



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:43 PM UTC

PDB ID : 6SKP / pdb_00006skp
Title : OXA-10_IPM. Structural insight to the enhanced carbapenem efficiency of OXA-655 compared to OXA-10.
Authors : Leiros, H.-K.S.
Deposited on : 2019-08-16
Resolution : 1.89 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

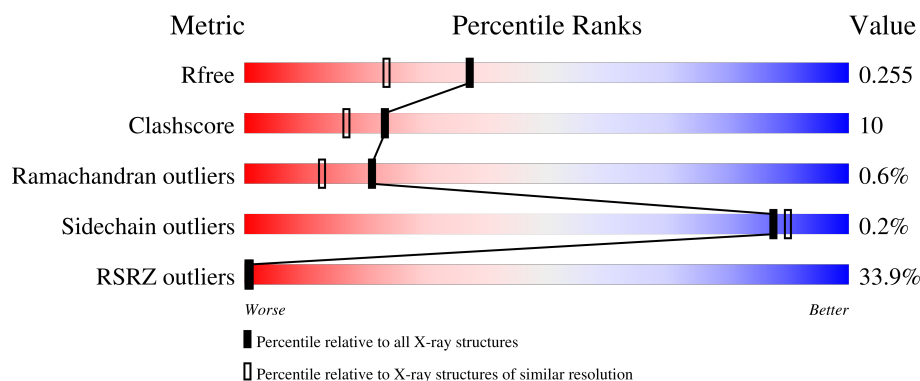
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	266	20% 74% 17% 8%
1	B	266	42% 74% 17% 8%

2 Entry composition [i](#)

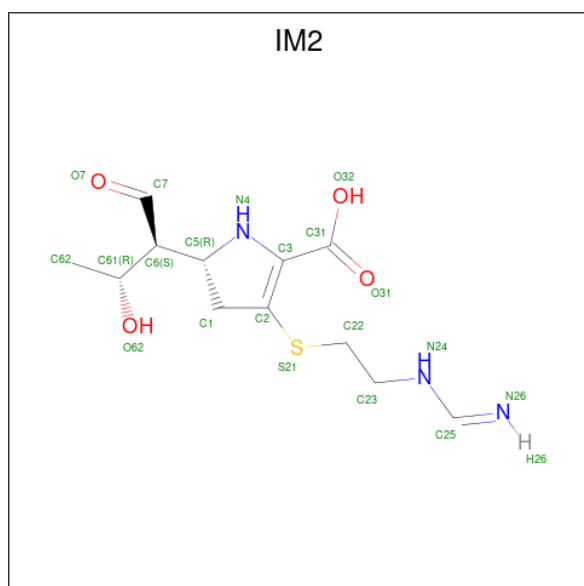
There are 5 unique types of molecules in this entry. The entry contains 8294 atoms, of which 3980 are hydrogens and 0 are deuteriums.

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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	H	N	O	S	20	11	0
			3953	1264	1972	332	379	6			
1	B	246	Total	C	H	N	O	S	38	6	0
			3921	1255	1956	329	375	6			

- Molecule 2 is (5R)-5-[(1S,2R)-1-formyl-2-hydroxypropyl]-3-[(2-[(E)-iminomethyl]amino)ethyl)sulfanyl]-4,5-dihydro-1H-pyrrole-2-carboxylic acid (CCD ID: IM2) (formula: C₁₂H₁₉N₃O₄S) (labeled as "Ligand of Interest" by depositor).

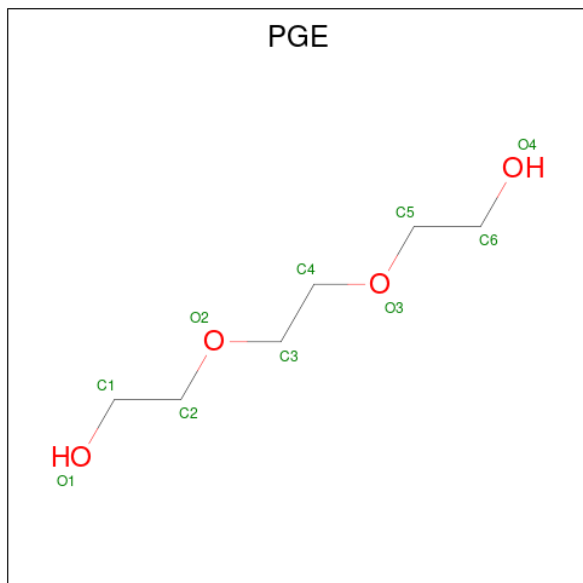


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	2	0
			39	12	19	3	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			39	12	19	3	4	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			24	6	14	4		

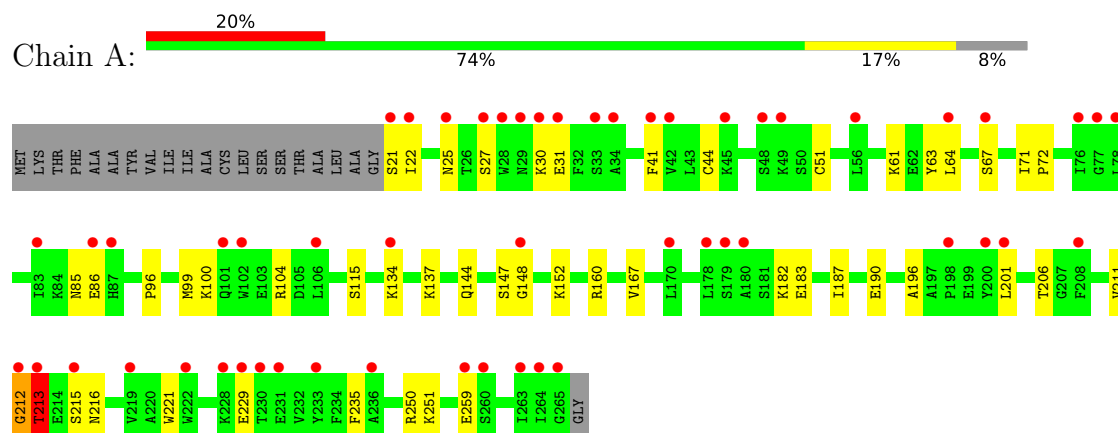
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		
5	B	123	Total	O	0	0
			123	123		

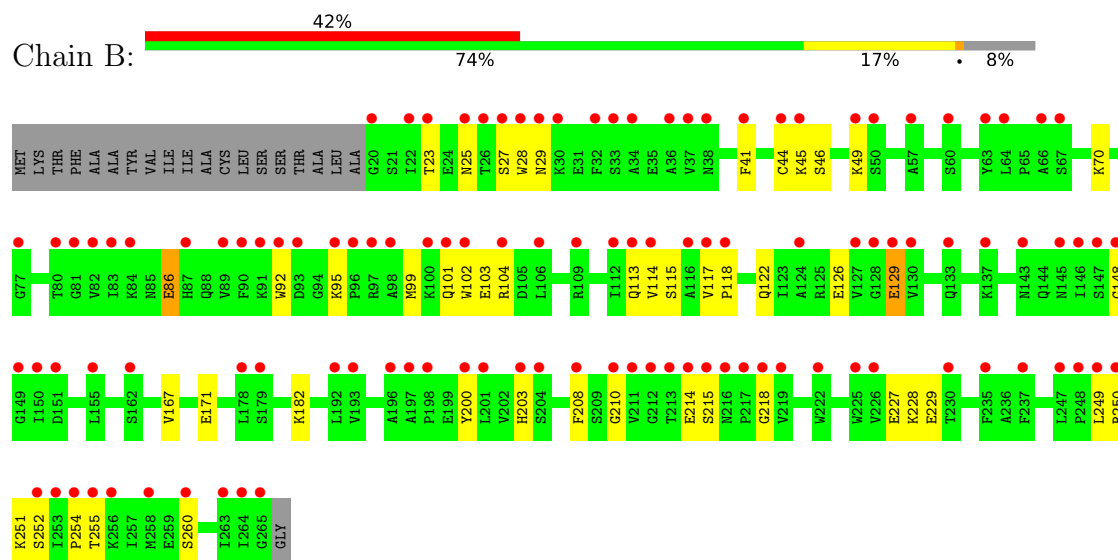
3 Residue-property plots [i](#)

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: Beta-lactamase



• Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.93Å 124.79Å 48.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 1.89 45.00 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.00-1.89) 99.2 (45.00-1.89)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.216 , 0.248 0.223 , 0.255	Depositor DCC
R_{free} test set	2100 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8294	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: IM2, KCX, PGE, NA

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	0.58	0/2044	0.75	0/2761
1	B	0.55	2/2022 (0.1%)	0.72	0/2732
All	All	0.57	2/4066 (0.0%)	0.73	0/5493

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	GLU	CD-OE2	6.95	1.38	1.25
1	B	129	GLU	CB-CG	-5.69	1.35	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213[B]	THR	Peptide

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	1981	1972	1924	36	2
1	B	1965	1956	1933	47	0
2	A	20	19	16	2	0
2	B	20	19	16	4	0
3	A	1	0	0	0	0
4	B	10	14	14	2	0
5	A	194	0	0	11	5
5	B	123	0	0	16	3
All	All	4314	3980	3903	81	7

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 (81) 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:147:SER:O	5:A:401:HOH:O	1.70	1.09
1:B:251:LYS:O	5:B:401:HOH:O	1.72	1.06
1:A:31:GLU:OE2	5:A:402:HOH:O	1.77	1.02
1:B:171:GLU:OE1	5:B:402:HOH:O	1.81	0.98
1:B:255:THR:N	5:B:401:HOH:O	2.00	0.95
4:B:302:PGE:O2	5:B:403:HOH:O	1.87	0.90
4:B:302:PGE:O1	5:B:404:HOH:O	1.91	0.89
1:A:21:SER:N	5:A:405:HOH:O	2.06	0.88
1:B:25:ASN:OD1	1:B:27:SER:OG	1.92	0.85
1:A:86:GLU:OE1	5:A:404:HOH:O	2.05	0.75
1:A:104:ARG:NH1	5:A:409:HOH:O	2.23	0.70
1:B:228:LYS:HD3	1:B:229:GLU:HG3	1.72	0.70
1:A:190:GLU:OE2	5:A:406:HOH:O	2.11	0.69
1:B:148:GLY:O	5:B:405:HOH:O	2.11	0.67
1:A:134:LYS:NZ	5:A:403:HOH:O	1.94	0.66
1:B:250:ARG:NH2	2:B:301:IM2:O31	2.18	0.65
1:A:182:LYS:NZ	1:B:86[B]:GLU:OE1	2.17	0.65
1:A:211:VAL:O	1:A:213[B]:THR:OG1	2.16	0.64
1:A:259:GLU:OE2	5:A:407:HOH:O	2.15	0.64
1:A:148:GLY:O	1:A:152:LYS:HE3	1.98	0.63
1:B:203:HIS:HD2	5:B:456:HOH:O	1.83	0.61
1:B:23[B]:THR:HG23	5:B:454:HOH:O	1.99	0.61
1:B:46:SER:O	1:B:49:LYS:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LYS:NZ	5:B:412:HOH:O	2.38	0.56
1:B:27:SER:O	1:B:29:ASN:N	2.39	0.56
1:B:250:ARG:HH12	2:B:301:IM2:C31	2.19	0.55
1:A:221:TRP:O	1:A:250:ARG:HD2	2.07	0.55
1:B:101:GLN:HB2	1:B:114:VAL:CG2	2.37	0.55
1:B:45:LYS:NZ	5:B:414:HOH:O	2.39	0.54
1:B:208:PHE:N	2:B:301:IM2:O7	2.38	0.54
1:A:22:ILE:HD12	1:A:51:CYS:O	2.08	0.53
1:B:49:LYS:HE2	1:B:171:GLU:OE2	2.08	0.52
1:A:61:LYS:HD3	1:A:63:TYR:OH	2.09	0.52
1:A:213[B]:THR:HG22	1:A:215[B]:SER:H	1.75	0.51
1:B:129:GLU:HG3	5:B:504:HOH:O	2.11	0.50
1:A:25:ASN:OD1	1:A:27:SER:HB3	2.11	0.50
1:B:92:TRP:CZ3	1:B:95:LYS:O	2.64	0.50
1:A:86:GLU:HB2	1:A:187:ILE:HG12	1.94	0.49
1:A:100:LYS:NZ	5:A:418:HOH:O	2.45	0.49
1:A:67:SER:OG	1:A:115[B]:SER:OG	2.27	0.49
1:A:183:GLU:OE2	1:B:182:LYS:HD3	2.13	0.49
1:A:213[B]:THR:HA	1:A:216:ASN:H	1.76	0.49
1:B:214:GLU:O	1:B:215:SER:CB	2.61	0.47
1:B:254:PRO:HG2	5:B:401:HOH:O	2.14	0.47
1:B:44:CYS:SG	1:B:167[A]:VAL:HG11	2.53	0.47
1:A:44:CYS:SG	1:A:167:VAL:HG11	2.55	0.47
1:B:122:GLN:O	1:B:126:GLU:HG3	2.14	0.47
1:B:41:PHE:CE2	1:B:254:PRO:HB3	2.50	0.46
1:B:113:GLN:OE1	5:B:407:HOH:O	2.20	0.46
1:B:86[B]:GLU:H	1:B:86[B]:GLU:CD	2.24	0.46
1:B:249:LEU:HA	1:B:252:SER:OG	2.16	0.46
1:B:200:TYR:HA	1:B:227:GLU:O	2.16	0.45
1:A:183:GLU:CD	1:B:182:LYS:HD3	2.42	0.44
1:B:115:SER:HB3	2:B:301:IM2:H51	1.99	0.44
1:A:229:GLU:OE2	1:B:104:ARG:NH2	2.51	0.44
1:A:85:ASN:HB2	5:B:412:HOH:O	2.18	0.43
1:B:103:GLU:C	1:B:104:ARG:HG3	2.44	0.43
1:B:49:LYS:HD2	1:B:49:LYS:HA	1.83	0.43
1:B:101:GLN:HB2	1:B:114:VAL:HG21	2.01	0.43
1:A:64:LEU:HD22	1:A:160:ARG:NH1	2.34	0.43
1:B:117:VAL:N	1:B:118:PRO:CD	2.82	0.42
1:B:210:GLY:O	1:B:218:GLY:HA3	2.19	0.42
1:A:71:ILE:HB	1:A:72:PRO:CD	2.49	0.42
1:A:137:LYS:HG2	1:A:144:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ALA:HA	1:A:201:LEU:HD23	2.01	0.42
1:A:27:SER:O	1:A:30:LYS:HG2	2.20	0.42
5:A:406:HOH:O	1:B:227:GLU:CD	2.62	0.42
1:B:260:SER:OG	5:B:406:HOH:O	2.19	0.42
1:A:41:PHE:CE2	1:A:235:PHE:HB2	2.54	0.42
1:A:99:MET:HE1	2:A:301:IM2:H11	2.02	0.41
1:B:99:MET:HE3	1:B:102:TRP:CZ2	2.56	0.41
1:A:212[B]:GLY:C	1:A:213[B]:THR:OG1	2.64	0.41
1:B:27:SER:C	1:B:29:ASN:N	2.79	0.41
5:A:406:HOH:O	1:B:227:GLU:OE1	2.22	0.41
1:B:227:GLU:HG3	5:B:456:HOH:O	2.21	0.41
1:A:206:THR:CG2	1:A:251:LYS:HE2	2.51	0.41
1:A:250:ARG:HH12	2:A:301:IM2:C31	2.34	0.40
1:B:27:SER:C	1:B:29:ASN:H	2.29	0.40

All (7) 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:96:PRO:O	1:A:137:LYS:NZ[2_455]	1.97	0.23
5:A:593:HOH:O	5:B:523:HOH:O[3_547]	1.97	0.23
5:A:561:HOH:O	5:B:425:HOH:O[3_547]	2.08	0.12
5:A:480:HOH:O	5:A:514:HOH:O[2_454]	2.16	0.04
1:A:96:PRO:O	1:A:137:LYS:HZ2[2_455]	1.57	0.03
5:A:547:HOH:O	5:B:499:HOH:O[3_547]	2.18	0.02
5:A:408:HOH:O	5:A:510:HOH:O[2_455]	2.19	0.01

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	253/266 (95%)	241 (95%)	8 (3%)	4 (2%)	7 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	249/266 (94%)	239 (96%)	9 (4%)	1 (0%)	30	22
All	All	502/532 (94%)	480 (96%)	17 (3%)	5 (1%)	21	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213[A]	THR
1	A	213[B]	THR
1	A	212[A]	GLY
1	A	212[B]	GLY
1	B	28	TRP

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	218/223 (98%)	218 (100%)	0	100	100
1	B	215/223 (96%)	213 (99%)	2 (1%)	70	73
All	All	433/446 (97%)	431 (100%)	2 (0%)	87	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86[A]	GLU
1	B	86[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	KCX	B	70	1	10,11,12	0.96	1 (10%)	6,12,14	0.73	0
1	KCX	A	70	1	10,11,12	1.03	0	6,12,14	0.58	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
1	KCX	B	70	1	-	0/9/10/12	-
1	KCX	A	70	1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	KCX	CE-NZ	2.13	1.51	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	PGE	B	302	-	9,9,9	0.40	0	8,8,8	0.40	0
2	IM2	B	301	1	15,20,20	0.83	1 (6%)	8,26,26	0.91	1 (12%)
2	IM2	A	301	1	15,20,20	0.48	0	8,26,26	1.44	1 (12%)

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	PGE	B	302	-	-	4/7/7/7	-
2	IM2	B	301	1	-	4/18/32/32	0/1/1/1
2	IM2	A	301	1	-	3/18/32/32	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	IM2	O7-C7	-2.26	1.11	1.20

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	IM2	O7-C7-C6	-3.85	116.08	125.27
2	B	301	IM2	C3-C2-S21	2.04	127.24	124.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

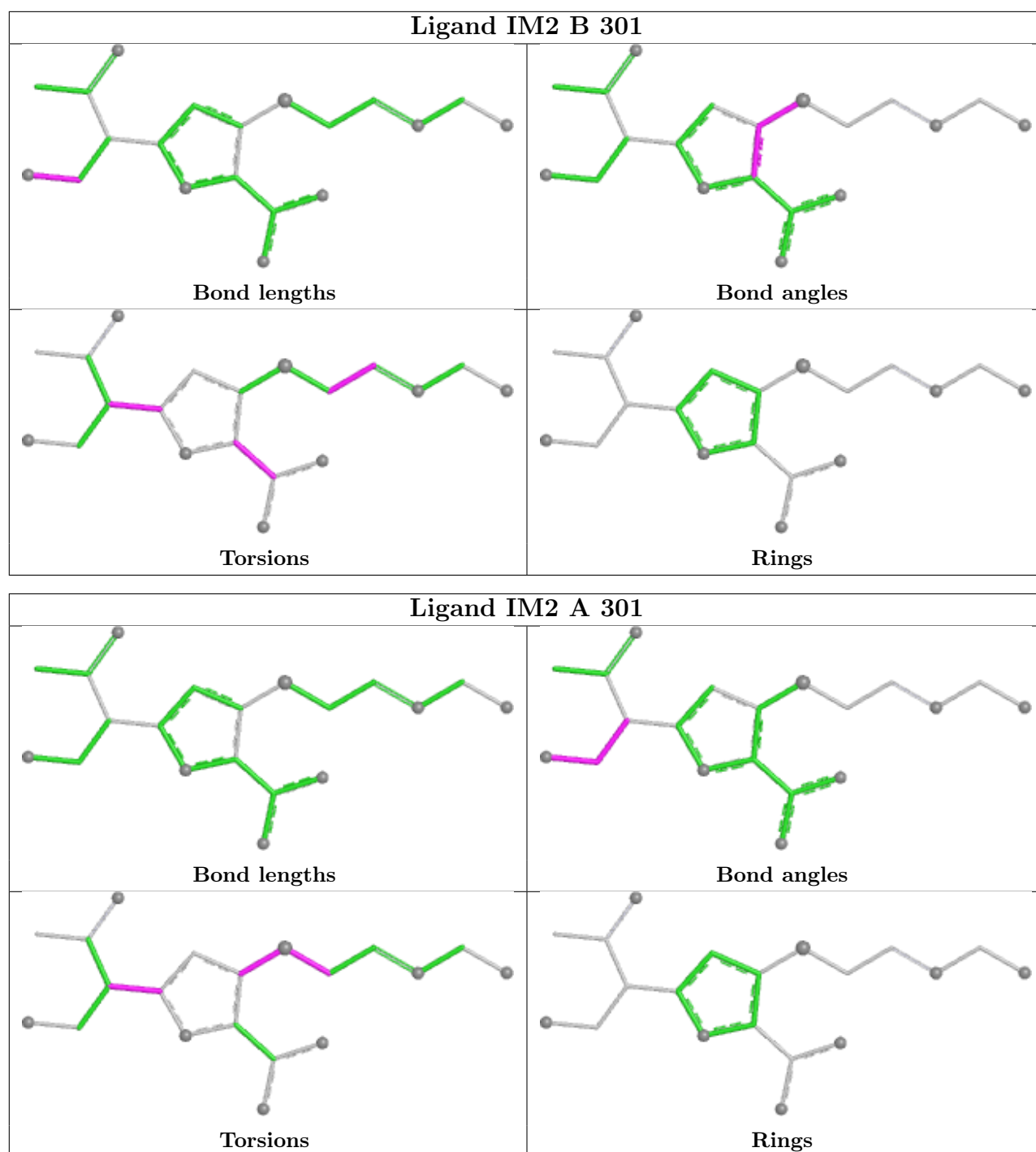
Mol	Chain	Res	Type	Atoms
2	A	301	IM2	C1-C5-C6-C7
2	A	301	IM2	C23-C22-S21-C2
2	B	301	IM2	C1-C5-C6-C7
2	B	301	IM2	S21-C22-C23-N24
4	B	302	PGE	O1-C1-C2-O2
4	B	302	PGE	O2-C3-C4-O3
4	B	302	PGE	C4-C3-O2-C2
2	B	301	IM2	N4-C3-C31-O32
2	A	301	IM2	C1-C2-S21-C22
2	B	301	IM2	N4-C3-C31-O31
4	B	302	PGE	C3-C4-O3-C5

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	PGE	2	0
2	B	301	IM2	4	0
2	A	301	IM2	2	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	244/266 (91%)	1.32	53 (21%) 2 2	12, 31, 58, 82	11 (4%)
1	B	245/266 (92%)	2.02	113 (46%) 0 0	14, 43, 70, 84	11 (4%)
All	All	489/532 (91%)	1.68	166 (33%) 1 1	12, 36, 66, 84	22 (4%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ILE	6.4
1	B	28	TRP	6.0
1	B	117	VAL	6.0
1	B	148	GLY	5.6
1	B	211	VAL	5.3
1	A	48	SER	5.1
1	B	23[A]	THR	5.0
1	B	106	LEU	5.0
1	A	213[A]	THR	4.8
1	B	26	THR	4.8
1	B	149	GLY	4.6
1	B	25	ASN	4.6
1	A	30	LYS	4.6
1	A	230	THR	4.5
1	B	127	VAL	4.5
1	A	265	GLY	4.5
1	B	98	ALA	4.5
1	A	215[A]	SER	4.4
1	B	82	VAL	4.4
1	A	180	ALA	4.4
1	B	66	ALA	4.4
1	A	134	LYS	4.2
1	A	42	VAL	4.2
1	B	210	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	81	GLY	4.1
1	B	254	PRO	4.0
1	A	27	SER	4.0
1	B	92	TRP	3.9
1	A	264	ILE	3.9
1	A	259	GLU	3.9
1	A	28	TRP	3.9
1	A	198	PRO	3.9
1	B	201	LEU	3.8
1	B	90	PHE	3.8
1	B	192	LEU	3.8
1	B	101	GLN	3.7
1	B	263	ILE	3.6
1	B	20	GLY	3.6
1	A	260	SER	3.6
1	B	252	SER	3.5
1	B	265	GLY	3.5
1	B	146	ILE	3.4
1	B	213	THR	3.4
1	A	34	ALA	3.4
1	B	102	TRP	3.4
1	B	104	ARG	3.4
1	A	76	ILE	3.3
1	B	130	VAL	3.3
1	B	235	PHE	3.3
1	B	84	LYS	3.3
1	B	113	GLN	3.3
1	B	249	LEU	3.3
1	A	33	SER	3.3
1	A	31	GLU	3.2
1	B	253	ILE	3.2
1	B	36	ALA	3.2
1	B	196	ALA	3.2
1	B	198	PRO	3.2
1	B	32	PHE	3.2
1	B	204	SER	3.2
1	A	200	TYR	3.1
1	B	67	SER	3.1
1	A	41	PHE	3.1
1	A	179	SER	3.1
1	A	231	GLU	3.1
1	A	49	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	100	LYS	3.1
1	B	215	SER	3.1
1	B	250	ARG	3.0
1	B	247	LEU	3.0
1	B	22	ILE	3.0
1	B	193	VAL	3.0
1	B	133	GLN	3.0
1	B	80	THR	2.9
1	B	87[A]	HIS	2.9
1	B	96	PRO	2.9
1	B	222	TRP	2.9
1	B	38	ASN	2.9
1	B	256	LYS	2.9
1	A	208	PHE	2.8
1	B	29	ASN	2.8
1	B	64	LEU	2.8
1	B	197	ALA	2.8
1	B	155	LEU	2.8
1	B	179	SER	2.8
1	B	34	ALA	2.8
1	B	57	ALA	2.8
1	B	124	ALA	2.8
1	B	216	ASN	2.7
1	B	30	LYS	2.7
1	B	208	PHE	2.7
1	B	248	PRO	2.7
1	A	29	ASN	2.7
1	A	77	GLY	2.7
1	B	178	LEU	2.7
1	A	229	GLU	2.7
1	B	95	LYS	2.7
1	B	116	ALA	2.6
1	A	21	SER	2.6
1	A	102	TRP	2.6
1	B	44	CYS	2.6
1	B	255	THR	2.6
1	A	263	ILE	2.5
1	B	150	ILE	2.5
1	B	162	SER	2.5
1	A	56	LEU	2.5
1	A	45	LYS	2.5
1	A	219	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	201	LEU	2.4
1	B	258	MET	2.4
1	B	217	PRO	2.4
1	B	260	SER	2.4
1	B	118	PRO	2.4
1	B	37	VAL	2.4
1	B	219	VAL	2.4
1	B	27	SER	2.4
1	B	60	SER	2.4
1	B	264	ILE	2.4
1	B	50	SER	2.4
1	A	233	TYR	2.3
1	A	83[A]	ILE	2.3
1	A	25	ASN	2.3
1	B	33	SER	2.3
1	B	109	ARG	2.3
1	A	87	HIS	2.3
1	A	86	GLU	2.3
1	B	129	GLU	2.3
1	B	214	GLU	2.3
1	B	97	ARG	2.3
1	A	170	LEU	2.3
1	B	41	PHE	2.2
1	B	63	TYR	2.2
1	A	178	LEU	2.2
1	A	148	GLY	2.2
1	B	212	GLY	2.2
1	B	200	TYR	2.2
1	B	89	VAL	2.2
1	B	128	GLY	2.2
1	A	236	ALA	2.2
1	B	225	TRP	2.2
1	B	226	VAL	2.2
1	A	212[A]	GLY	2.2
1	B	145	ASN	2.1
1	B	114	VAL	2.1
1	B	230	THR	2.1
1	B	147	SER	2.1
1	B	77	GLY	2.1
1	B	218	GLY	2.1
1	B	91	LYS	2.1
1	A	106	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	143	ASN	2.1
1	A	67	SER	2.1
1	B	49	LYS	2.1
1	A	222	TRP	2.1
1	A	64	LEU	2.1
1	B	93	ASP	2.1
1	B	112	ILE	2.0
1	B	137	LYS	2.0
1	B	237	PHE	2.0
1	A	101	GLN	2.0
1	A	78	LEU	2.0
1	B	151	ASP	2.0
1	A	228	LYS	2.0
1	B	45	LYS	2.0
1	B	83	ILE	2.0
1	B	203	HIS	2.0

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	KCX	A	70	12/13	0.90	0.11	19,24,31,32	0
1	KCX	B	70	12/13	0.93	0.10	29,36,46,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

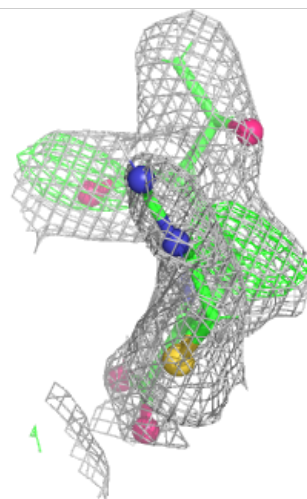
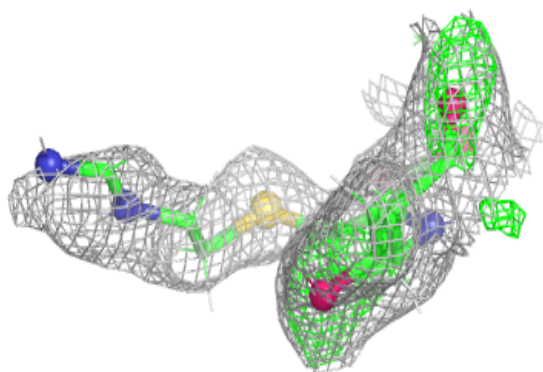
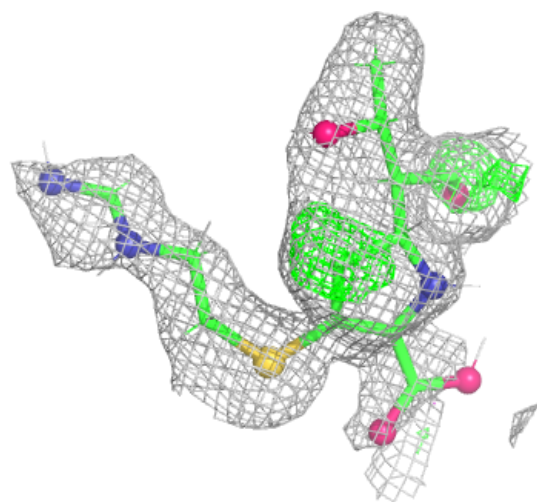
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	IM2	B	301	20/20	0.65	0.30	39,49,62,62	39
3	NA	A	302	1/1	0.74	0.36	66,66,66,66	0
4	PGE	B	302	10/10	0.75	0.23	56,67,77,77	0
2	IM2	A	301	20/20	0.87	0.18	34,47,57,62	4

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.

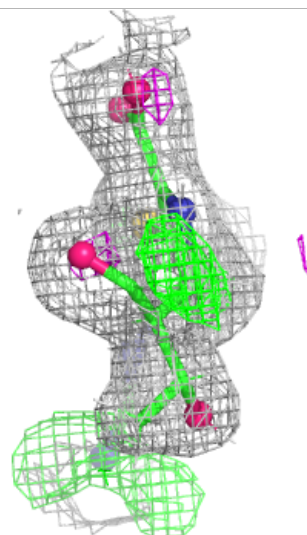
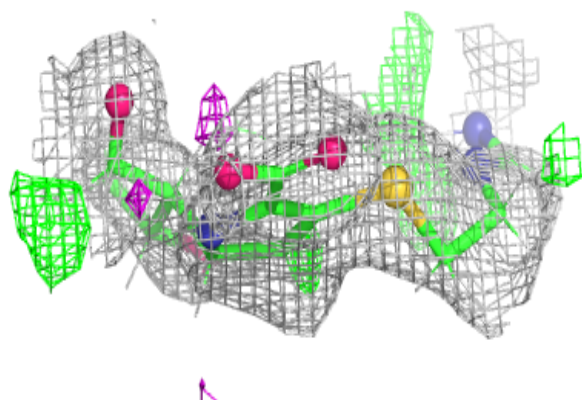
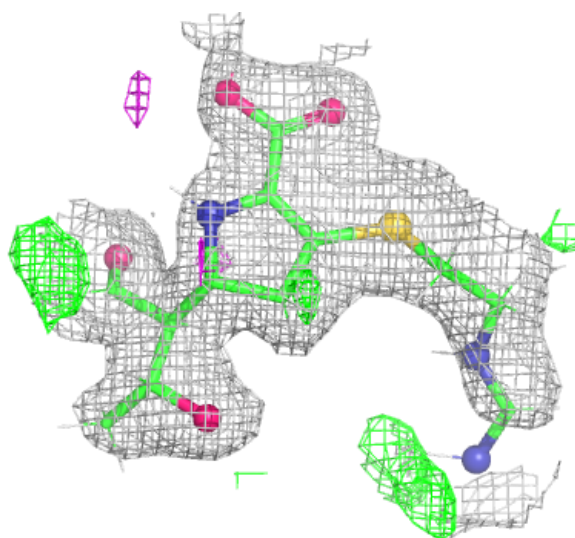
Electron density around IM2 B 301:

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 IM2 A 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.