

wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2024 – 02:33 PM EDT

PDB ID	:	9B2P
Title	:	Structure of the quorum quenching lactonase GcL D122N mutant - bimetallic
		metal center - C2 space group
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Deposited on	:	2024-03-15
Resolution	:	2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

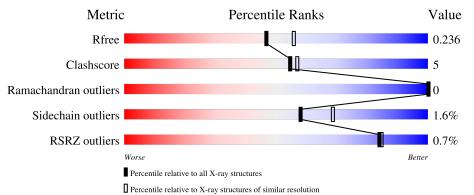
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.25 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	А	276	90%	9%	•
1	Р	276	87%	12%	•
1	Х	276	89%	10%	•



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6947 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.

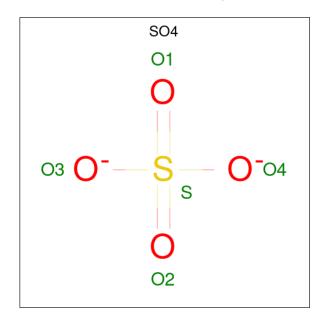
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	1 1	976	Total	С	Ν	0	S	0	0	0
	A	276	2237	1423	391	409	14			
1	D	275	Total	С	Ν	0	S	0	3	0
		215	2257	1435	395	413	14			
1	v	276	Total	С	Ν	0	S	0	2	0
	270	2257	1434	397	412	14	0		U	

• Molecule 1 is a protein called quorum-quenching N-acyl-homoserine lactonase.

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	122	ASN	ASP	engineered mutation	UNP A0A023DFE8
Р	122	ASN	ASP	engineered mutation	UNP A0A023DFE8
Х	122	ASN	ASP	engineered mutation	UNP A0A023DFE8

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Р	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Р	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Х	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Х	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

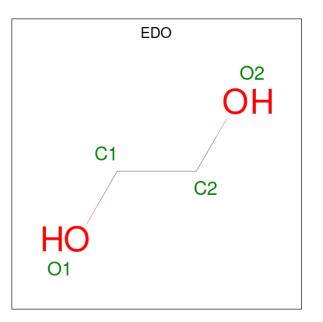
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Co 1 1	0	0
3	Р	1	Total Co 1 1	0	0
3	Х	1	Total Co 1 1	0	0

• Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Fe 1 1	0	0
4	Р	1	Total Fe 1 1	0	0
4	Х	1	Total Fe 1 1	0	0

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Р	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Р	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 6 is water.

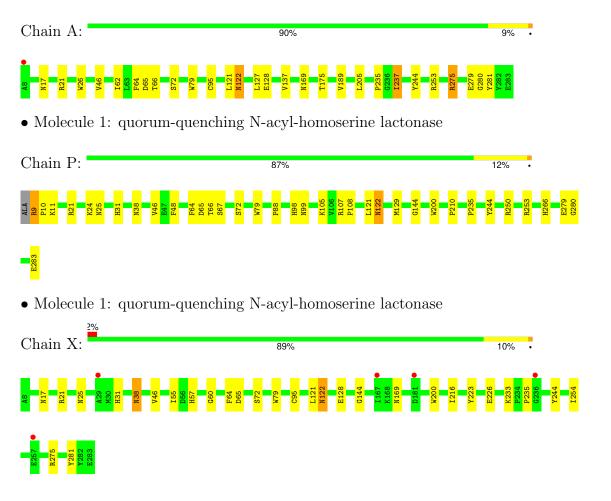
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0
6	Р	49	Total O 49 49	0	0
6	Х	46	Total O 46 46	0	0



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: quorum-quenching N-acyl-homoserine lactonase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	160.77Å 109.11Å 97.17Å	Denesiten
a, b, c, α , β , γ	90.00° 116.42° 90.00°	Depositor
Resolution (Å)	73.93 - 2.25	Depositor
Resolution (A)	73.93 - 2.25	EDS
% Data completeness	98.7 (73.93-2.25)	Depositor
(in resolution range)	98.4 (73.93-2.25)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.37 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
D D	0.208 , 0.234	Depositor
R, R_{free}	0.212 , 0.236	DCC
R_{free} test set	3516 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.3	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 29.2	EDS
L-test for twinning ²	$< L > = 0.51, < L^2 > = 0.35$	Xtriage
	0.437 for -1/2 *h+1/2 *k+l, 1/2 *h-1/2 *k+l, 1	
Estimated twinning fraction	/2*h+1/2*k 0.439 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2	Xtriage
	0.439 for $-1/2$ *h $-1/2$ *k $+1,-1/2$ *h $-1/2$ *k $-1,1/2$	11011080
E.E. completion	*h-1/2*k	EDC
F_o, F_c correlation	0.96	EDS
Total number of atoms	6947	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: FE, EDO, CO, SO4

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/2300	0.50	0/3122	
1	Р	0.27	0/2323	0.49	0/3151	
1	Х	0.27	0/2320	0.50	0/3148	
All	All	0.27	0/6943	0.50	0/9421	

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	А	0	1
1	Р	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	275	ARG	Sidechain
1	Р	107	ARG	Sidechain

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2237	0	2153	18	0
1	Р	2257	0	2168	25	0
1	Х	2257	0	2172	20	0
2	А	10	0	0	0	0
2	Р	10	0	0	0	0
2	Х	10	0	0	0	0
3	А	1	0	0	0	0
3	Р	1	0	0	0	0
3	Х	1	0	0	0	0
4	А	1	0	0	0	0
4	Р	1	0	0	0	0
4	Х	1	0	0	0	0
5	Р	8	0	12	0	0
6	А	57	0	0	0	0
6	Р	49	0	0	0	0
6	Х	46	0	0	1	0
All	All	6947	0	6505	62	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 5.

The worst 5 of 62 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:P:122:ASN:HD22	1:P:122:ASN:H	1.46	0.62
1:A:280:GLY:HA3	1:P:280:GLY:HA3	1.84	0.59
1:P:9:ARG:NE	1:P:9:ARG:HA	2.16	0.59
1:X:55:ILE:HD12	1:X:55:ILE:N	2.20	0.57
1:P:121:LEU:H	1:P:121:LEU:HD23	1.69	0.56

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	А	274/276~(99%)	264 (96%)	10 (4%)	0	100	100
1	Р	275/276~(100%)	266 (97%)	9 (3%)	0	100	100
1	Х	276/276~(100%)	265 (96%)	11 (4%)	0	100	100
All	All	825/828~(100%)	795 (96%)	30 (4%)	0	100	100

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

There are no Ramachandran outliers to report.

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	Perce	ntiles
1	А	236/236~(100%)	233~(99%)	3~(1%)	65	74
1	Р	239/236~(101%)	234 (98%)	5(2%)	48	57
1	Х	238/236~(101%)	235~(99%)	3 (1%)	65	74
All	All	713/708 (101%)	702~(98%)	11 (2%)	58	70

5 of 11 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	Р	279	GLU
1	Х	38	ASN
1	Х	223	TYR
1	Х	122	ASN
1	Р	38	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such side chains are listed below:

Mol	Chain	Res	Type
1	Х	69	ASN
1	Х	38	ASN
1	Р	69	ASN

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Mol	Chain	Res	Type
1	Х	31	HIS
1	Р	38	ASN

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 (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	Turne	Chain	in Res Link		Bond lengths			Bond angles		
	Type	Chain	Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	Р	302	-	4,4,4	0.35	0	$6,\!6,\!6$	0.08	0
5	EDO	Р	304	-	3,3,3	0.07	0	$2,\!2,\!2$	0.14	0
5	EDO	Р	303	-	3,3,3	0.07	0	$2,\!2,\!2$	0.15	0
2	SO4	Х	302	-	4,4,4	0.34	0	$6,\!6,\!6$	0.08	0
2	SO4	А	301	-	4,4,4	0.34	0	$6,\!6,\!6$	0.06	0
2	SO4	Р	301	-	4,4,4	0.33	0	$6,\!6,\!6$	0.08	0
2	SO4	А	302	-	4,4,4	0.34	0	$6,\!6,\!6$	0.07	0
2	SO4	Х	301	-	4,4,4	0.34	0	$6,\!6,\!6$	0.08	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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	Р	303	-	-	0/1/1/1	-
5	EDO	Р	304	-	-	0/1/1/1	-

'-' means no outliers of that kind were identified.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	А	276/276~(100%)	-0.36	1 (0%) 89 90	18, 53, 80, 101	11 (3%)
1	Р	275/276~(99%)	-0.49	0 100 100	19, 53, 78, 102	12 (4%)
1	Х	$276/276\ (100\%)$	-0.50	5 (1%) 67 68	19, 53, 81, 106	11 (3%)
All	All	827/828~(99%)	-0.45	6 (0%) 84 85	18, 53, 80, 106	34 (4%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Х	236	GLY	2.6
1	Х	29	ALA	2.5
1	А	8	ALA	2.2
1	Х	167	ILE	2.2
1	Х	181	ASP	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

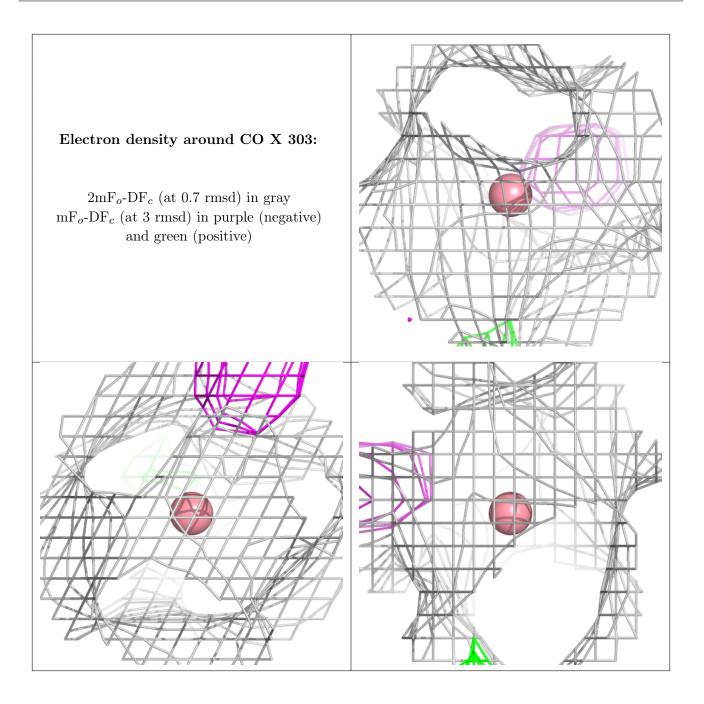
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



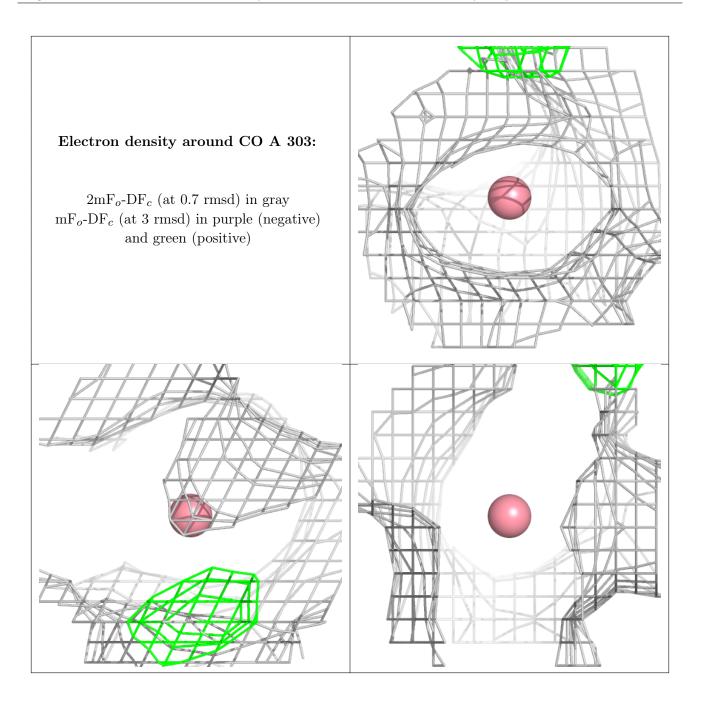
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
2	SO4	Х	301	5/5	0.97	0.09	$55,\!56,\!59,\!64$	5
2	SO4	А	302	5/5	0.98	0.07	67,74,81,100	0
2	SO4	Р	301	5/5	0.98	0.05	69,70,76,80	0
2	SO4	Р	302	5/5	0.98	0.06	45,60,64,72	5
2	SO4	А	301	5/5	0.98	0.07	56,59,62,66	5
2	SO4	Х	302	5/5	0.98	0.06	$65,\!80,\!88,\!98$	0
5	EDO	Р	303	4/4	0.98	0.10	66,68,69,72	0
5	EDO	Р	304	4/4	0.98	0.08	70,80,81,82	0
3	CO	Х	303	1/1	1.00	0.02	48,48,48,48	0
4	FE	А	304	1/1	1.00	0.02	41,41,41,41	0
4	FE	Р	306	1/1	1.00	0.02	42,42,42,42	0
4	FE	Х	304	1/1	1.00	0.04	41,41,41,41	0
3	CO	А	303	1/1	1.00	0.01	48,48,48,48	0
3	CO	Р	305	1/1	1.00	0.01	46,46,46,46	0

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

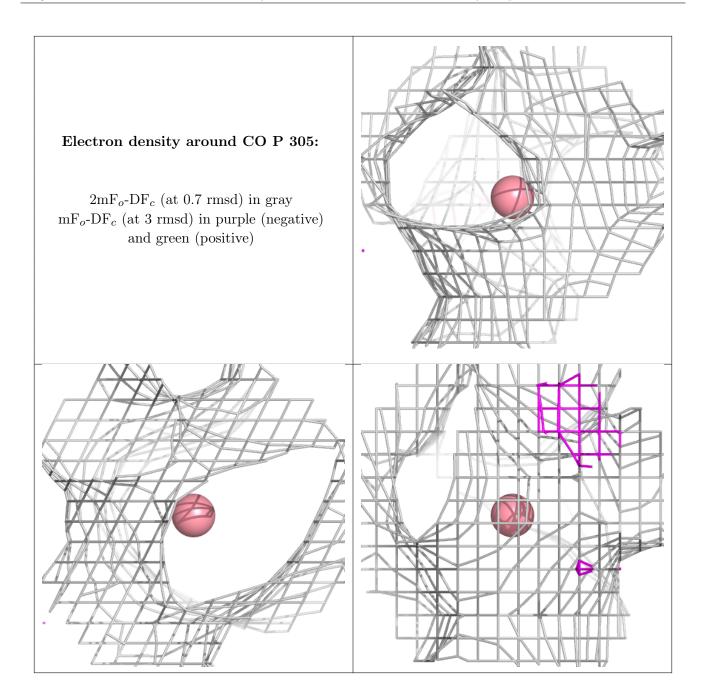












6.5 Other polymers (i)

There are no such residues in this entry.

