Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2026 – 09:25 pm GMT

PDB ID	:	29KJ / pdb_000029kj
Title	:	Putative Polyurethane Degrading Esterase in Triple Liganded State
Authors	:	Bicer, D.; Otzen, D.E.; Morth, J.P.; Thirup, S.S.
Deposited on	:	2026-03-18
Resolution	:	1.25 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 (i) 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 (i)) were used in the production of this report:

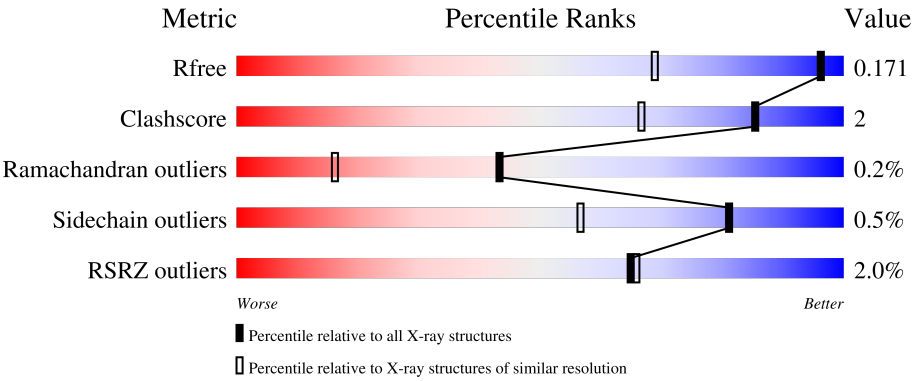
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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 <=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	530	2% 91%
2	B	5	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8338 atoms, of which 3844 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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	508	7735	2495	3775	713	734	18	6	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A9Q3ZCR3
A	2	ALA	-	expression tag	UNP A0A9Q3ZCR3
A	38	CYS	HIS	conflict	UNP A0A9Q3ZCR3
A	89	ASP	GLY	conflict	UNP A0A9Q3ZCR3
A	229	ALA	THR	conflict	UNP A0A9Q3ZCR3
A	472	THR	ALA	conflict	UNP A0A9Q3ZCR3
A	475	GLY	SER	conflict	UNP A0A9Q3ZCR3
A	490	THR	ALA	conflict	UNP A0A9Q3ZCR3
A	491	GLU	ALA	conflict	UNP A0A9Q3ZCR3
A	495	GLN	GLU	conflict	UNP A0A9Q3ZCR3
A	496	GLU	GLN	conflict	UNP A0A9Q3ZCR3
A	503	ARG	VAL	conflict	UNP A0A9Q3ZCR3
A	507	ARG	-	expression tag	UNP A0A9Q3ZCR3
A	508	PRO	-	expression tag	UNP A0A9Q3ZCR3
A	509	GLU	-	expression tag	UNP A0A9Q3ZCR3
A	510	THR	-	expression tag	UNP A0A9Q3ZCR3
A	511	ALA	-	expression tag	UNP A0A9Q3ZCR3
A	512	LYS	-	expression tag	UNP A0A9Q3ZCR3
A	513	SER	-	expression tag	UNP A0A9Q3ZCR3
A	514	SER	-	expression tag	UNP A0A9Q3ZCR3
A	515	GLY	-	expression tag	UNP A0A9Q3ZCR3
A	516	GLU	-	expression tag	UNP A0A9Q3ZCR3
A	517	ASN	-	expression tag	UNP A0A9Q3ZCR3
A	518	LEU	-	expression tag	UNP A0A9Q3ZCR3
A	519	TYR	-	expression tag	UNP A0A9Q3ZCR3
A	520	PHE	-	expression tag	UNP A0A9Q3ZCR3
A	521	GLN	-	expression tag	UNP A0A9Q3ZCR3

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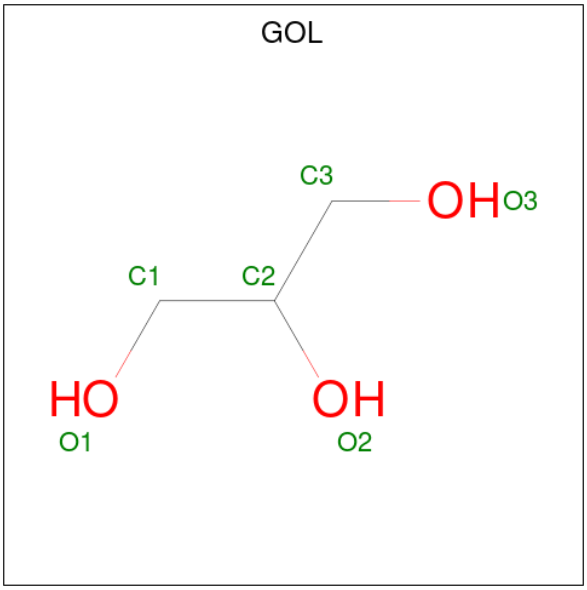
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Chain	Residue	Modelled	Actual	Comment	Reference
A	522	GLY	-	expression tag	UNP A0A9Q3ZCR3
A	523	HIS	-	expression tag	UNP A0A9Q3ZCR3
A	524	HIS	-	expression tag	UNP A0A9Q3ZCR3
A	525	HIS	-	expression tag	UNP A0A9Q3ZCR3
A	526	HIS	-	expression tag	UNP A0A9Q3ZCR3
A	527	HIS	-	expression tag	UNP A0A9Q3ZCR3
A	528	HIS	-	expression tag	UNP A0A9Q3ZCR3
A	529	HIS	-	expression tag	UNP A0A9Q3ZCR3
A	530	HIS	-	expression tag	UNP A0A9Q3ZCR3

- Molecule 2 is a protein called ASN-LEU-TYR-ALA-GLN.

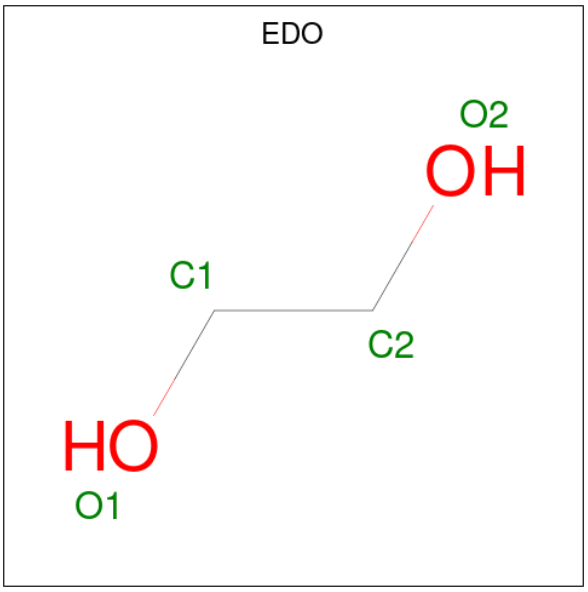
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	H	N	O	83	0	0
			83	27	41	7	8			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



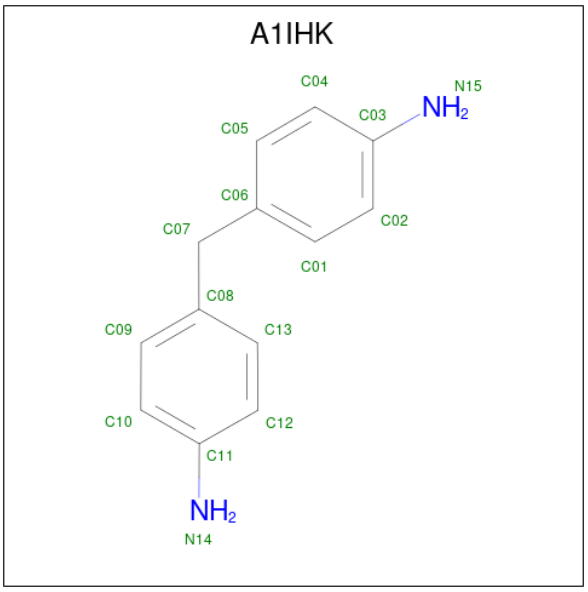
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



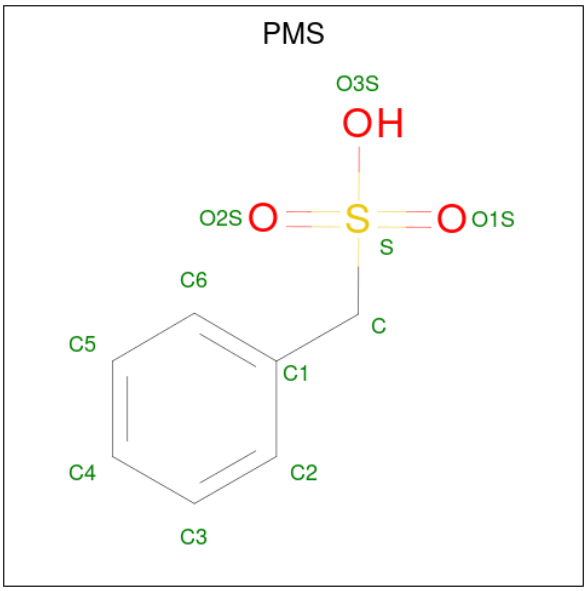
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is 4-[(4-aminophenyl)methyl]aniline (CCD ID: A1IHK) (formula: $C_{13}H_{14}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	N	29	0
			29	13	14	2		

- Molecule 6 is phenylmethanesulfonic acid (CCD ID: PMS) (formula: $C_7H_8O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 10 7 2 1	10	0

- Molecule 7 is water.

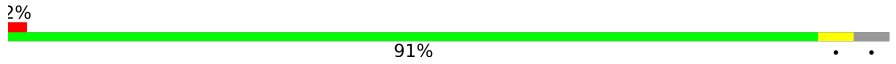
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	456	Total O 456 456	0	0
7	B	1	Total O 1 1	0	0

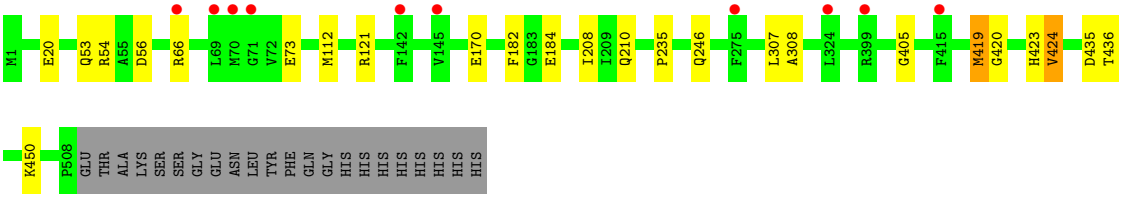
3 Residue-property plots (i)

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: Carboxylic ester hydrolase

Chain A:





- Molecule 2: ASN-LEU-TYR-ALA-GLN

Chain B:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.26Å 92.61Å 99.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.24 – 1.25 31.24 – 1.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.24-1.25) 100.0 (31.24-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.25Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.147 , 0.171 0.147 , 0.171	Depositor DCC
R_{free} test set	6981 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.46 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8338	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, A1IHK, PMS, EDO

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	0.43	0/4069	0.62	1/5533 (0.0%)
2	B	0.13	0/42	0.30	0/56
All	All	0.43	0/4111	0.62	1/5589 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	419	MET	CG-SD-CE	-6.69	86.18	100.90

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	3960	3775	3778	17	1
2	B	42	41	41	0	0
3	A	6	8	8	0	0
4	A	4	6	6	0	0
5	A	15	14	0	0	0
6	A	10	0	7	0	0
7	A	456	0	0	5	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4494	3844	3840	17	1

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 2.

All (17) 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:435:ASP:OD2	1:A:450:LYS:HE3	2.00	0.61
1:A:170:GLU:OE2	7:A:701:HOH:O	2.16	0.59
1:A:20:GLU:O	1:A:121:ARG:HD3	2.05	0.57
1:A:170:GLU:CG	7:A:880:HOH:O	2.57	0.51
1:A:308:ALA:O	1:A:405:GLY:HA2	2.13	0.49
1:A:170:GLU:HG2	7:A:991:HOH:O	2.14	0.48
1:A:66:ARG:NH1	1:A:73:GLU:HG3	2.30	0.47
1:A:112:MET:HE2	1:A:436:THR:HG21	1.98	0.44
1:A:170:GLU:HG3	7:A:880:HOH:O	2.16	0.44
1:A:435:ASP:OD2	1:A:450:LYS:CE	2.65	0.43
1:A:184:GLU:HA	1:A:210:GLN:O	2.18	0.43
1:A:208:ILE:HA	1:A:307:LEU:O	2.20	0.41
1:A:235:PRO:HD3	7:A:857:HOH:O	2.20	0.41
1:A:423:HIS:C	1:A:424:VAL:HG23	2.46	0.41
1:A:112:MET:HE3	1:A:112:MET:O	2.20	0.41
1:A:54:ARG:HD3	1:A:56:ASP:OD2	2.21	0.41
1:A:419:MET:HB3	1:A:419:MET:HE3	1.90	0.40

All (1) 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:246:GLN:HE22	1:A:420:GLY:H[2_455]	1.33	0.27

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	506/530 (96%)	491 (97%)	14 (3%)	1 (0%)	43 16
2	B	3/5 (60%)	3 (100%)	0	0	100 100
All	All	509/535 (95%)	494 (97%)	14 (3%)	1 (0%)	43 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	402/421 (96%)	400 (100%)	2 (0%)	81 56
2	B	4/4 (100%)	4 (100%)	0	100 100
All	All	406/425 (96%)	404 (100%)	2 (0%)	81 56

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

Mol	Chain	Res	Type
1	A	53	GLN
1	A	182	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	122	ASN
1	A	166	ASN
1	A	354	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands 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	$\#\|Z\| > 2$
3	GOL	A	601	-	5,5,5	0.39	0	5,5,5	0.47	0
4	EDO	A	602	-	3,3,3	0.33	0	2,2,2	0.23	0
5	A1IHK	A	603	-	16,16,16	0.19	0	21,21,21	0.28	0
6	PMS	A	604	1	7,10,11	0.36	0	11,12,15	1.02	1 (9%)

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
3	GOL	A	601	-	-	0/4/4/4	-
4	EDO	A	602	-	-	0/1/1/1	-
5	A1IHK	A	603	-	-	0/4/4/4	0/2/2/2
6	PMS	A	604	1	-	1/4/4/5	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	604	PMS	O2S-S-C	2.47	109.57	105.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

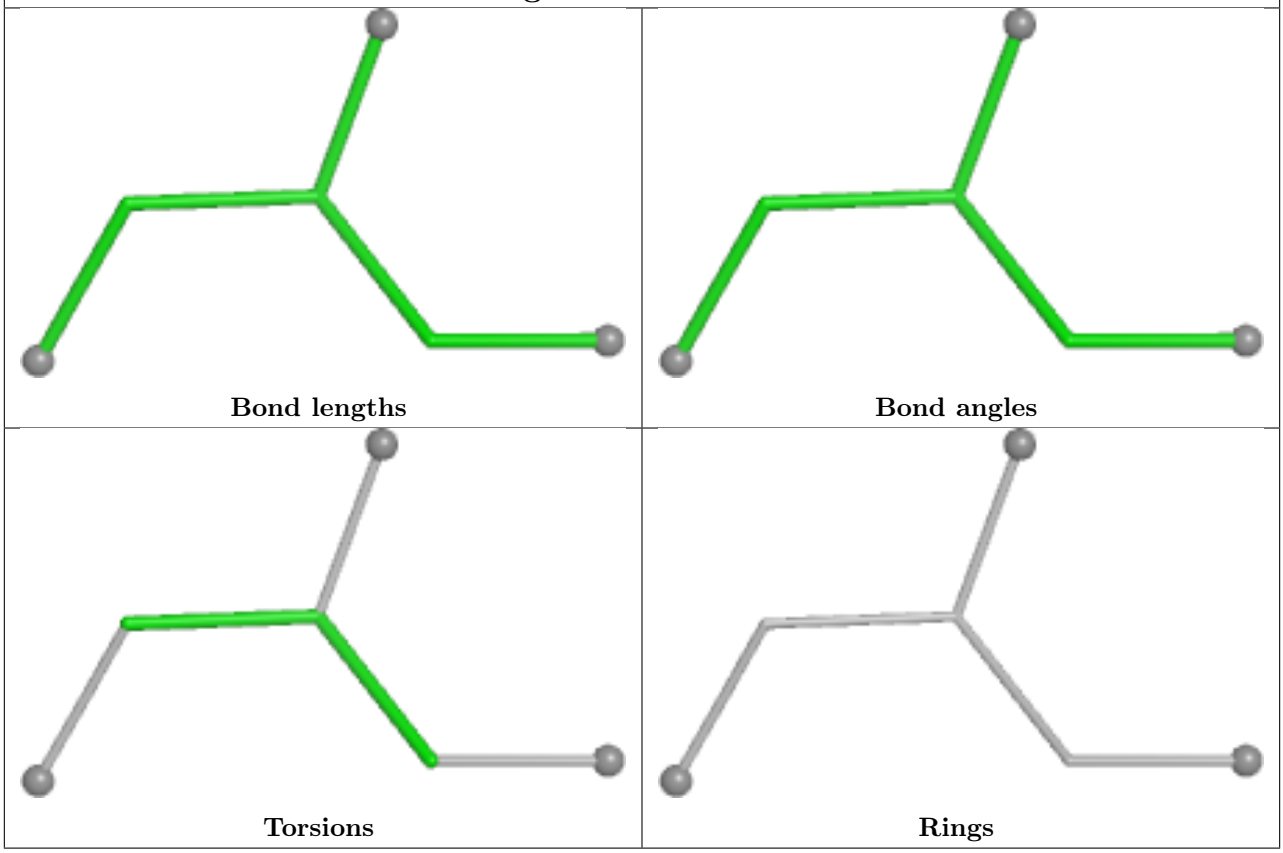
Mol	Chain	Res	Type	Atoms
6	A	604	PMS	C1-C-S-O1S

There are no ring outliers.

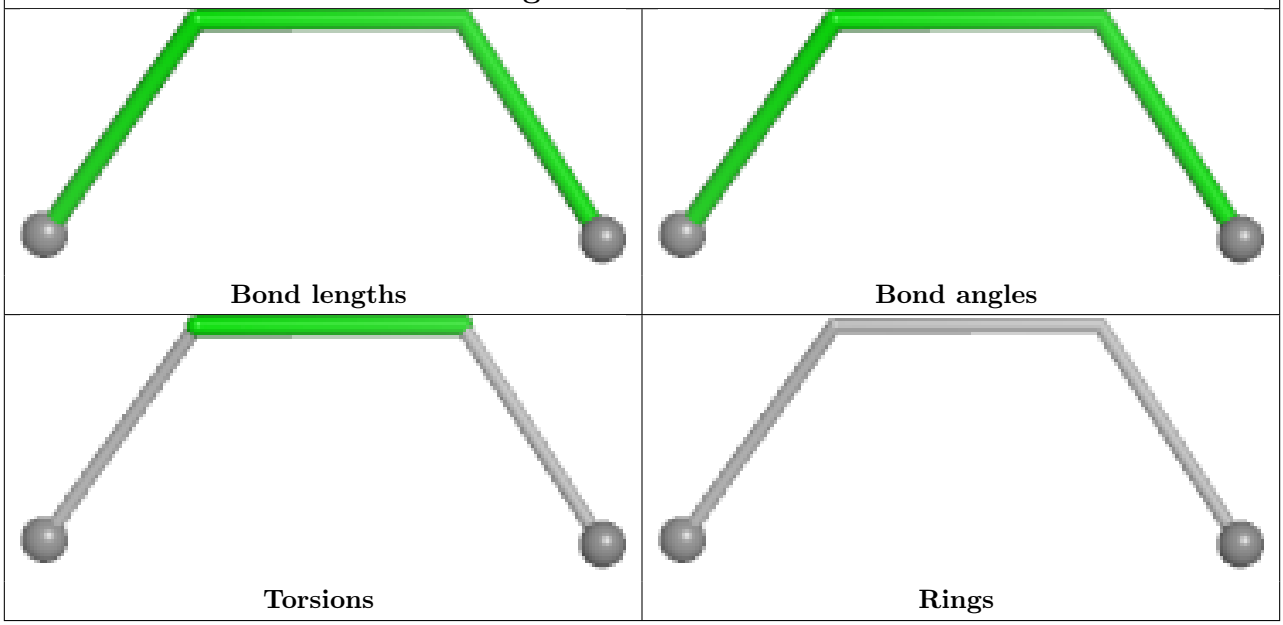
No monomer is involved in short contacts.

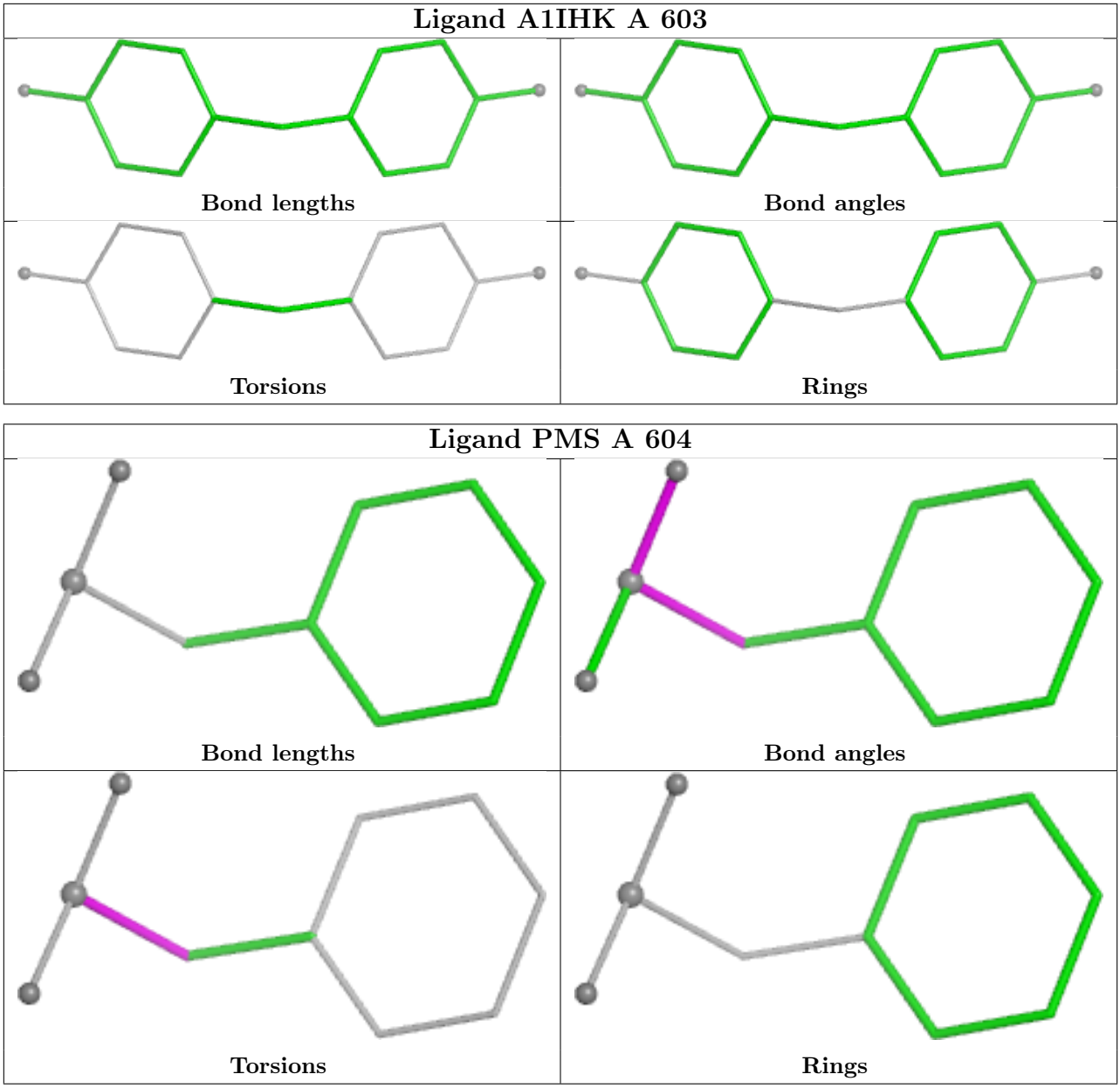
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand GOL A 601



Ligand EDO A 602





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, 95^{th} 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	507/530 (95%)	-0.22	10 (1%) 65 66	12, 21, 36, 51	0
2	B	0/5	-	-	-	-
All	All	507/535 (94%)	-0.22	10 (1%) 65 66	12, 21, 36, 51	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	LEU	3.6
1	A	69	LEU	3.4
1	A	275	PHE	2.8
1	A	142	PHE	2.7
1	A	71	GLY	2.7
1	A	415	PHE	2.4
1	A	70	MET	2.3
1	A	145	VAL	2.3
1	A	66	ARG	2.2
1	A	399	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

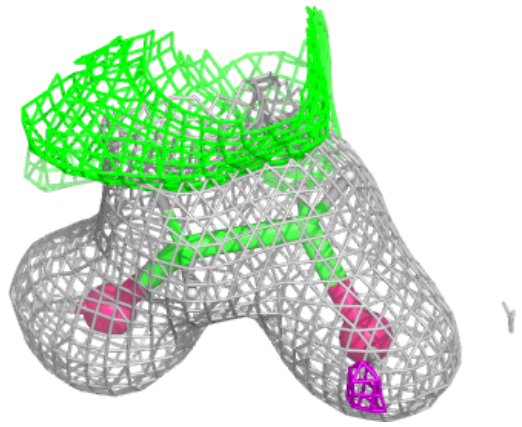
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

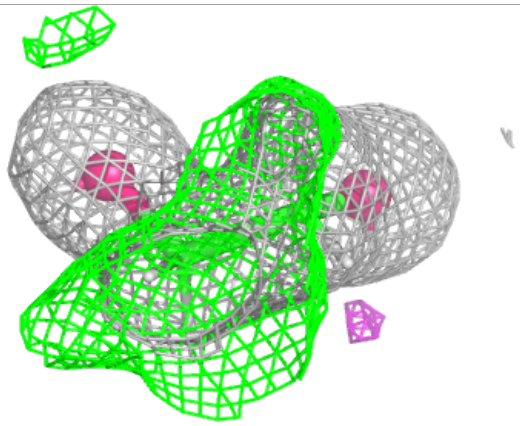
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	602	4/4	0.96	0.06	18,22,27,27	0
3	GOL	A	601	6/6	0.98	0.04	17,20,22,26	0
5	A1IHK	A	603	15/15	-	-	18,24,29,33	29
6	PMS	A	604	10/11	-	-	19,19,19,19	10

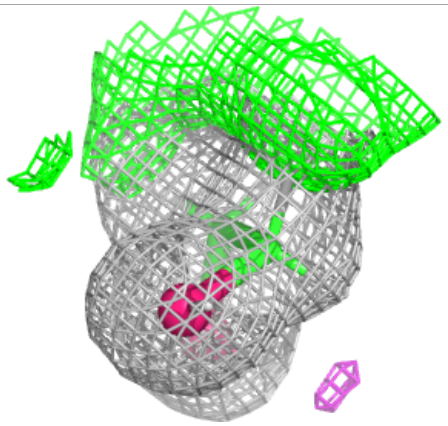
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO A 602:

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

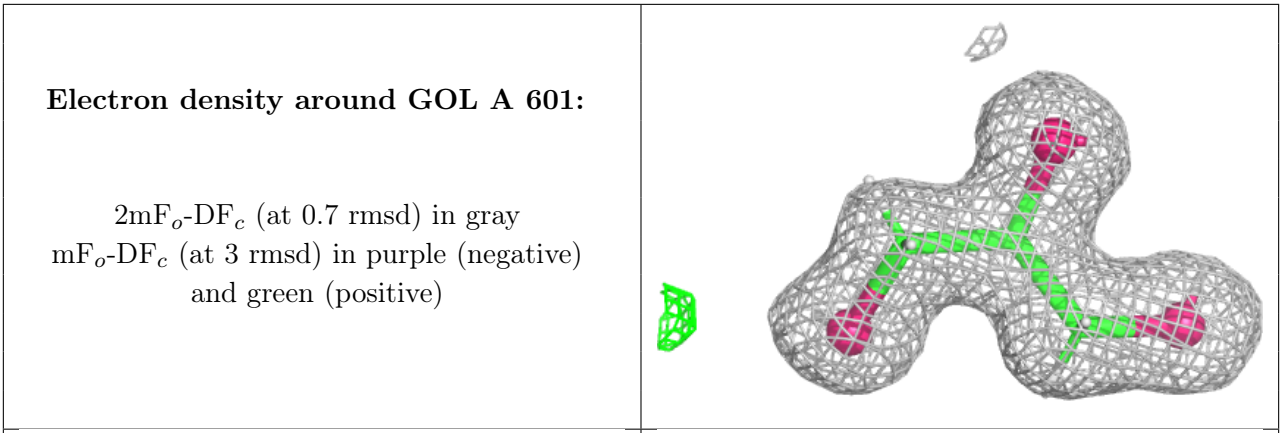


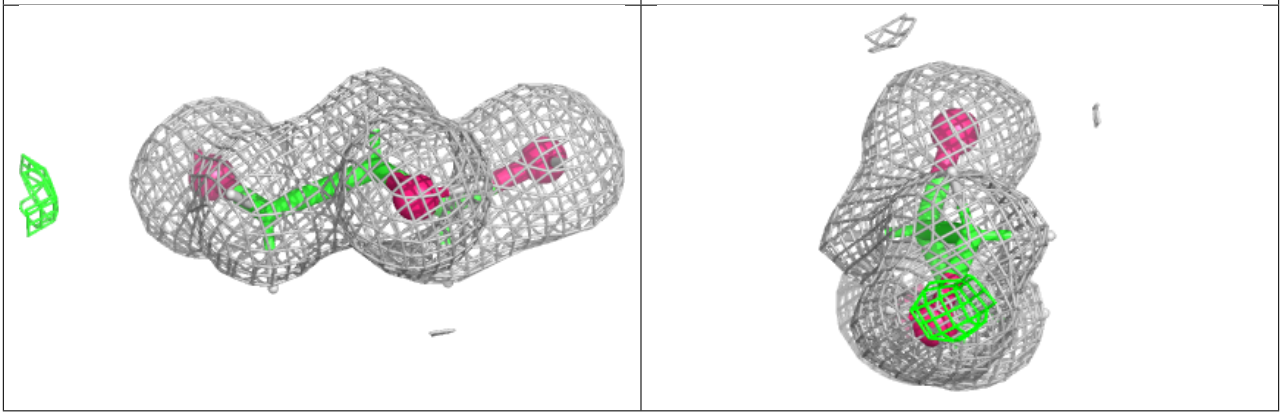




Electron density around GOL A 601:

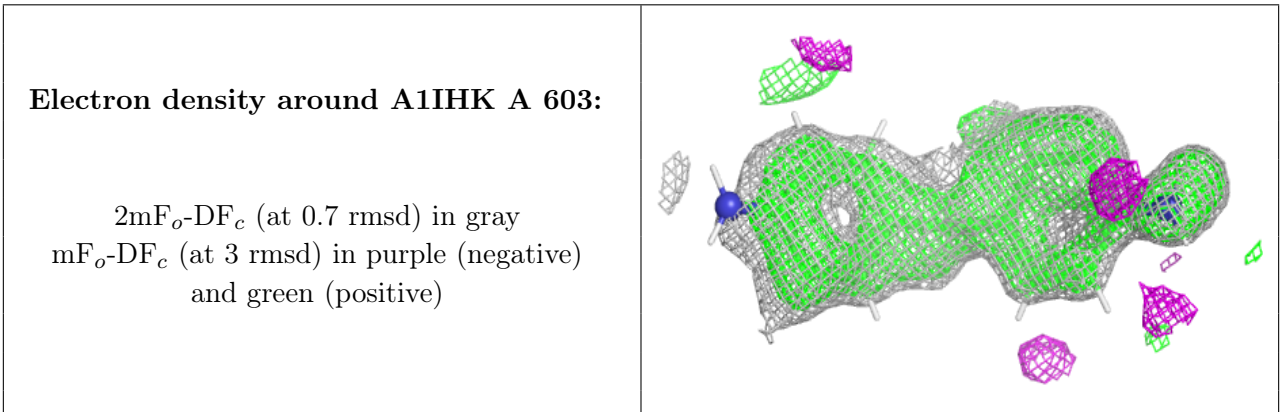
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

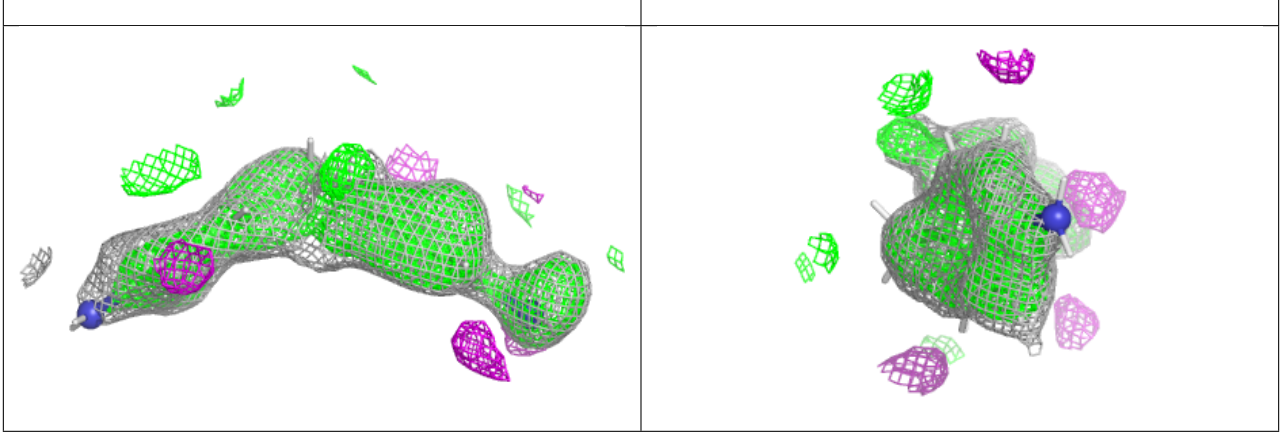




Electron density around A1IHK A 603:

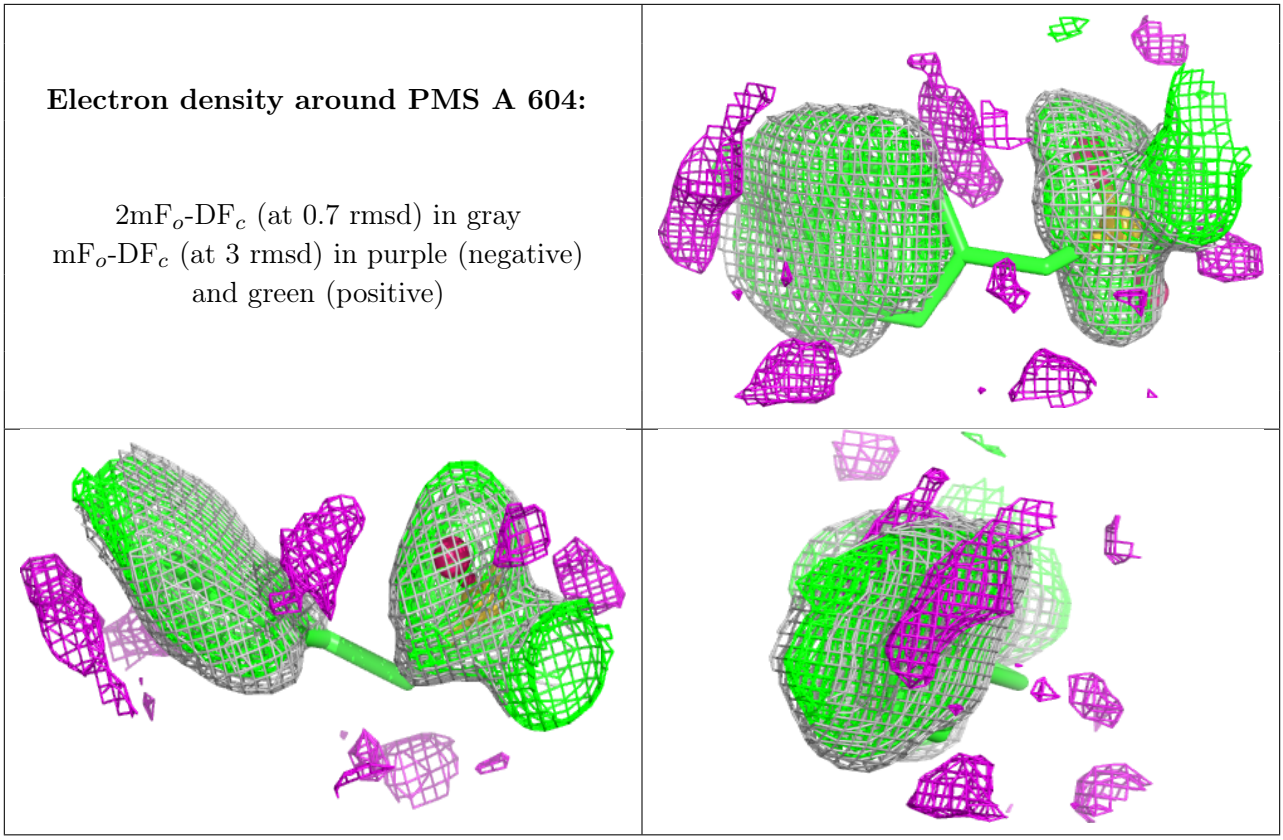
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around PMS A 604:

$2mF_o$-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.