



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:43 AM UTC

PDB ID : 1XMY / pdb_00001xmy
Title : Catalytic Domain Of Human Phosphodiesterase 4B In Complex With (R)-Rolipram
Authors : Card, G.L.; England, B.P.; Suzuki, Y.; Fong, D.; Powell, B.; Lee, B.; Luu, C.; Tabrizizad, M.; Gillette, S.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn, M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.
Deposited on : 2004-10-04
Resolution : 2.40 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](#) ①) 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

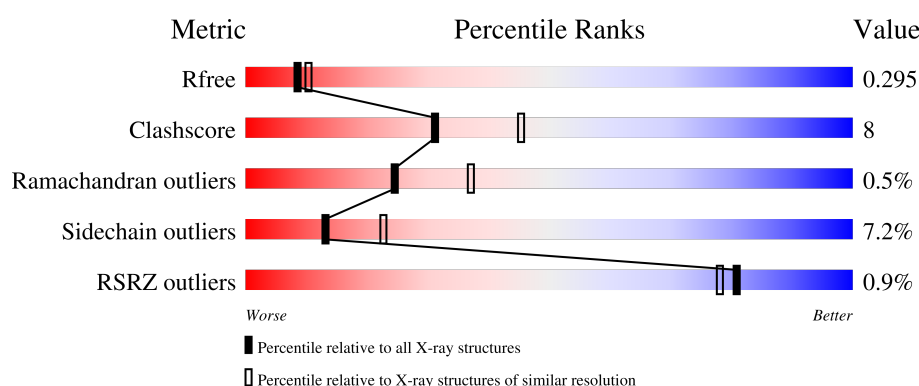
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	398	
2	B	398	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5331 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2613	1651	441	502	19	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	initiating methionine	UNP Q07343
A	132	GLY	-	cloning artifact	UNP Q07343
A	133	SER	-	cloning artifact	UNP Q07343
A	134	SER	-	cloning artifact	UNP Q07343
A	135	HIS	-	expression tag	UNP Q07343
A	136	HIS	-	expression tag	UNP Q07343
A	137	HIS	-	expression tag	UNP Q07343
A	138	HIS	-	expression tag	UNP Q07343
A	139	HIS	-	expression tag	UNP Q07343
A	140	HIS	-	expression tag	UNP Q07343
A	141	SER	-	cloning artifact	UNP Q07343
A	142	SER	-	cloning artifact	UNP Q07343
A	143	GLY	-	cloning artifact	UNP Q07343
A	144	LEU	-	cloning artifact	UNP Q07343
A	145	VAL	-	cloning artifact	UNP Q07343
A	146	PRO	-	cloning artifact	UNP Q07343
A	147	ARG	-	cloning artifact	UNP Q07343
A	148	GLY	-	cloning artifact	UNP Q07343
A	149	SER	-	cloning artifact	UNP Q07343
A	150	HIS	-	cloning artifact	UNP Q07343
A	151	MET	-	cloning artifact	UNP Q07343
A	194	CME	CYS	modified residue	UNP Q07343
A	320	CME	CYS	modified residue	UNP Q07343

- Molecule 2 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	323	Total	C	N	O	S	0	0	0
			2613	1651	441	502	19			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	131	MET	-	initiating methionine	UNP Q07343
B	132	GLY	-	cloning artifact	UNP Q07343
B	133	SER	-	cloning artifact	UNP Q07343
B	134	SER	-	cloning artifact	UNP Q07343
B	135	HIS	-	expression tag	UNP Q07343
B	136	HIS	-	expression tag	UNP Q07343
B	137	HIS	-	expression tag	UNP Q07343
B	138	HIS	-	expression tag	UNP Q07343
B	139	HIS	-	expression tag	UNP Q07343
B	140	HIS	-	expression tag	UNP Q07343
B	141	SER	-	cloning artifact	UNP Q07343
B	142	SER	-	cloning artifact	UNP Q07343
B	143	GLY	-	cloning artifact	UNP Q07343
B	144	LEU	-	cloning artifact	UNP Q07343
B	145	VAL	-	cloning artifact	UNP Q07343
B	146	PRO	-	cloning artifact	UNP Q07343
B	147	ARG	-	cloning artifact	UNP Q07343
B	148	GLY	-	cloning artifact	UNP Q07343
B	149	SER	-	cloning artifact	UNP Q07343
B	150	HIS	-	cloning artifact	UNP Q07343
B	151	MET	-	cloning artifact	UNP Q07343
B	194	CME	CYS	modified residue	UNP Q07343
B	432	CME	CYS	modified residue	UNP Q07343

- 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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

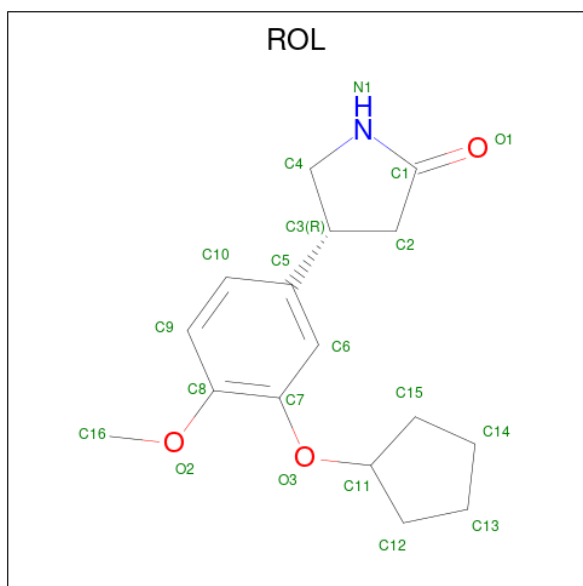
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

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

- Molecule 5 is ROLIPRAM (CCD ID: ROL) (formula: $C_{16}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	16	1	3		
5	B	1	Total	C	N	O	0	0
			20	16	1	3		

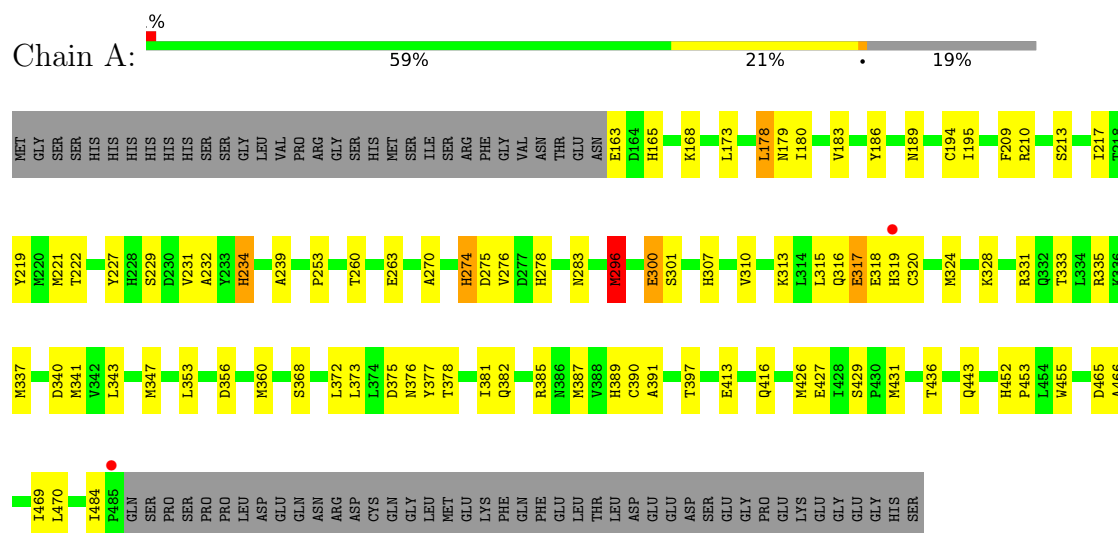
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	33	Total	O	0	0
			33	33		

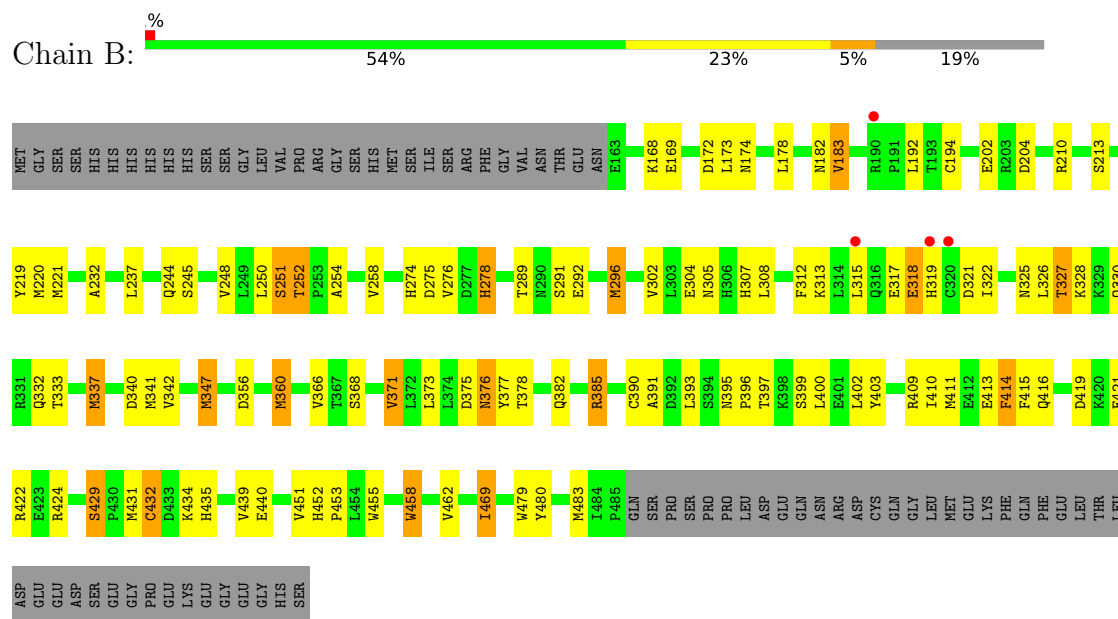
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



- Molecule 2: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.67Å 94.63Å 106.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.40 70.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (70.71-2.40) 99.1 (70.71-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.243 , 0.298 0.243 , 0.295	Depositor DCC
R_{free} test set	1792 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5331	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 54.00 % 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 3.8896e-05. 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CME, ROL, MG

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	1.38	12/2654 (0.5%)	1.34	10/3597 (0.3%)
2	B	1.47	22/2654 (0.8%)	1.38	15/3597 (0.4%)
All	All	1.43	34/5308 (0.6%)	1.36	25/7194 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	MET	SD-CE	8.29	2.00	1.79
1	A	324	MET	SD-CE	8.04	1.99	1.79
1	A	276	VAL	CA-CB	7.56	1.62	1.54
2	B	250	LEU	C-O	-6.87	1.15	1.24
1	A	426	MET	SD-CE	6.66	1.96	1.79
1	A	221	MET	SD-CE	6.59	1.96	1.79
2	B	483	MET	SD-CE	6.48	1.95	1.79
1	A	387	MET	SD-CE	-6.41	1.63	1.79
2	B	296	MET	SD-CE	6.32	1.95	1.79
2	B	469	ILE	CA-CB	-6.21	1.46	1.54
2	B	337	MET	SD-CE	-6.13	1.64	1.79
1	A	391	ALA	CA-CB	6.10	1.62	1.53
1	A	466	ALA	CA-CB	-6.08	1.44	1.53
2	B	245	SER	C-O	-5.87	1.17	1.24
2	B	252	THR	CA-CB	5.87	1.61	1.53
1	A	229	SER	CA-C	5.76	1.60	1.52
1	A	234	HIS	CA-C	5.75	1.60	1.53
2	B	292	GLU	CA-C	-5.73	1.45	1.52
2	B	220	MET	C-O	-5.57	1.17	1.24
2	B	183	VAL	CA-CB	5.46	1.62	1.54
2	B	431	MET	SD-CE	5.32	1.92	1.79
1	A	431	MET	SD-CE	5.31	1.92	1.79
2	B	391	ALA	C-O	-5.31	1.17	1.24
2	B	192	LEU	C-O	-5.31	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	347	MET	CG-SD	5.31	1.94	1.80
2	B	304	GLU	CA-C	-5.27	1.45	1.52
1	A	360	MET	SD-CE	5.25	1.92	1.79
2	B	414	PHE	CA-C	5.15	1.59	1.52
2	B	393	LEU	CA-C	5.12	1.59	1.52
2	B	385	ARG	C-O	-5.12	1.18	1.24
1	A	296	MET	CA-C	5.08	1.59	1.52
2	B	278	HIS	C-O	-5.05	1.17	1.24
2	B	402	LEU	CA-C	5.04	1.59	1.52
2	B	289	THR	CA-CB	5.03	1.62	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	ILE	CB-CA-C	-9.91	101.72	110.94
2	B	312	PHE	N-CA-C	-6.35	105.36	113.23
1	A	283	ASN	N-CA-C	-6.25	104.38	111.07
1	A	232	ALA	N-CA-C	5.72	117.98	111.11
1	A	378	THR	N-CA-C	5.55	118.05	111.33
2	B	424	ARG	N-CA-C	5.55	119.68	113.02
2	B	276	VAL	N-CA-C	5.55	117.44	109.51
2	B	305	ASN	N-CA-C	-5.53	105.25	111.28
1	A	347	MET	N-CA-C	5.50	119.09	112.38
2	B	435	HIS	N-CA-C	5.49	118.19	111.82
2	B	302	VAL	CA-C-O	-5.39	115.67	121.27
1	A	310	VAL	CB-CA-C	-5.32	105.16	111.81
2	B	451	VAL	N-CA-C	5.32	116.09	110.72
2	B	251	SER	N-CA-C	5.31	119.61	113.18
1	A	341	MET	N-CA-C	5.26	117.09	111.36
2	B	252	THR	N-CA-CB	5.24	117.44	109.75
2	B	376	ASN	N-CA-C	5.22	114.49	108.49
2	B	421	GLU	N-CA-C	-5.16	105.74	111.36
1	A	274	HIS	N-CA-C	5.14	119.18	113.01
2	B	220	MET	CG-SD-CE	-5.10	89.68	100.90
2	B	232	ALA	N-CA-C	5.10	116.84	111.28
1	A	416	GLN	N-CA-C	-5.07	105.93	111.82
1	A	222	THR	OG1-CB-CG2	-5.06	99.18	109.30
2	B	458	TRP	N-CA-C	-5.03	105.99	111.82
2	B	376	ASN	N-CA-CB	5.02	114.63	109.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2613	0	2541	38	0
2	B	2613	0	2541	51	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	21	0	0
5	B	20	0	21	1	0
6	A	28	0	0	0	0
6	B	33	0	0	2	0
All	All	5331	0	5124	85	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 8.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:THR:HB	2:B:469:ILE:HG23	1.54	0.88
2:B:356:ASP:HB3	2:B:382:GLN:NE2	2.04	0.72
2:B:333:THR:HG22	2:B:337:MET:HE2	1.72	0.69
2:B:340:ASP:OD1	2:B:385:ARG:HD3	1.92	0.69
1:A:234:HIS:ND1	1:A:413:GLU:OE2	2.26	0.69
5:B:102:ROL:H101	6:B:12:HOH:O	1.93	0.68
2:B:414:PHE:O	2:B:432:CME:HB2	1.93	0.68
1:A:270:ALA:O	1:A:274:HIS:HB3	1.95	0.67
2:B:219:TYR:CE1	2:B:315:LEU:HD23	2.30	0.67
2:B:356:ASP:HB3	2:B:382:GLN:HE22	1.61	0.65
2:B:327:THR:HG23	2:B:330:GLN:H	1.61	0.63
1:A:296:MET:SD	2:B:296:MET:SD	2.97	0.63
2:B:419:ASP:HA	2:B:422:ARG:NH1	2.14	0.63
1:A:397:THR:HB	1:A:469:ILE:HG23	1.79	0.63
1:A:317:GLU:OE2	1:A:319:HIS:HB2	2.00	0.62
1:A:356:ASP:HB3	1:A:382:GLN:NE2	2.15	0.62
2:B:337:MET:O	2:B:341:MET:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:HIS:HB3	1:A:186:TYR:CE2	2.40	0.56
1:A:213:SER:O	1:A:217:ILE:HG12	2.06	0.55
1:A:234:HIS:HD1	1:A:413:GLU:CD	2.15	0.54
1:A:313:LYS:O	1:A:316:GLN:HG2	2.07	0.54
2:B:274:HIS:O	2:B:307:HIS:CD2	2.61	0.54
2:B:415:PHE:CG	2:B:434:LYS:HB3	2.43	0.53
1:A:179:ASN:C	1:A:179:ASN:OD1	2.51	0.53
2:B:376:ASN:CG	2:B:377:TYR:H	2.18	0.52
1:A:340:ASP:OD1	1:A:385:ARG:HD3	2.10	0.52
2:B:419:ASP:CG	2:B:434:LYS:HZ3	2.18	0.51
2:B:400:LEU:HD11	2:B:479:TRP:CE3	2.45	0.51
1:A:253:PRO:HD2	1:A:465:ASP:CG	2.36	0.50
1:A:381:ILE:O	1:A:385:ARG:HG3	2.12	0.50
1:A:296:MET:CE	2:B:313:LYS:NZ	2.74	0.50
1:A:353:LEU:HD23	1:A:389:HIS:CD2	2.46	0.50
2:B:248:VAL:O	2:B:251:SER:HB2	2.12	0.50
1:A:260:THR:OG1	1:A:263:GLU:HG3	2.12	0.50
1:A:452:HIS:HB3	1:A:453:PRO:HD3	1.93	0.49
2:B:410:ILE:HD11	2:B:414:PHE:CE1	2.48	0.49
2:B:322:ILE:O	6:B:8:HOH:O	2.20	0.49
2:B:419:ASP:OD2	2:B:434:LYS:NZ	2.46	0.49
2:B:411:MET:HG3	2:B:439:VAL:HG22	1.95	0.49
2:B:210:ARG:HB2	2:B:325:ASN:HD22	1.78	0.49
2:B:395:ASN:N	2:B:396:PRO:CD	2.76	0.49
1:A:275:ASP:O	1:A:278:HIS:HB2	2.13	0.48
2:B:172:ASP:O	2:B:178:LEU:HB2	2.13	0.48
2:B:419:ASP:HA	2:B:422:ARG:HH12	1.79	0.48
1:A:381:ILE:O	1:A:381:ILE:HG13	2.12	0.48
1:A:300:GLU:O	1:A:301:SER:C	2.56	0.48
2:B:318:GLU:OE2	2:B:319:HIS:N	2.46	0.48
2:B:254:ALA:O	2:B:371:VAL:HG22	2.14	0.47
1:A:296:MET:HE3	2:B:313:LYS:NZ	2.29	0.47
1:A:376:ASN:O	1:A:377:TYR:C	2.56	0.47
2:B:399:SER:O	2:B:400:LEU:C	2.57	0.47
1:A:219:TYR:CE1	1:A:315:LEU:HD23	2.49	0.47
2:B:315:LEU:O	2:B:321:ASP:HB2	2.15	0.47
2:B:452:HIS:HB3	2:B:453:PRO:HD3	1.96	0.47
1:A:296:MET:HE3	1:A:296:MET:HB2	1.88	0.46
2:B:413:GLU:O	2:B:416:GLN:HB2	2.15	0.46
1:A:227:TYR:CZ	1:A:239:ALA:HB2	2.50	0.46
2:B:237:LEU:HD23	2:B:409:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:MET:HE3	2:B:360:MET:HA	1.98	0.45
1:A:195:ILE:HD12	1:A:195:ILE:HA	1.81	0.45
2:B:440:GLU:H	2:B:440:GLU:CD	2.25	0.45
2:B:390:CYS:HB3	2:B:455:TRP:CZ2	2.52	0.44
1:A:353:LEU:HD23	1:A:389:HIS:HD2	1.82	0.44
1:A:390:CYS:HB3	1:A:455:TRP:CZ2	2.53	0.44
1:A:333:THR:O	1:A:337:MET:HG3	2.18	0.44
2:B:429:SER:O	2:B:432:CME:N	2.51	0.43
2:B:376:ASN:CG	2:B:377:TYR:N	2.76	0.43
2:B:308:LEU:HG	2:B:342:VAL:HG11	2.01	0.43
1:A:296:MET:HE3	2:B:313:LYS:HZ3	1.83	0.42
1:A:296:MET:CE	2:B:313:LYS:HZ1	2.32	0.42
2:B:397:THR:CB	2:B:469:ILE:HG23	2.37	0.42
1:A:165:HIS:HB3	1:A:186:TYR:CZ	2.54	0.42
2:B:174:ASN:ND2	2:B:202:GLU:OE2	2.46	0.42
1:A:173:LEU:HA	1:A:178:LEU:HD13	2.01	0.42
2:B:403:TYR:CE2	2:B:480:TYR:CE2	3.08	0.42
1:A:209:PHE:O	1:A:210:ARG:C	2.63	0.42
2:B:173:LEU:O	2:B:244:GLN:NE2	2.53	0.42
2:B:219:TYR:CD2	2:B:219:TYR:C	2.98	0.42
2:B:275:ASP:O	2:B:278:HIS:HB2	2.19	0.41
1:A:165:HIS:CB	1:A:186:TYR:CZ	3.03	0.41
2:B:169:GLU:OE2	2:B:182:ASN:HB3	2.21	0.41
2:B:403:TYR:CE2	2:B:480:TYR:HE2	2.38	0.41
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.96	0.40
1:A:275:ASP:HA	1:A:307:HIS:CD2	2.56	0.40
2:B:458:TRP:O	2:B:462:VAL:HG22	2.21	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	319/398 (80%)	305 (96%)	13 (4%)	1 (0%)	36	50
2	B	319/398 (80%)	306 (96%)	11 (3%)	2 (1%)	21	32
All	All	638/796 (80%)	611 (96%)	24 (4%)	3 (0%)	24	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ASP
2	B	291	SER
2	B	375	ASP

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	291/358 (81%)	269 (92%)	22 (8%)	12	21
2	B	291/358 (81%)	271 (93%)	20 (7%)	14	24
All	All	582/716 (81%)	540 (93%)	42 (7%)	13	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	A	168	LYS
1	A	178	LEU
1	A	180	ILE
1	A	183	VAL
1	A	189	ASN
1	A	231	VAL
1	A	296	MET
1	A	300	GLU
1	A	317	GLU
1	A	318	GLU
1	A	328	LYS
1	A	331	ARG

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	368	SER
1	A	372	LEU
1	A	373	LEU
1	A	427	GLU
1	A	429	SER
1	A	436	THR
1	A	443	GLN
1	A	470	LEU
2	B	168	LYS
2	B	183	VAL
2	B	204	ASP
2	B	213	SER
2	B	221	MET
2	B	252	THR
2	B	258	VAL
2	B	317	GLU
2	B	318	GLU
2	B	326	LEU
2	B	327	THR
2	B	328	LYS
2	B	332	GLN
2	B	347	MET
2	B	366	VAL
2	B	368	SER
2	B	371	VAL
2	B	373	LEU
2	B	378	THR
2	B	429	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
2	B	182	ASN
2	B	284	GLN
2	B	288	ASN
2	B	382	GLN
2	B	478	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are 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
1	CME	A	320	1	4,5,10	1.58	1 (25%)	1,5,11	2.23	1 (100%)
2	CME	B	432	2	4,5,10	2.26	1 (25%)	1,5,11	3.19	1 (100%)
2	CME	B	194	2	4,5,10	1.66	1 (25%)	1,5,11	0.32	0
1	CME	A	194	1	4,5,10	1.87	1 (25%)	1,5,11	5.40	1 (100%)

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
1	CME	A	320	1	-	0/1/4/10	-
2	CME	B	432	2	-	1/1/4/10	-
2	CME	B	194	2	-	1/1/4/10	-
1	CME	A	194	1	-	1/1/4/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	432	CME	CB-CA	3.95	1.57	1.53
1	A	194	CME	CB-SG	-2.80	1.75	1.81
2	B	194	CME	CB-CA	-2.44	1.50	1.53
1	A	320	CME	CB-SG	-2.03	1.77	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	CME	CA-CB-SG	-5.40	102.86	114.40
2	B	432	CME	CA-CB-SG	3.19	121.21	114.40
1	A	320	CME	CA-CB-SG	-2.23	109.63	114.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	194	CME	N-CA-CB-SG
2	B	194	CME	N-CA-CB-SG
2	B	432	CME	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	432	CME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ROL	B	102	-	22,22,22	1.53	3 (13%)	30,30,30	2.14	6 (20%)
5	ROL	A	101	-	22,22,22	1.43	4 (18%)	30,30,30	3.09	13 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ROL	B	102	-	-	0/10/26/26	0/3/3/3
5	ROL	A	101	-	-	4/10/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	102	ROL	C4-C3	-4.64	1.49	1.54
5	B	102	ROL	O3-C7	3.13	1.42	1.37
5	A	101	ROL	O3-C7	2.82	1.42	1.37
5	A	101	ROL	C4-C3	-2.82	1.51	1.54
5	A	101	ROL	C5-C3	2.64	1.57	1.52
5	A	101	ROL	O2-C8	2.57	1.41	1.37
5	B	102	ROL	C5-C3	2.37	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	101	ROL	C3-C4-N1	-9.21	95.41	103.09
5	B	102	ROL	C16-O2-C8	6.61	127.20	117.51
5	A	101	ROL	C3-C2-C1	-5.69	97.54	104.96
5	A	101	ROL	C2-C3-C5	-5.14	104.70	115.29
5	A	101	ROL	C4-C3-C2	4.94	110.93	104.03
5	B	102	ROL	O3-C11-C12	-4.86	91.97	108.71
5	A	101	ROL	O2-C8-C7	4.83	121.95	115.40
5	A	101	ROL	O3-C11-C12	-4.71	92.48	108.71
5	B	102	ROL	O1-C1-C2	-4.25	121.06	126.48
5	A	101	ROL	C16-O2-C8	3.76	123.02	117.51
5	B	102	ROL	C4-C3-C5	-3.74	104.60	114.04
5	B	102	ROL	C3-C4-N1	3.49	106.00	103.09
5	A	101	ROL	O1-C1-C2	-3.36	122.20	126.48
5	A	101	ROL	C6-C5-C3	3.04	128.41	120.88
5	A	101	ROL	O2-C8-C9	-2.96	119.30	124.30
5	A	101	ROL	C10-C5-C3	-2.63	114.42	121.09
5	A	101	ROL	C2-C1-N1	2.40	110.97	108.68
5	B	102	ROL	C4-N1-C1	-2.13	112.06	114.13
5	A	101	ROL	C14-C13-C12	-2.11	98.96	105.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

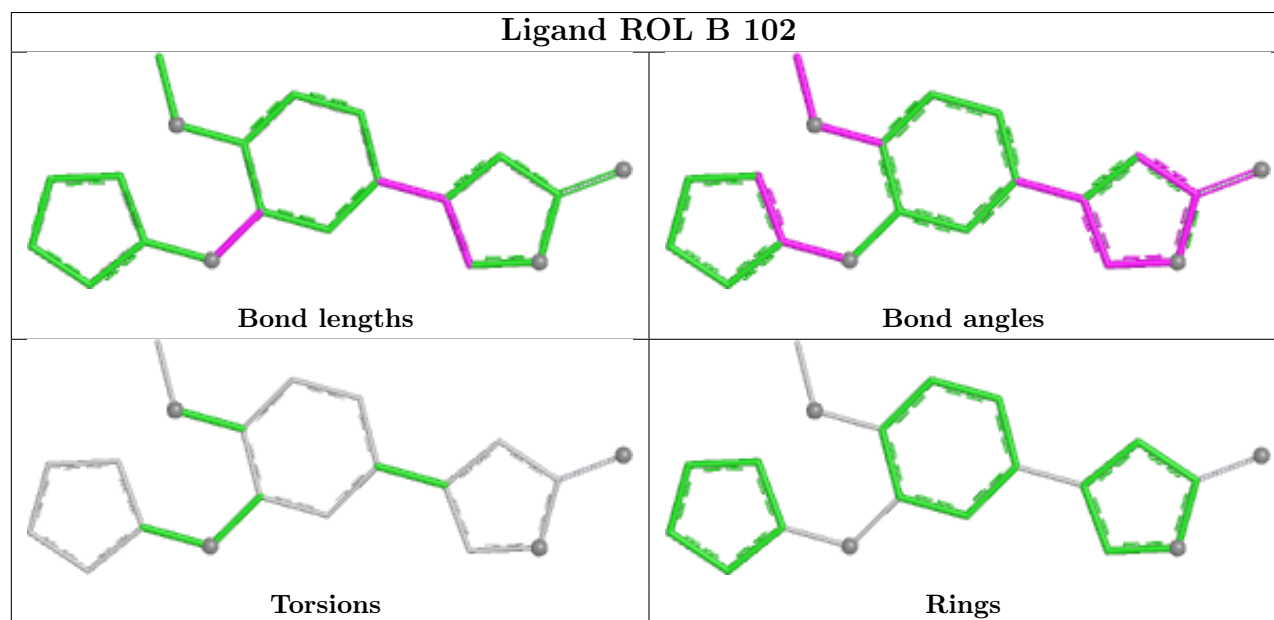
Mol	Chain	Res	Type	Atoms
5	A	101	ROL	C15-C11-O3-C7
5	A	101	ROL	C7-C8-O2-C16
5	A	101	ROL	C12-C11-O3-C7
5	A	101	ROL	C9-C8-O2-C16

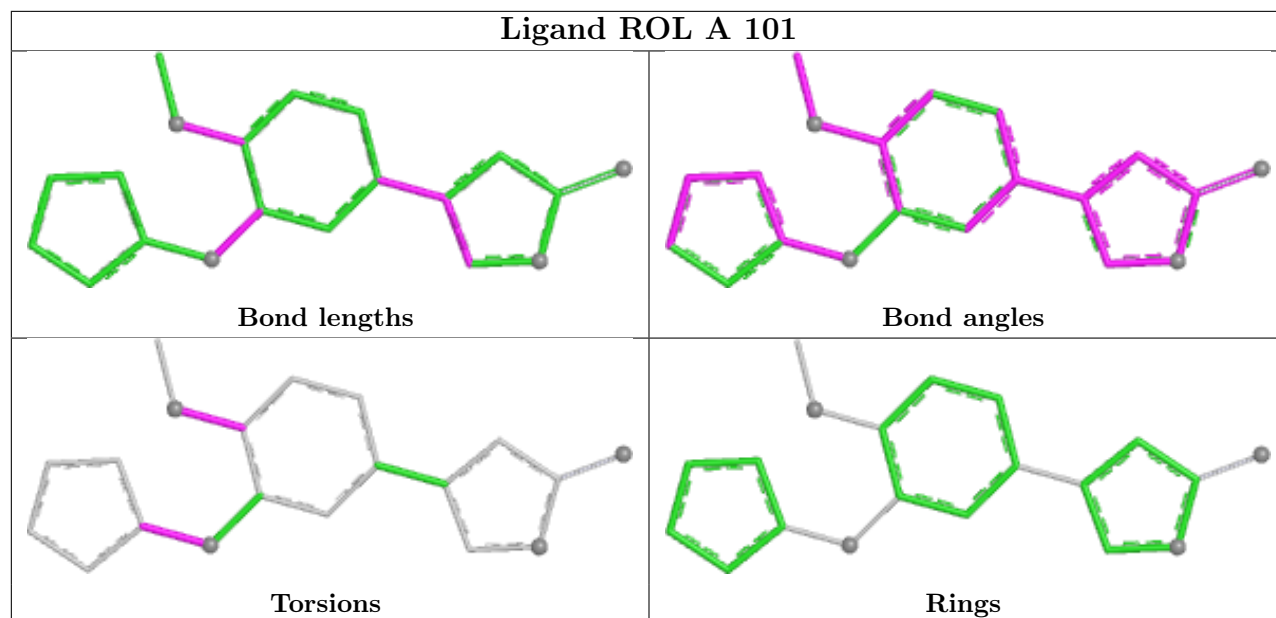
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	102	ROL	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 [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	321/398 (80%)	0.22	2 (0%) 85 83	14, 23, 29, 42	0
2	B	321/398 (80%)	0.35	4 (1%) 76 73	15, 23, 29, 33	0
All	All	642/796 (80%)	0.28	6 (0%) 81 78	14, 23, 29, 42	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	PRO	3.7
2	B	190	ARG	3.1
2	B	320	CYS	2.4
2	B	315	LEU	2.4
1	A	319	HIS	2.2
2	B	319	HIS	2.1

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
1	CME	A	320	6/11	0.83	0.14	44,46,46,55	0
2	CME	B	432	6/11	0.85	0.10	33,36,38,48	0
2	CME	B	194	6/11	0.92	0.09	30,32,34,44	0
1	CME	A	194	6/11	0.92	0.11	31,32,35,44	0

6.3 Carbohydrates [i](#)

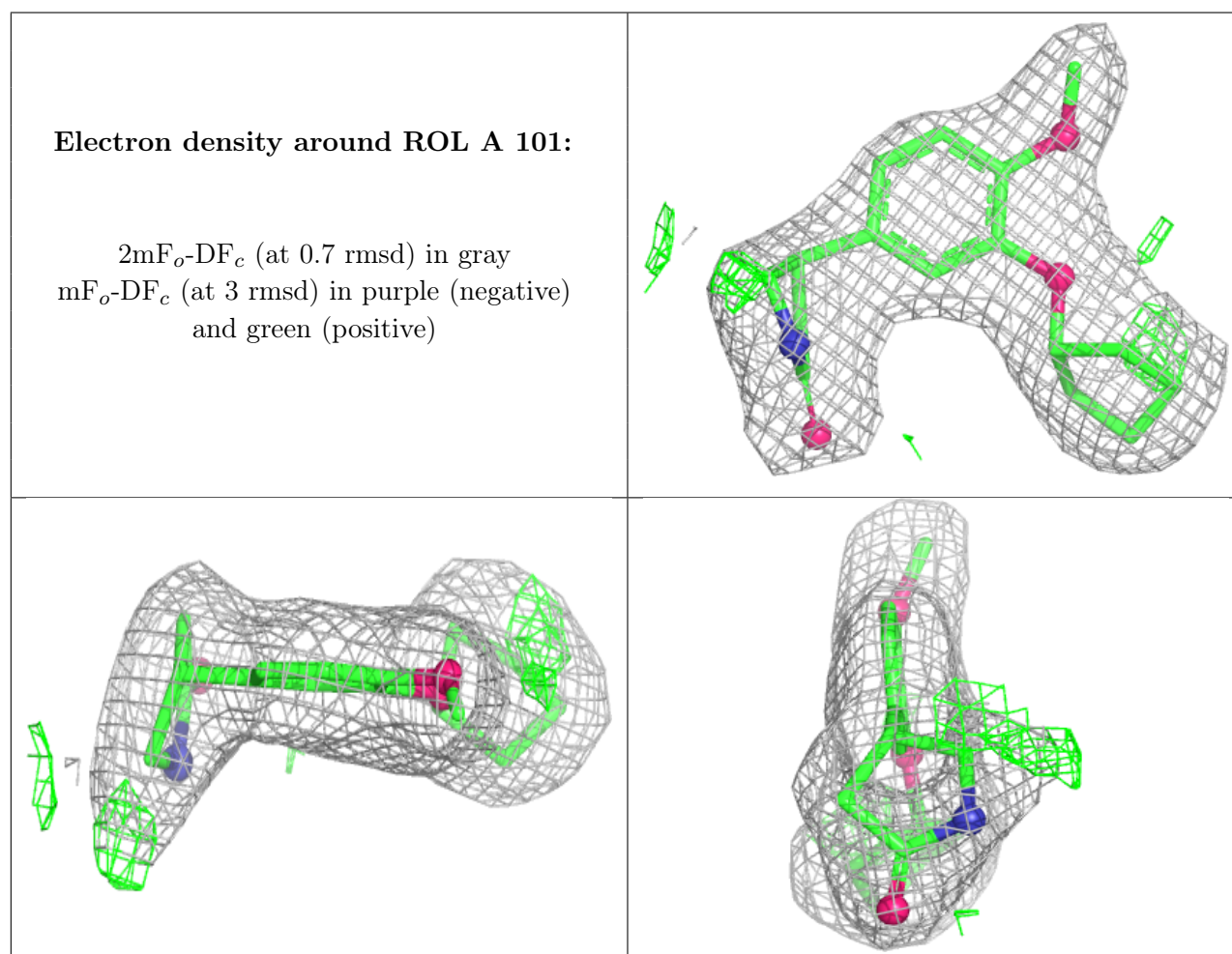
There are no oligosaccharides in this entry.

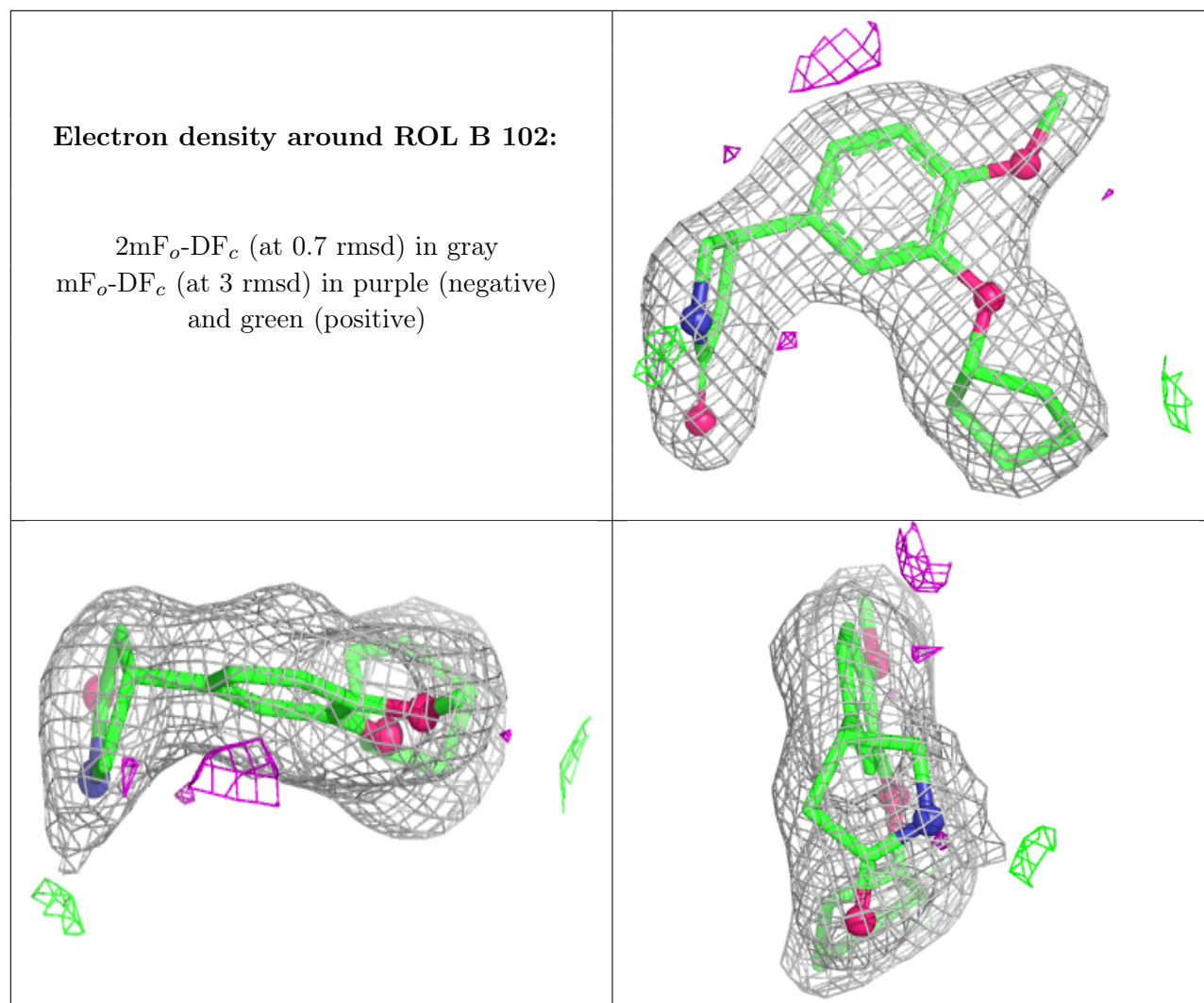
6.4 Ligands [i](#)

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
5	ROL	A	101	20/20	0.88	0.13	40,44,46,53	0
5	ROL	B	102	20/20	0.92	0.11	38,43,48,49	0
3	ZN	B	1001	1/1	0.97	0.04	41,41,41,41	0
4	MG	B	1002	1/1	0.97	0.04	26,26,26,26	0
3	ZN	A	1001	1/1	0.98	0.04	39,39,39,39	0
4	MG	A	1002	1/1	0.99	0.06	30,30,30,30	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 ⓘ

There are no such residues in this entry.