



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:29 PM UTC

PDB ID : 9I8O / pdb_00009i8o
Title : Beta-Catenin R4 with Compound 1
Authors : Skowron, A.N.; Klejnot, M.; Pastok, M.W.; Gorecka-Minakowska, K.M.; Wisniewski, J.; Walczak, M.J.
Deposited on : 2025-02-05
Resolution : 2.65 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:

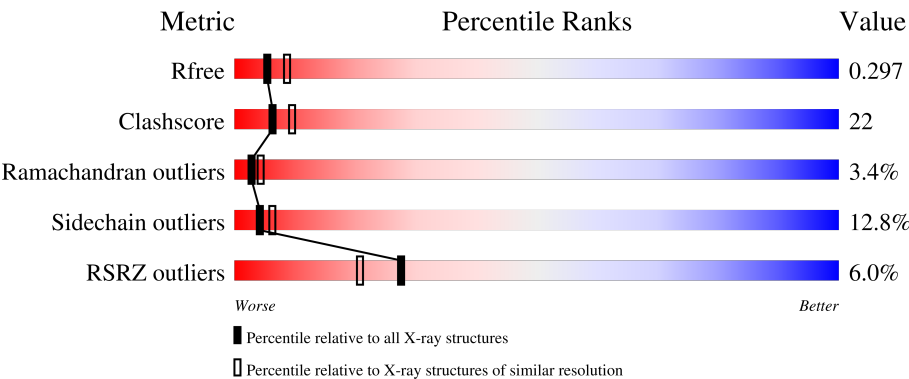
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	169	<div><div>2%</div><div>54%</div><div>34%</div><div>9%</div><div>.</div></div>
1	B	169	<div><div>2%</div><div>59%</div><div>34%</div><div>.</div><div>..</div></div>
1	C	169	<div><div>2%</div><div>44%</div><div>44%</div><div>8%</div><div>..</div></div>
1	D	169	<div><div>16%</div><div>46%</div><div>40%</div><div>8%</div><div>5%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5008 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.

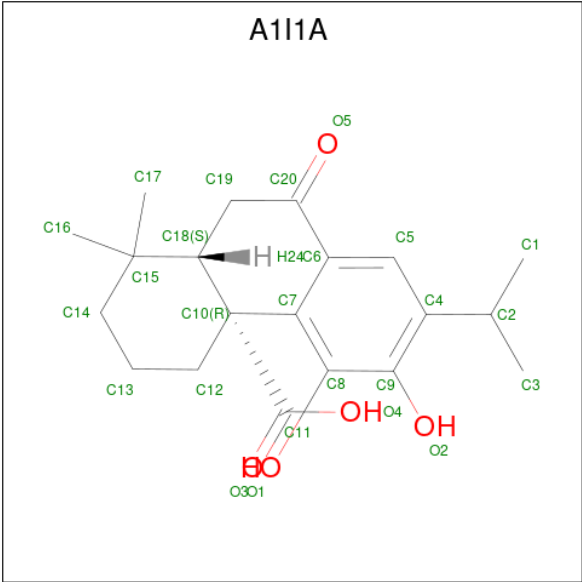
- Molecule 1 is a protein called Catenin beta 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1250	786	225	230	9			
1	B	165	Total	C	N	O	S	0	0	0
			1258	790	227	232	9			
1	C	166	Total	C	N	O	S	0	0	0
			1262	792	228	233	9			
1	D	160	Total	C	N	O	S	0	0	0
			1213	764	220	220	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	SER	-	expression tag	UNP A0A2R8Y815
A	138	TRP	-	expression tag	UNP A0A2R8Y815
A	139	SER	-	expression tag	UNP A0A2R8Y815
A	140	GLY	-	expression tag	UNP A0A2R8Y815
B	137	SER	-	expression tag	UNP A0A2R8Y815
B	138	TRP	-	expression tag	UNP A0A2R8Y815
B	139	SER	-	expression tag	UNP A0A2R8Y815
B	140	GLY	-	expression tag	UNP A0A2R8Y815
C	137	SER	-	expression tag	UNP A0A2R8Y815
C	138	TRP	-	expression tag	UNP A0A2R8Y815
C	139	SER	-	expression tag	UNP A0A2R8Y815
C	140	GLY	-	expression tag	UNP A0A2R8Y815
D	137	SER	-	expression tag	UNP A0A2R8Y815
D	138	TRP	-	expression tag	UNP A0A2R8Y815
D	139	SER	-	expression tag	UNP A0A2R8Y815
D	140	GLY	-	expression tag	UNP A0A2R8Y815

- Molecule 2 is (4 {a} {R}),10 {a} {S})-1,1-dimethyl-5,6-bis(oxidanyl)-9-oxidanylidene-7-propan-2-yl-3,4,10,10 {a}-tetrahydro-2 {H}-phenanthrene-4 {a}-carboxylic acid (CCD ID: A1I1A) (formula: C₂₀H₂₆O₅) (labeled as "Ligand of Interest" by depositor).

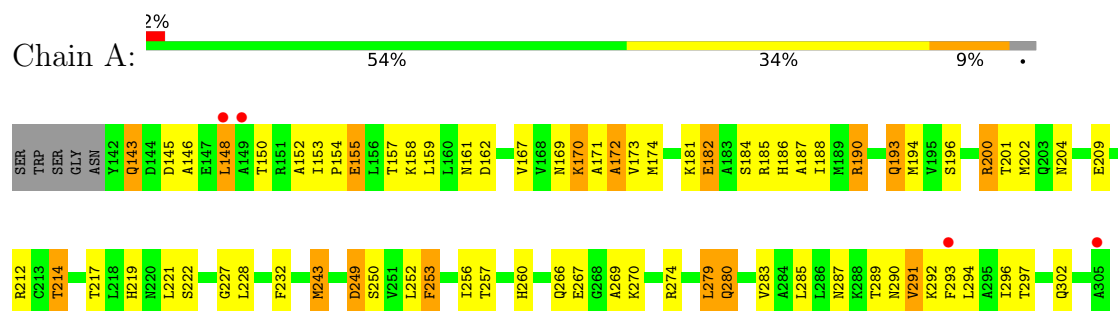


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			25	20	5		

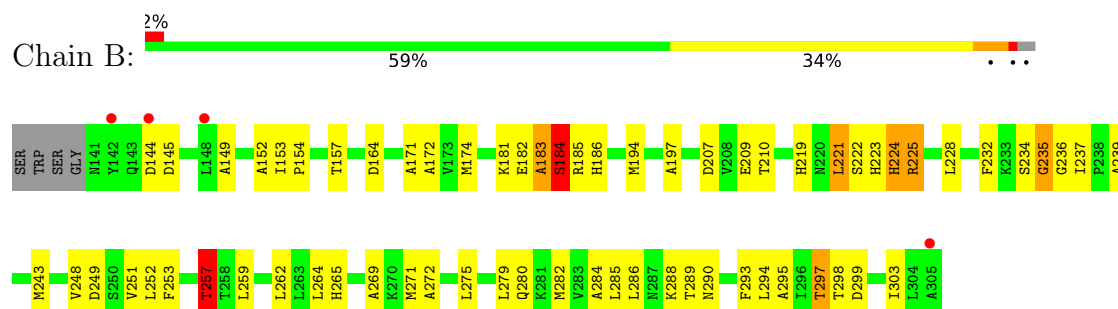
3 Residue-property plots

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.

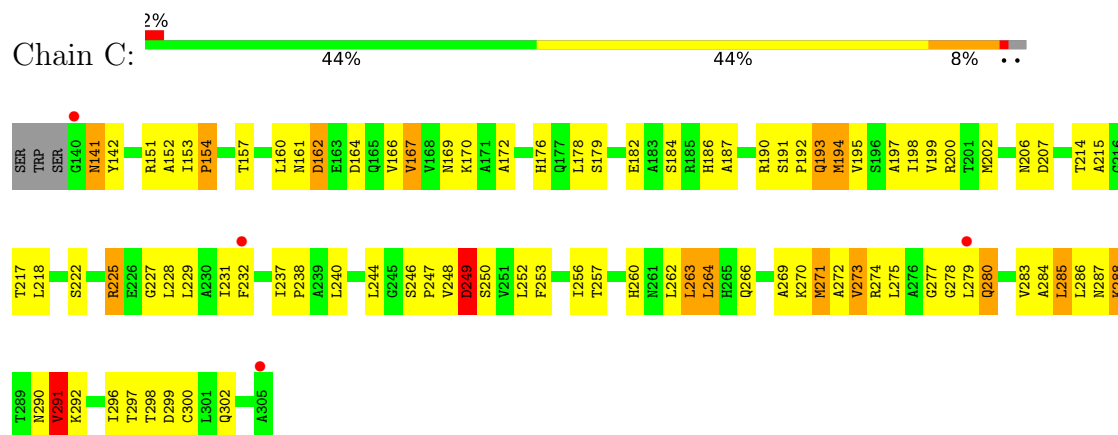
• Molecule 1: Catenin beta 1



• Molecule 1: Catenin beta 1

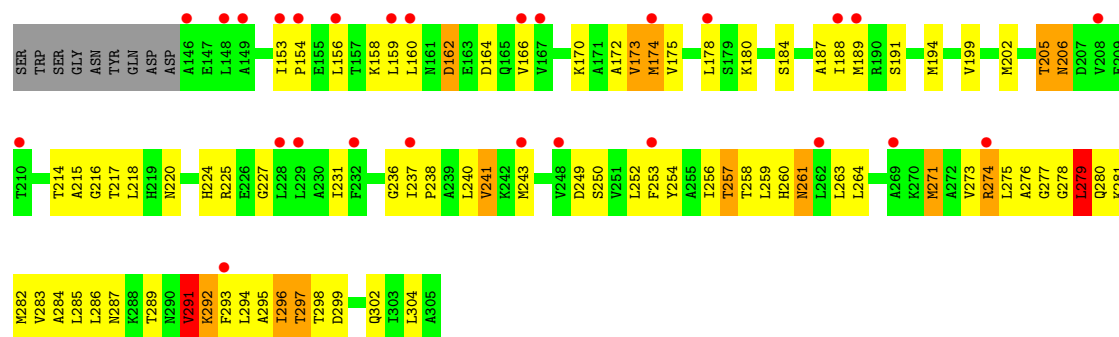


• Molecule 1: Catenin beta 1



• Molecule 1: Catenin beta 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.07Å 98.07Å 232.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.38 – 2.65 90.38 – 2.65	Depositor EDS
% Data completeness (in resolution range)	51.5 (90.38-2.65) 47.9 (90.38-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.212 , 0.305 0.213 , 0.297	Depositor DCC
R_{free} test set	815 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5008	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7189e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1I1A

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	0.54	0/1265	1.15	3/1711 (0.2%)
1	B	0.62	0/1273	1.16	2/1722 (0.1%)
1	C	0.53	0/1277	1.07	0/1727
1	D	0.49	0/1227	1.09	0/1659
All	All	0.55	0/5042	1.12	5/6819 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ARG	CB-CA-C	5.69	118.63	109.07
1	B	257	THR	CA-CB-OG1	-5.53	101.31	109.60
1	A	253	PHE	CA-CB-CG	5.48	119.28	113.80
1	B	144	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	200	ARG	N-CA-C	-5.04	105.67	111.07

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	1250	0	1307	52	0
1	B	1258	0	1313	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1262	0	1316	72	0
1	D	1213	0	1282	63	0
2	C	25	0	0	1	0
All	All	5008	0	5218	227	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 22.

All (227) 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:B:253:PHE:O	1:B:257:THR:HG23	1.67	0.92
1:B:280:GLN:H	1:B:280:GLN:CD	1.86	0.83
1:B:219:HIS:O	1:B:222:SER:OG	1.96	0.83
1:B:293:PHE:O	1:B:297:THR:OG1	2.02	0.78
1:A:212:ARG:HH12	1:B:209:GLU:CD	1.95	0.75
1:B:284:ALA:O	1:B:288:LYS:HG3	1.88	0.74
1:C:286:LEU:HD23	1:D:298:THR:HG22	1.69	0.74
1:D:279:LEU:O	1:D:283:VAL:HG13	1.91	0.70
1:C:194:MET:O	1:C:197:ALA:N	2.26	0.68
1:B:299:ASP:O	1:B:303:ILE:HG13	1.93	0.68
1:D:295:ALA:O	1:D:298:THR:OG1	2.12	0.67
1:B:184:SER:O	1:B:185:ARG:C	2.38	0.67
1:C:161:ASN:O	1:C:162:ASP:C	2.37	0.67
1:C:141:ASN:C	1:C:141:ASN:OD1	2.37	0.66
1:C:202:MET:HE1	1:C:240:LEU:HD23	1.77	0.66
1:D:227:GLY:O	1:D:231:ILE:HG13	1.95	0.66
1:A:157:THR:O	1:A:161:ASN:ND2	2.28	0.65
1:D:299:ASP:O	1:D:302:GLN:HB2	1.98	0.64
1:C:279:LEU:O	1:C:283:VAL:HG23	1.97	0.64
1:A:182:GLU:O	1:A:186:HIS:ND1	2.31	0.63
1:D:282:MET:HA	1:D:285:LEU:HD12	1.79	0.63
1:A:249:ASP:N	1:A:249:ASP:OD1	2.32	0.63
1:C:157:THR:HG23	1:C:194:MET:HA	1.80	0.62
1:C:193:GLN:CD	1:C:193:GLN:H	2.06	0.62
1:A:169:ASN:O	1:A:173:VAL:HG23	2.00	0.62
1:C:271:MET:O	1:C:274:ARG:N	2.32	0.62
1:D:256:ILE:O	1:D:257:THR:C	2.42	0.61
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.82	0.61
1:C:190:ARG:O	1:C:192:PRO:HD3	2.02	0.60
1:D:293:PHE:O	1:D:297:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:O	1:A:253:PHE:C	2.45	0.59
1:D:278:GLY:O	1:D:279:LEU:C	2.45	0.59
1:A:219:HIS:O	1:A:222:SER:OG	2.19	0.59
1:A:184:SER:O	1:A:185:ARG:C	2.45	0.59
1:D:240:LEU:O	1:D:241:VAL:C	2.46	0.59
1:D:253:PHE:HB2	1:D:293:PHE:CZ	2.38	0.58
1:B:145:ASP:O	1:B:149:ALA:N	2.35	0.58
1:A:285:LEU:O	1:A:289:THR:HG23	2.04	0.57
1:C:260:HIS:O	1:C:264:LEU:HB2	2.04	0.57
1:D:253:PHE:O	1:D:257:THR:OG1	2.20	0.57
1:C:290:ASN:O	1:C:291:VAL:C	2.48	0.57
1:B:157:THR:HG23	1:B:194:MET:HA	1.85	0.57
1:D:153:ILE:HB	1:D:154:PRO:HD3	1.87	0.57
1:A:161:ASN:OD1	1:A:200:ARG:NH1	2.38	0.56
1:A:202:MET:HB2	1:A:214:THR:HB	1.86	0.56
1:C:161:ASN:O	1:C:162:ASP:O	2.23	0.56
1:B:295:ALA:O	1:B:298:THR:HB	2.06	0.56
1:C:298:THR:HG23	1:D:286:LEU:HB3	1.88	0.55
1:D:240:LEU:O	1:D:243:MET:N	2.38	0.55
1:D:256:ILE:HD11	1:D:282:MET:HE2	1.88	0.55
1:B:153:ILE:O	1:B:154:PRO:C	2.47	0.55
1:A:201:THR:O	1:A:204:ASN:N	2.35	0.55
1:B:280:GLN:CD	1:B:280:GLN:N	2.61	0.54
1:A:145:ASP:HB3	1:A:148:LEU:HD22	1.90	0.54
1:D:191:SER:O	1:D:194:MET:N	2.36	0.54
1:C:248:VAL:O	1:C:249:ASP:C	2.49	0.54
1:C:232:PHE:HB2	1:C:266:GLN:HE21	1.72	0.53
1:B:280:GLN:H	1:B:280:GLN:NE2	2.06	0.53
1:B:183:ALA:O	1:B:186:HIS:N	2.40	0.53
1:B:183:ALA:O	1:B:184:SER:C	2.51	0.53
1:C:278:GLY:O	1:C:279:LEU:C	2.51	0.53
1:A:291:VAL:O	1:A:292:LYS:C	2.51	0.53
1:D:257:THR:O	1:D:261:ASN:ND2	2.42	0.53
1:A:186:HIS:O	1:A:187:ALA:C	2.52	0.53
1:D:172:ALA:O	1:D:173:VAL:C	2.52	0.53
1:D:217:THR:O	1:D:220:ASN:N	2.42	0.53
1:C:169:ASN:O	1:C:170:LYS:C	2.52	0.52
1:B:234:SER:O	1:B:235:GLY:C	2.51	0.52
1:C:280:GLN:CD	1:C:280:GLN:H	2.16	0.52
1:C:237:ILE:O	1:C:238:PRO:C	2.53	0.52
1:A:266:GLN:HG3	1:A:267:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ASN:O	1:C:292:LYS:N	2.43	0.52
1:D:172:ALA:HA	1:D:175:VAL:HG12	1.91	0.52
1:C:263:LEU:HD21	1:C:273:VAL:HG21	1.92	0.52
1:D:237:ILE:HB	1:D:238:PRO:HD3	1.91	0.52
1:D:156:LEU:O	1:D:159:LEU:N	2.40	0.52
1:D:174:MET:O	1:D:178:LEU:HG	2.10	0.51
1:C:164:ASP:OD2	1:C:166:VAL:HB	2.10	0.51
1:D:296:ILE:HD13	1:D:296:ILE:N	2.25	0.51
1:C:176:HIS:O	1:C:179:SER:OG	2.28	0.51
1:A:171:ALA:O	1:A:172:ALA:C	2.54	0.51
1:A:221:LEU:N	1:A:221:LEU:HD23	2.26	0.50
1:C:271:MET:O	1:C:275:LEU:HG	2.12	0.50
1:A:280:GLN:H	1:A:280:GLN:CD	2.19	0.50
1:C:249:ASP:O	1:C:250:SER:C	2.54	0.50
1:A:293:PHE:O	1:A:294:LEU:C	2.54	0.50
1:B:252:LEU:HD23	1:B:293:PHE:CD2	2.46	0.50
1:C:291:VAL:O	1:C:292:LYS:C	2.55	0.50
1:A:154:PRO:O	1:A:158:LYS:HG3	2.10	0.50
1:A:243:MET:HA	1:A:243:MET:HE2	1.93	0.50
1:A:209:GLU:HB2	1:B:209:GLU:HB2	1.94	0.50
1:B:285:LEU:HD23	1:B:297:THR:CG2	2.42	0.50
1:D:285:LEU:O	1:D:289:THR:HG23	2.12	0.50
1:A:186:HIS:O	1:A:190:ARG:HG3	2.12	0.49
1:D:299:ASP:HA	1:D:302:GLN:HB2	1.93	0.49
1:A:188:ILE:C	1:A:190:ARG:H	2.20	0.49
1:C:206:ASN:OD1	1:C:207:ASP:N	2.44	0.49
1:C:296:ILE:HD12	1:C:296:ILE:H	1.77	0.49
1:D:282:MET:O	1:D:283:VAL:C	2.55	0.49
1:C:225:ARG:NE	1:C:225:ARG:H	2.10	0.49
1:D:189:MET:HE1	1:D:224:HIS:HB2	1.94	0.49
1:C:227:GLY:O	1:C:228:LEU:C	2.56	0.49
1:C:153:ILE:O	1:C:154:PRO:C	2.55	0.49
1:C:198:ILE:CG2	1:C:218:LEU:HD21	2.42	0.49
1:D:202:MET:HB2	1:D:214:THR:HB	1.93	0.49
1:A:279:LEU:O	1:A:283:VAL:HG23	2.13	0.49
1:C:262:LEU:O	1:C:264:LEU:N	2.41	0.48
1:C:273:VAL:O	1:C:275:LEU:N	2.46	0.48
1:D:250:SER:O	1:D:254:TYR:CD2	2.66	0.48
1:A:227:GLY:O	1:A:228:LEU:C	2.56	0.48
1:B:207:ASP:HB3	1:B:210:THR:OG1	2.13	0.48
1:A:169:ASN:O	1:A:172:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LEU:HD23	1:B:297:THR:HG23	1.95	0.48
1:C:202:MET:HE1	1:C:240:LEU:CD2	2.43	0.48
1:B:234:SER:O	1:B:236:GLY:N	2.47	0.48
1:B:239:ALA:O	1:B:243:MET:HG2	2.13	0.48
1:C:296:ILE:HD12	1:C:296:ILE:N	2.29	0.48
1:D:296:ILE:O	1:D:297:THR:C	2.56	0.47
1:C:152:ALA:O	1:C:153:ILE:C	2.56	0.47
1:C:269:ALA:O	1:C:272:ALA:N	2.46	0.47
1:A:270:LYS:O	1:A:274:ARG:HG3	2.14	0.47
1:C:256:ILE:HG23	1:C:257:THR:N	2.29	0.47
1:A:153:ILE:O	1:A:155:GLU:N	2.48	0.47
1:B:153:ILE:HG23	1:B:194:MET:HE2	1.96	0.47
1:D:283:VAL:O	1:D:286:LEU:HG	2.14	0.47
1:B:149:ALA:O	1:B:152:ALA:N	2.48	0.46
1:C:298:THR:HG23	1:D:286:LEU:CB	2.46	0.46
1:D:275:LEU:C	1:D:277:GLY:N	2.72	0.46
1:D:216:GLY:O	1:D:220:ASN:ND2	2.45	0.46
1:C:153:ILE:N	1:C:154:PRO:HD2	2.31	0.46
1:C:298:THR:O	1:C:299:ASP:C	2.59	0.46
1:A:155:GLU:O	1:A:158:LYS:N	2.49	0.46
1:B:232:PHE:CD1	1:B:232:PHE:C	2.93	0.46
1:B:264:LEU:HB3	1:B:265:HIS:CE1	2.50	0.46
1:D:217:THR:O	1:D:218:LEU:C	2.58	0.46
1:C:247:PRO:HG2	2:C:401:A1I1A:C4	2.46	0.46
1:A:184:SER:O	1:A:187:ALA:N	2.49	0.46
1:A:188:ILE:HG23	1:A:194:MET:HG2	1.98	0.46
1:B:232:PHE:C	1:B:232:PHE:HD1	2.24	0.46
1:D:260:HIS:O	1:D:263:LEU:N	2.49	0.45
1:B:279:LEU:O	1:B:280:GLN:C	2.59	0.45
1:C:273:VAL:C	1:C:275:LEU:N	2.74	0.45
1:C:244:LEU:HD22	1:C:285:LEU:HD13	1.98	0.45
1:B:171:ALA:O	1:B:172:ALA:C	2.60	0.45
1:D:202:MET:O	1:D:205:THR:HG22	2.16	0.45
1:D:240:LEU:HB2	1:D:259:LEU:HD21	1.99	0.45
1:D:261:ASN:HA	1:D:264:LEU:HD12	1.98	0.45
1:A:167:VAL:O	1:A:170:LYS:N	2.50	0.45
1:A:152:ALA:O	1:A:153:ILE:C	2.61	0.44
1:A:170:LYS:CE	1:A:174:MET:HE2	2.47	0.44
1:C:178:LEU:O	1:C:184:SER:OG	2.35	0.44
1:A:159:LEU:O	1:A:162:ASP:HB3	2.16	0.44
1:D:299:ASP:C	1:D:302:GLN:HB2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LEU:HD12	1:C:194:MET:HE2	1.99	0.44
1:B:271:MET:HE3	1:B:275:LEU:HG	1.99	0.44
1:D:256:ILE:HD11	1:D:282:MET:CE	2.48	0.44
1:B:294:LEU:O	1:B:295:ALA:C	2.60	0.44
1:C:191:SER:OG	1:C:193:GLN:NE2	2.51	0.44
1:C:194:MET:O	1:C:195:VAL:C	2.61	0.44
1:D:187:ALA:O	1:D:188:ILE:C	2.61	0.44
1:B:224:HIS:O	1:B:225:ARG:C	2.61	0.44
1:D:297:THR:O	1:D:298:THR:C	2.61	0.44
1:A:143:GLN:O	1:A:146:ALA:HB2	2.18	0.43
1:A:159:LEU:O	1:A:162:ASP:CB	2.65	0.43
1:C:302:GLN:OE1	1:D:287:ASN:ND2	2.51	0.43
1:D:254:TYR:O	1:D:258:THR:OG1	2.22	0.43
1:A:267:GLU:C	1:A:269:ALA:H	2.27	0.43
1:A:292:LYS:O	1:A:296:ILE:CD1	2.66	0.43
1:D:215:ALA:O	1:D:216:GLY:C	2.60	0.43
1:D:291:VAL:O	1:D:292:LYS:C	2.61	0.43
1:D:294:LEU:O	1:D:298:THR:HG23	2.18	0.43
1:A:214:THR:O	1:A:217:THR:HB	2.19	0.43
1:C:199:VAL:O	1:C:200:ARG:C	2.61	0.43
1:D:236:GLY:O	1:D:237:ILE:C	2.61	0.43
1:D:162:ASP:OD1	1:D:164:ASP:HB3	2.19	0.43
1:B:194:MET:O	1:B:197:ALA:N	2.51	0.43
1:C:141:ASN:O	1:C:142:TYR:C	2.61	0.43
1:C:169:ASN:O	1:C:172:ALA:N	2.52	0.43
1:D:240:LEU:HA	1:D:243:MET:CG	2.49	0.43
1:C:198:ILE:HG21	1:C:218:LEU:HD21	2.01	0.43
1:D:227:GLY:O	1:D:231:ILE:CG1	2.66	0.43
1:A:257:THR:O	1:A:260:HIS:HB3	2.18	0.42
1:D:158:LYS:C	1:D:160:LEU:H	2.25	0.42
1:D:256:ILE:HG23	1:D:257:THR:N	2.34	0.42
1:B:221:LEU:HD23	1:B:221:LEU:N	2.34	0.42
1:A:200:ARG:O	1:A:204:ASN:ND2	2.52	0.42
1:A:193:GLN:H	1:A:193:GLN:HE21	1.67	0.42
1:A:212:ARG:NH1	1:B:209:GLU:OE1	2.53	0.42
1:C:231:ILE:O	1:C:232:PHE:C	2.62	0.42
1:B:164:ASP:OD1	1:B:164:ASP:C	2.62	0.42
1:D:257:THR:O	1:D:260:HIS:HB3	2.20	0.42
1:C:195:VAL:HA	1:C:198:ILE:HD12	2.02	0.42
1:A:290:ASN:OD1	1:A:291:VAL:N	2.52	0.42
1:B:182:GLU:O	1:B:185:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LEU:HA	1:C:266:GLN:HE22	1.84	0.42
1:D:282:MET:O	1:D:284:ALA:N	2.53	0.42
1:B:209:GLU:O	1:B:210:THR:C	2.61	0.42
1:A:232:PHE:CD1	1:A:232:PHE:C	2.98	0.41
1:B:224:HIS:O	1:B:228:LEU:HD12	2.19	0.41
1:C:277:GLY:O	1:C:280:GLN:NE2	2.53	0.41
1:C:207:ASP:OD1	1:C:207:ASP:C	2.63	0.41
1:C:273:VAL:O	1:C:274:ARG:C	2.62	0.41
1:C:253:PHE:CD1	1:C:253:PHE:C	2.97	0.41
1:C:284:ALA:O	1:C:287:ASN:N	2.52	0.41
1:D:205:THR:OG1	1:D:206:ASN:N	2.54	0.41
1:D:271:MET:O	1:D:275:LEU:HG	2.19	0.41
1:C:273:VAL:C	1:C:275:LEU:H	2.27	0.41
1:D:166:VAL:O	1:D:170:LYS:HG2	2.20	0.41
1:A:171:ALA:O	1:A:174:MET:N	2.54	0.41
1:A:296:ILE:N	1:A:296:ILE:HD12	2.35	0.41
1:C:141:ASN:OD1	1:C:142:TYR:N	2.53	0.41
1:C:194:MET:CG	1:C:195:VAL:N	2.84	0.41
1:D:273:VAL:O	1:D:274:ARG:C	2.64	0.41
1:A:196:SER:O	1:A:200:ARG:HB2	2.20	0.41
1:B:223:HIS:C	1:B:224:HIS:CD2	2.99	0.41
1:C:186:HIS:O	1:C:187:ALA:C	2.62	0.41
1:C:246:SER:HA	1:C:247:PRO:HD3	1.94	0.41
1:B:251:VAL:O	1:B:252:LEU:C	2.64	0.40
1:B:280:GLN:N	1:B:280:GLN:NE2	2.69	0.40
1:C:237:ILE:N	1:C:238:PRO:HD2	2.37	0.40
1:D:237:ILE:CB	1:D:238:PRO:HD3	2.51	0.40
1:B:259:LEU:HA	1:B:262:LEU:HD12	2.04	0.40
1:B:269:ALA:O	1:B:272:ALA:HB3	2.21	0.40
1:C:162:ASP:HB3	1:C:167:VAL:HG11	2.02	0.40
1:B:271:MET:O	1:B:272:ALA:C	2.64	0.40
1:C:160:LEU:HD23	1:C:160:LEU:HA	1.94	0.40
1:C:214:THR:OG1	1:C:215:ALA:N	2.55	0.40

There are no symmetry-related clashes.

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	162/169 (96%)	126 (78%)	35 (22%)	1 (1%)	21	34
1	B	163/169 (96%)	140 (86%)	19 (12%)	4 (2%)	4	7
1	C	164/169 (97%)	129 (79%)	27 (16%)	8 (5%)	1	2
1	D	158/169 (94%)	114 (72%)	35 (22%)	9 (6%)	1	1
All	All	647/676 (96%)	509 (79%)	116 (18%)	22 (3%)	3	4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	SER
1	C	291	VAL
1	D	304	LEU
1	B	183	ALA
1	B	235	GLY
1	D	279	LEU
1	C	162	ASP
1	C	249	ASP
1	D	173	VAL
1	D	199	VAL
1	D	249	ASP
1	A	172	ALA
1	C	263	LEU
1	C	264	LEU
1	C	288	LYS
1	D	162	ASP
1	D	241	VAL
1	D	276	ALA
1	D	291	VAL
1	B	225	ARG
1	C	273	VAL
1	C	154	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	137/141 (97%)	118 (86%)	19 (14%)	3	5
1	B	138/141 (98%)	124 (90%)	14 (10%)	7	11
1	C	138/141 (98%)	119 (86%)	19 (14%)	3	5
1	D	133/141 (94%)	115 (86%)	18 (14%)	4	5
All	All	546/564 (97%)	476 (87%)	70 (13%)	4	6

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	148	LEU
1	A	150	THR
1	A	155	GLU
1	A	170	LYS
1	A	181	LYS
1	A	182	GLU
1	A	193	GLN
1	A	214	THR
1	A	243	MET
1	A	249	ASP
1	A	250	SER
1	A	256	ILE
1	A	279	LEU
1	A	280	GLN
1	A	287	ASN
1	A	291	VAL
1	A	297	THR
1	A	302	GLN
1	B	174	MET
1	B	181	LYS
1	B	184	SER
1	B	221	LEU
1	B	224	HIS

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Mol	Chain	Res	Type
1	B	237	ILE
1	B	248	VAL
1	B	249	ASP
1	B	257	THR
1	B	282	MET
1	B	286	LEU
1	B	289	THR
1	B	290	ASN
1	B	297	THR
1	C	141	ASN
1	C	151	ARG
1	C	167	VAL
1	C	182	GLU
1	C	193	GLN
1	C	194	MET
1	C	217	THR
1	C	222	SER
1	C	225	ARG
1	C	249	ASP
1	C	252	LEU
1	C	270	LYS
1	C	271	MET
1	C	280	GLN
1	C	285	LEU
1	C	288	LYS
1	C	291	VAL
1	C	297	THR
1	C	300	CYS
1	D	174	MET
1	D	180	LYS
1	D	184	SER
1	D	205	THR
1	D	206	ASN
1	D	225	ARG
1	D	252	LEU
1	D	257	THR
1	D	261	ASN
1	D	271	MET
1	D	274	ARG
1	D	279	LEU
1	D	280	GLN
1	D	281	LYS

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Mol	Chain	Res	Type
1	D	291	VAL
1	D	292	LYS
1	D	296	ILE
1	D	297	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	204	ASN
1	A	219	HIS
1	A	223	HIS
1	A	265	HIS
1	B	141	ASN
1	B	287	ASN
1	C	176	HIS
1	C	204	ASN
1	C	219	HIS
1	C	220	ASN
1	C	265	HIS
1	C	290	ASN
1	D	161	ASN
1	D	219	HIS
1	D	260	HIS
1	D	261	ASN
1	D	265	HIS

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

1 ligand 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	A1I1A	C	401	-	27,27,27	0.75	1 (3%)	36,44,44	0.93	1 (2%)

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	A1I1A	C	401	-	-	0/10/44/44	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	A1I1A	O4-C11	-2.86	1.20	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	A1I1A	O4-C11-C10	2.60	119.60	113.94

There are no chirality outliers.

There are no torsion outliers.

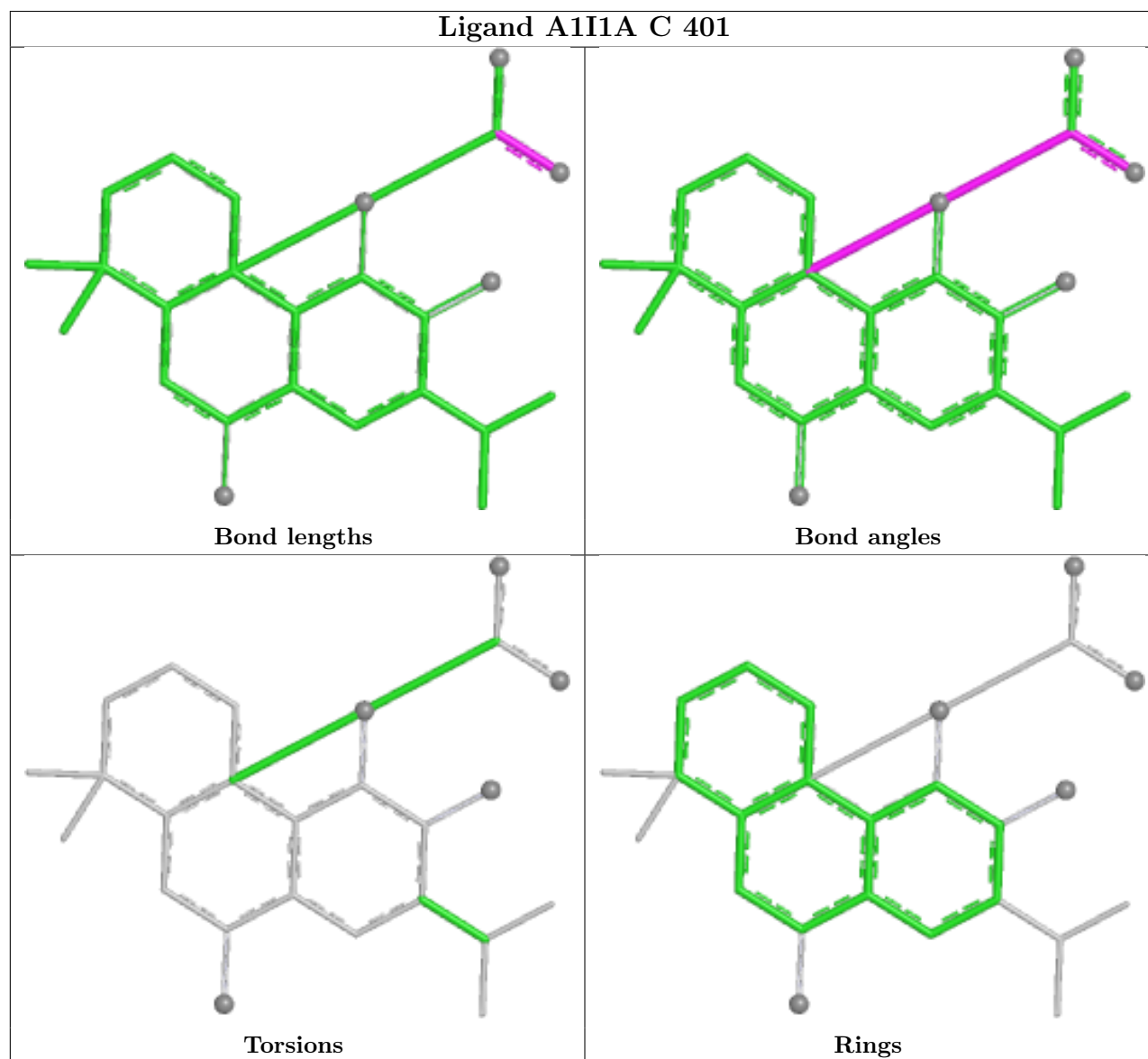
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	A1I1A	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 ⓘ

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	164/169 (97%)	0.14	4 (2%) 59 53	37, 66, 129, 162	0
1	B	165/169 (97%)	-0.04	4 (2%) 59 53	31, 53, 112, 188	0
1	C	166/169 (98%)	0.08	4 (2%) 59 53	44, 72, 102, 116	0
1	D	160/169 (94%)	0.98	27 (16%) 4 3	53, 121, 173, 200	0
All	All	655/676 (96%)	0.29	39 (5%) 27 21	31, 72, 155, 200	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	ILE	4.2
1	B	142	TYR	4.1
1	D	293	PHE	4.0
1	C	232	PHE	3.5
1	B	148	LEU	3.5
1	D	154	PRO	3.3
1	A	293	PHE	3.2
1	D	153	ILE	3.1
1	A	148	LEU	3.1
1	D	148	LEU	3.1
1	D	160	LEU	3.0
1	D	156	LEU	2.8
1	D	188	ILE	2.8
1	C	279	LEU	2.7
1	D	178	LEU	2.7
1	D	243	MET	2.7
1	D	174	MET	2.7
1	D	146	ALA	2.6
1	A	149	ALA	2.6
1	D	228	LEU	2.5
1	A	305	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	166	VAL	2.5
1	D	262	LEU	2.4
1	B	144	ASP	2.4
1	D	269	ALA	2.4
1	C	140	GLY	2.4
1	D	159	LEU	2.3
1	D	149	ALA	2.3
1	B	305	ALA	2.3
1	D	167	VAL	2.3
1	D	253	PHE	2.3
1	D	210	THR	2.2
1	D	208	VAL	2.2
1	D	189	MET	2.2
1	D	274	ARG	2.1
1	D	229	LEU	2.1
1	D	232	PHE	2.1
1	D	248	VAL	2.0
1	C	305	ALA	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](#)

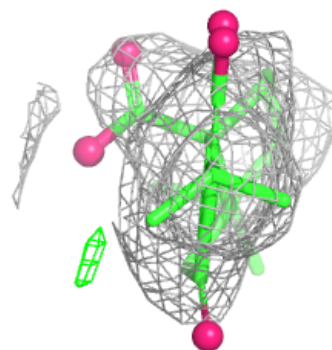
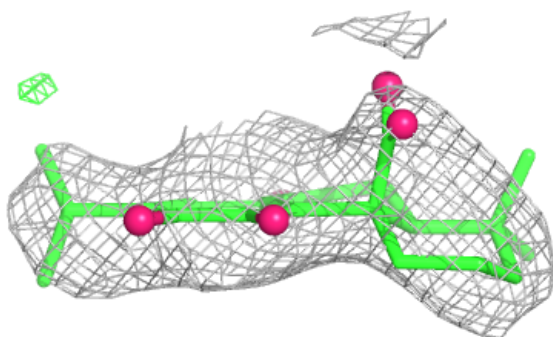
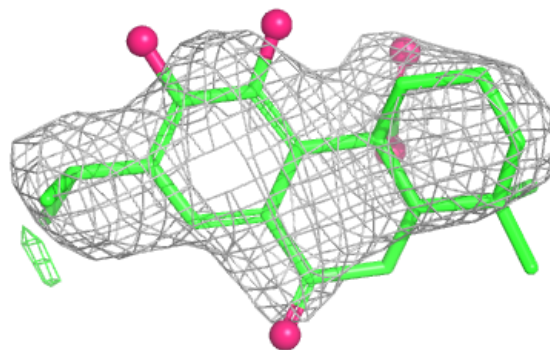
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1I1A	C	401	25/25	0.89	0.18	80,131,151,161	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 A1I1A C 401:

$2mF_o - DF_c$ (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.