:B:174:PRO:HB2	1:B:175:TYR:HD1	1.85	0.42
1:A:164:LEU:O	1:A:167:ASN:N	2.53	0.42
1:A:320:THR:HG23	1:A:322:LEU:HG	2.01	0.42
1:B:147:GLY:HA3	1:B:319:GLY:HA3	2.02	0.41
1:B:224:ARG:NH1	1:B:242:SER:O	2.53	0.41
1:B:297:PRO:HA	2:C:11:ILE:O	2.21	0.41
1:A:148:ILE:O	1:A:207:ASN:ND2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HB	1:B:148:ILE:HD13	2.02	0.41
1:A:145:GLY:C	1:A:147:GLY:H	2.29	0.41
1:A:353:TRP:CZ3	1:B:159:SER:HA	2.55	0.41
1:B:377:LEU:HD13	1:B:379:TRP:CZ3	2.56	0.41
1:A:165:TYR:O	1:A:169:GLN:HG3	2.21	0.40
1:B:314:LEU:HA	1:B:338:VAL:HG13	2.03	0.40
1:B:175:TYR:HB2	1:B:176:PRO:CD	2.51	0.40
2:C:2:PRO:O	2:C:2:PRO:HG2	2.22	0.40
1:B:342:LEU:O	1:B:362:GLN:N	2.54	0.40
1:B:298:LEU:CG	2:C:12:PRO:HA	2.52	0.40
2:C:9:LYS:HA	4:C:202:IMD:HN1	1.86	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	271/274 (99%)	266 (98%)	5 (2%)	0	100	100
1	B	272/274 (99%)	268 (98%)	4 (2%)	0	100	100
2	C	10/13 (77%)	8 (80%)	1 (10%)	1 (10%)	0	6
All	All	553/561 (99%)	542 (98%)	10 (2%)	1 (0%)	43	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	2	PRO

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	237/238 (100%)	230 (97%)	7 (3%)	36	57
1	B	238/238 (100%)	230 (97%)	8 (3%)	32	55
2	C	12/12 (100%)	11 (92%)	1 (8%)	10	35
All	All	487/488 (100%)	471 (97%)	16 (3%)	33	55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LEU
1	A	152	SER
1	A	154	ILE
1	A	158	ARG
1	A	164	LEU
1	A	282	VAL
1	A	283	CYS
1	B	152	SER
1	B	177	GLU
1	B	179	ILE
1	B	257	THR
1	B	279	ARG
1	B	280	CYS
1	B	282	VAL
1	B	345	ARG
2	C	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	B	210	HIS
1	B	368	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
2	D8R	C	10	2	12,13,14	1.75	3 (25%)	10,15,17	2.68	2 (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
2	D8R	C	10	2	-	4/13/14/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	10	D8R	C1-NZ	4.57	1.43	1.33
2	C	10	D8R	O-C	2.94	1.31	1.19
2	C	10	D8R	CE-NZ	2.17	1.51	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	10	D8R	CE-NZ-C1	-7.34	109.49	122.59
2	C	10	D8R	C2-C1-NZ	3.06	122.46	116.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	10	D8R	C2-C1-NZ-CE
2	C	10	D8R	O1-C1-C2-O2
2	C	10	D8R	O1-C1-NZ-CE
2	C	10	D8R	NZ-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	10	D8R	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	IMD	C	201	-	5,5,5	0.22	0	5,5,5	0.48	0
4	IMD	C	202	-	5,5,5	0.25	0	5,5,5	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMD	C	201	-	-	-	0/1/1/1
4	IMD	C	202	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

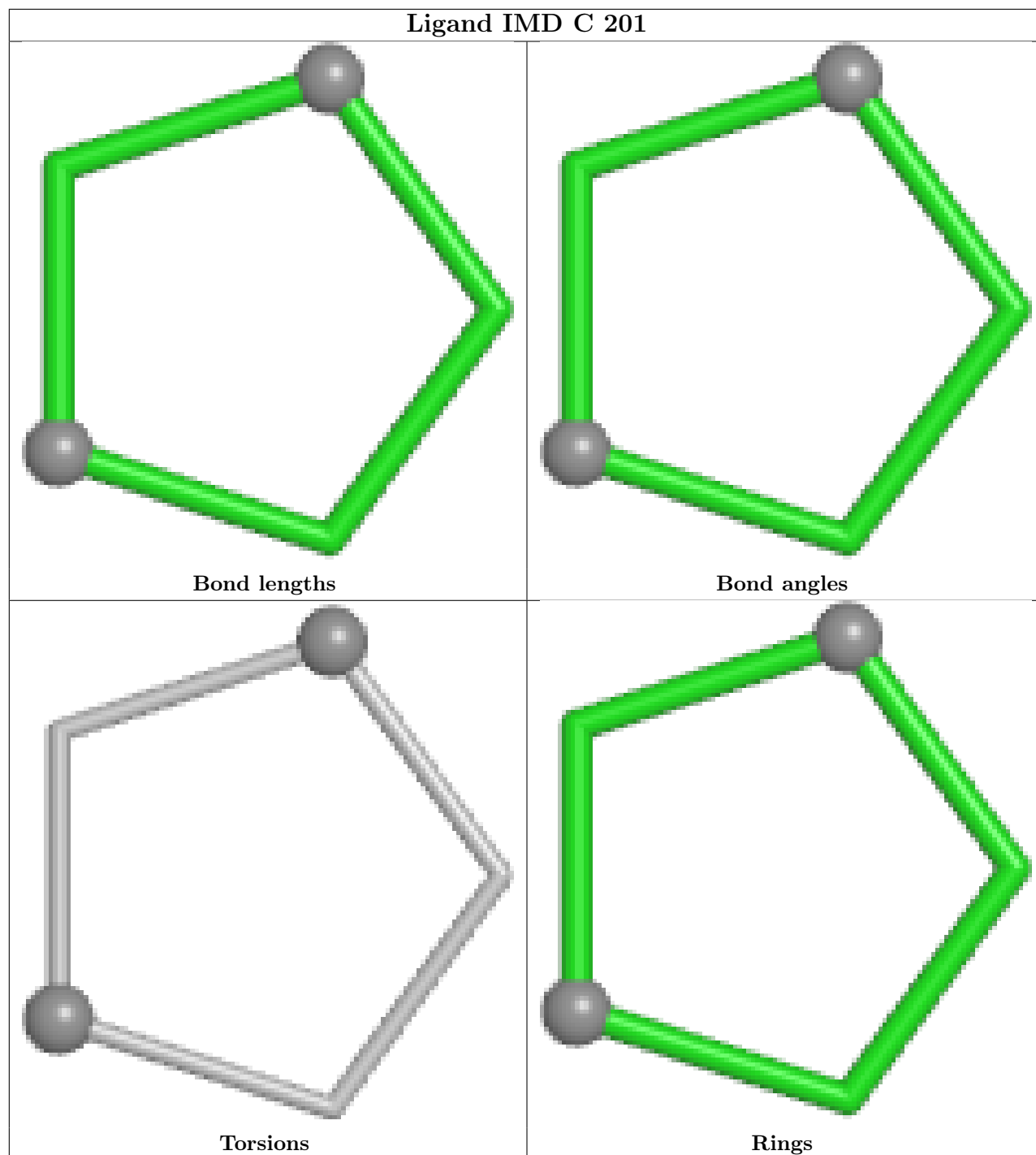
There are no torsion outliers.

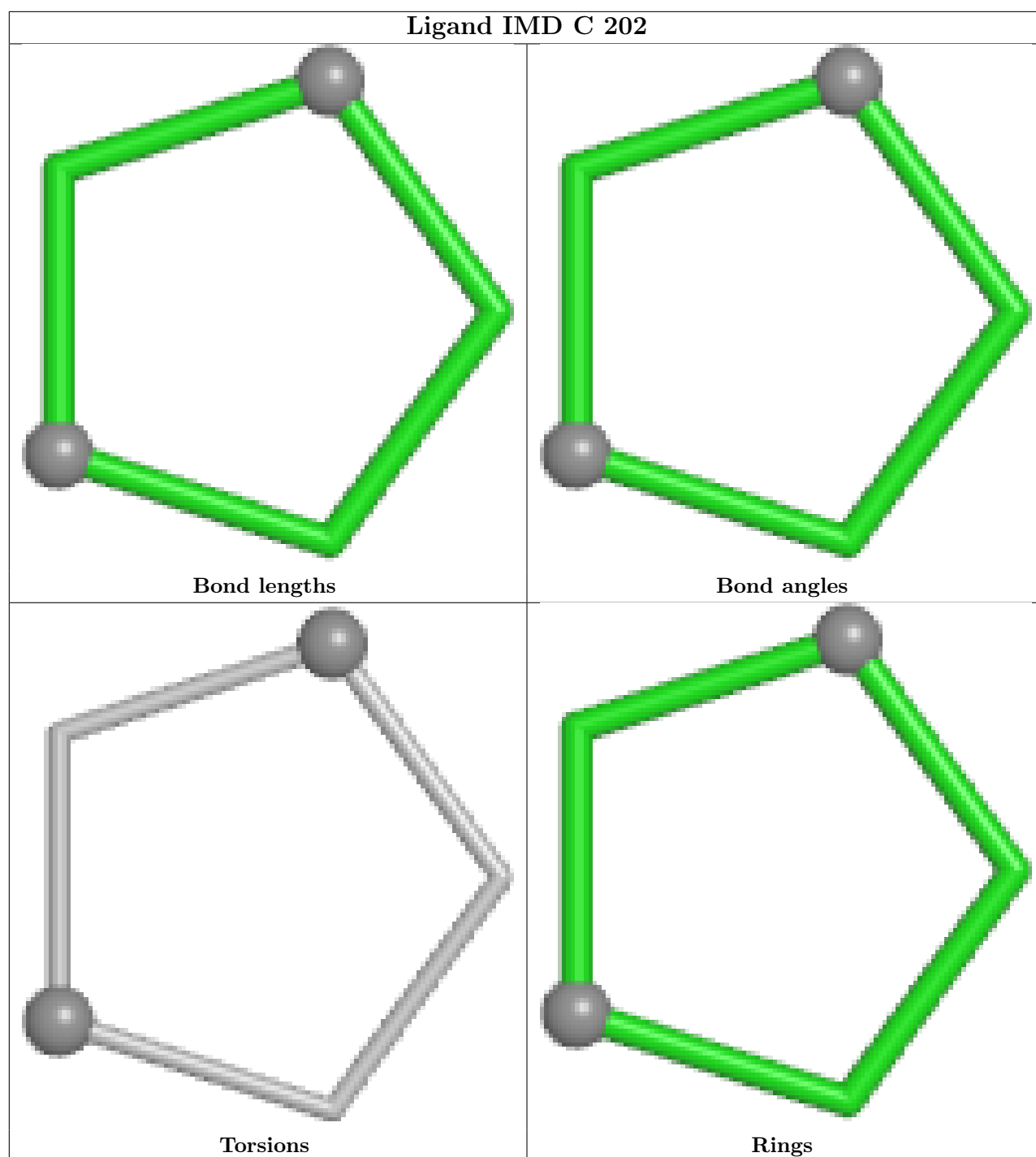
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	IMD	5	0
4	C	202	IMD	7	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 [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	273/274 (99%)	-1.42	0 100 100	31, 52, 80, 94	0
1	B	274/274 (100%)	-1.45	0 100 100	35, 56, 76, 90	0
2	C	12/13 (92%)	-0.86	0 100 100	92, 103, 112, 118	0
All	All	559/561 (99%)	-1.42	0 100 100	31, 54, 82, 118	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	D8R	C	10	14/15	0.99	0.07	76,94,114,118	0

6.3 Carbohydrates [i](#)

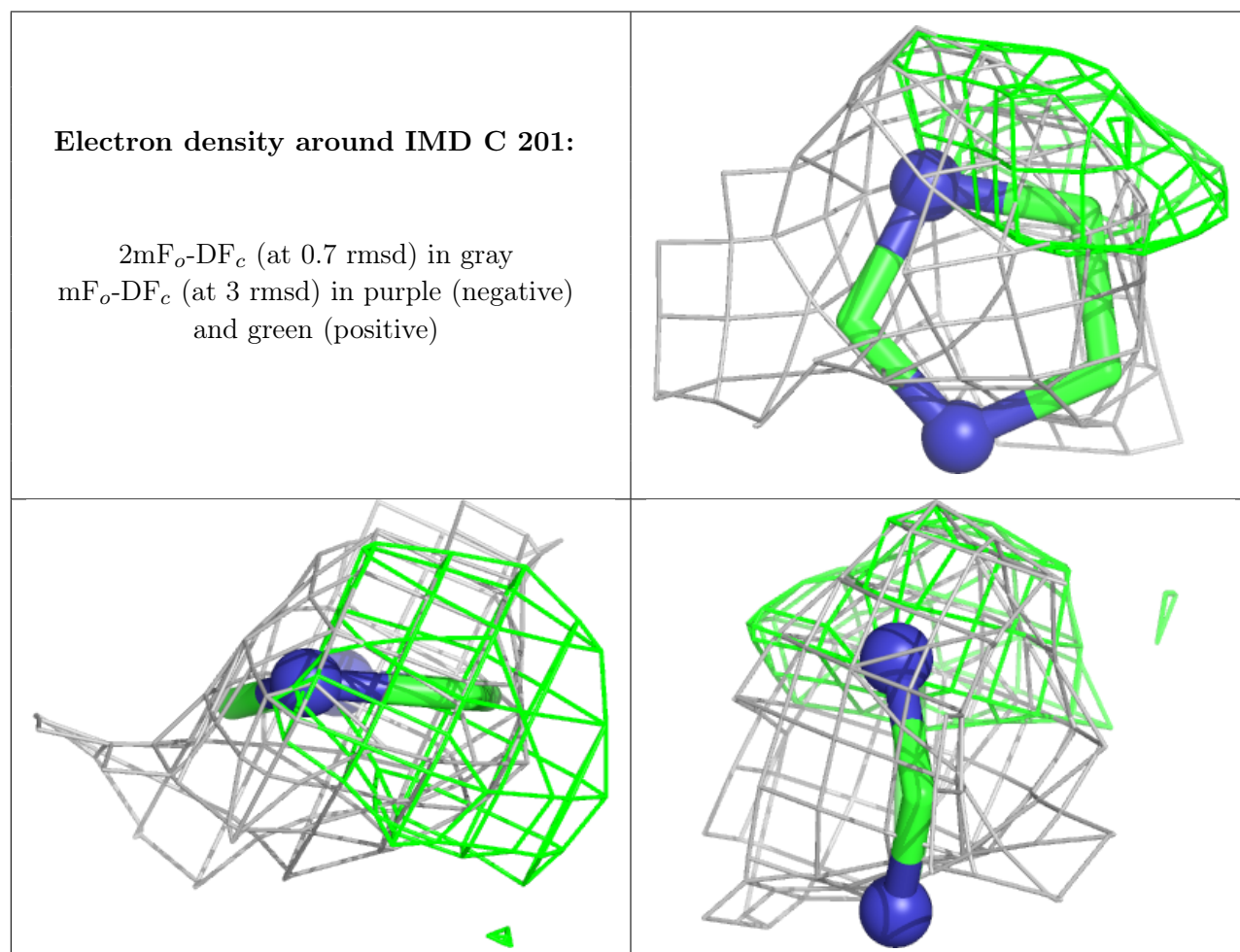
There are no oligosaccharides in this entry.

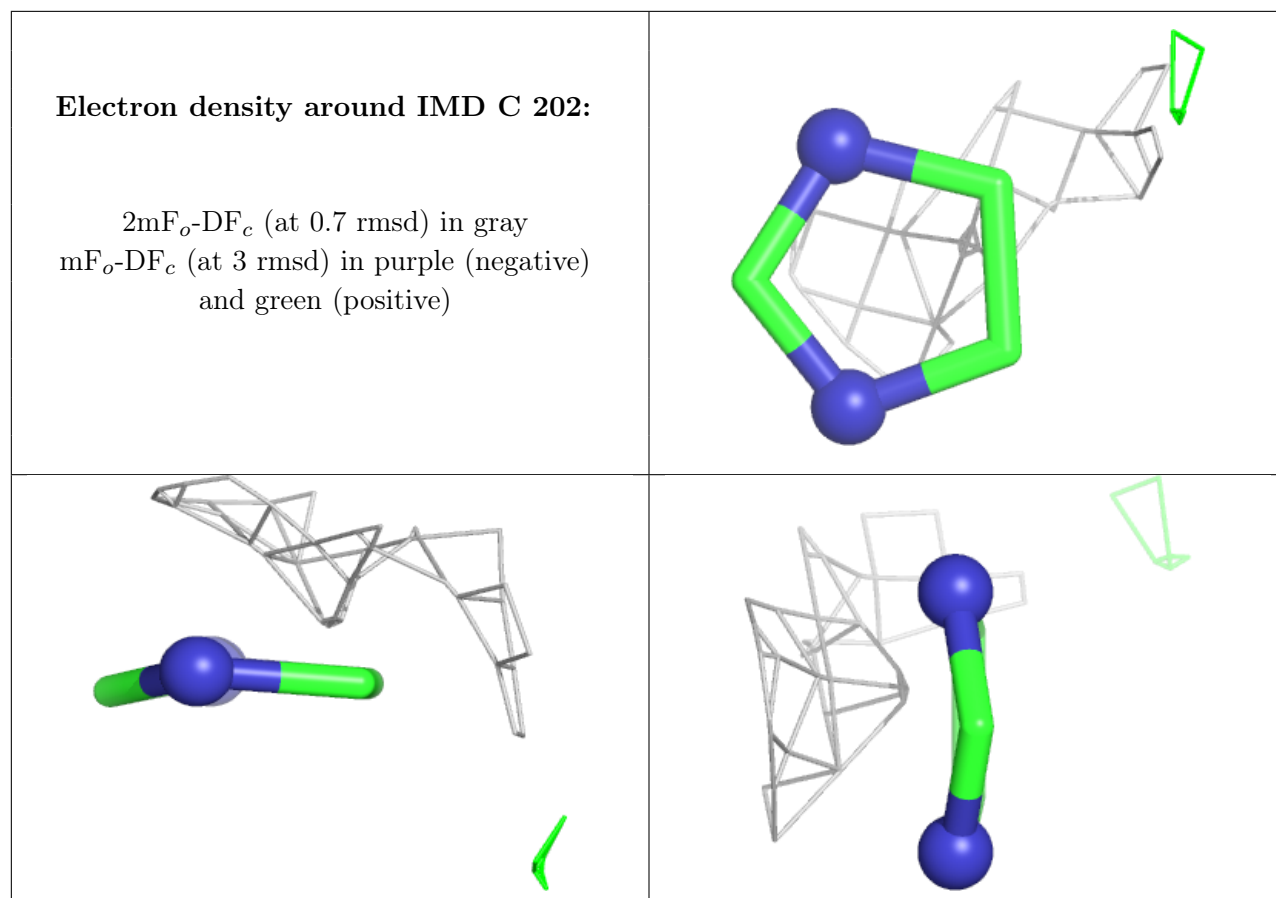
6.4 Ligands [i](#)

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	IMD	C	201	5/5	0.96	0.14	74,82,93,93	0
4	IMD	C	202	5/5	0.98	0.12	87,91,103,104	0
3	ZN	A	401	1/1	1.00	0.02	32,32,32,32	0
3	ZN	B	401	1/1	1.00	0.01	32,32,32,32	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.