



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:39 AM UTC

PDB ID : 8R2X / pdb_00008r2x
Title : Crystal structure of hydroxyquinol-1,2-dioxygenase from *Rhodococcus jostii* RHA1 (RjTsdC)
Authors : Zahn, M.; Kuatsjah, E.; Salvachua, D.
Deposited on : 2023-11-07
Resolution : 1.57 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

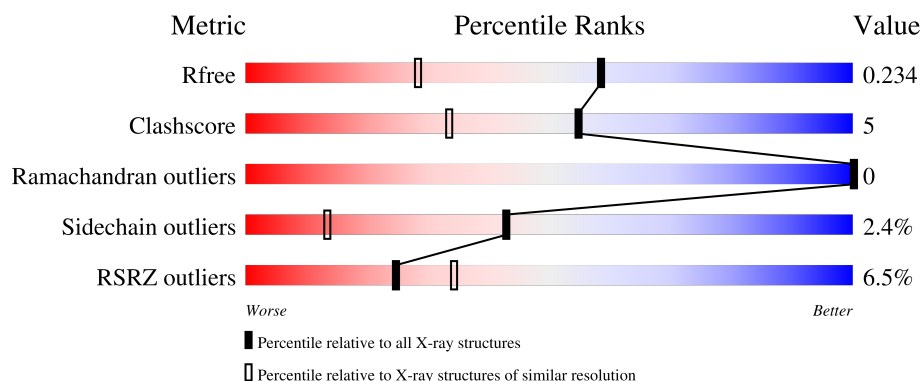
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	302	5% 80% 10% • 8%
1	B	302	7% 79% 12% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4775 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 6-chlorohydroxyquinol-1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	1	0
			2166	1356	379	422	9			
1	B	277	Total	C	N	O	S	0	1	0
			2163	1354	379	421	9			

There are 40 discrepancies between the modelled and reference sequences:

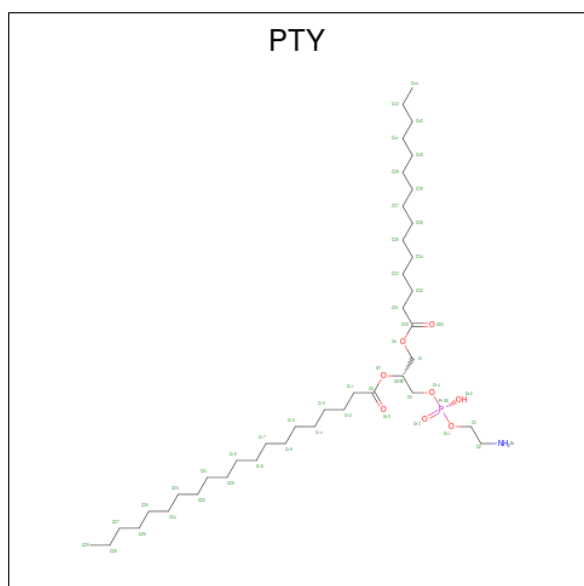
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q0SFL8
A	-18	GLY	-	expression tag	UNP Q0SFL8
A	-17	SER	-	expression tag	UNP Q0SFL8
A	-16	SER	-	expression tag	UNP Q0SFL8
A	-15	HIS	-	expression tag	UNP Q0SFL8
A	-14	HIS	-	expression tag	UNP Q0SFL8
A	-13	HIS	-	expression tag	UNP Q0SFL8
A	-12	HIS	-	expression tag	UNP Q0SFL8
A	-11	HIS	-	expression tag	UNP Q0SFL8
A	-10	HIS	-	expression tag	UNP Q0SFL8
A	-9	SER	-	expression tag	UNP Q0SFL8
A	-8	SER	-	expression tag	UNP Q0SFL8
A	-7	GLY	-	expression tag	UNP Q0SFL8
A	-6	LEU	-	expression tag	UNP Q0SFL8
A	-5	VAL	-	expression tag	UNP Q0SFL8
A	-4	PRO	-	expression tag	UNP Q0SFL8
A	-3	ARG	-	expression tag	UNP Q0SFL8
A	-2	GLY	-	expression tag	UNP Q0SFL8
A	-1	SER	-	expression tag	UNP Q0SFL8
A	0	HIS	-	expression tag	UNP Q0SFL8
B	-19	MET	-	initiating methionine	UNP Q0SFL8
B	-18	GLY	-	expression tag	UNP Q0SFL8
B	-17	SER	-	expression tag	UNP Q0SFL8
B	-16	SER	-	expression tag	UNP Q0SFL8
B	-15	HIS	-	expression tag	UNP Q0SFL8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q0SFL8
B	-13	HIS	-	expression tag	UNP Q0SFL8
B	-12	HIS	-	expression tag	UNP Q0SFL8
B	-11	HIS	-	expression tag	UNP Q0SFL8
B	-10	HIS	-	expression tag	UNP Q0SFL8
B	-9	SER	-	expression tag	UNP Q0SFL8
B	-8	SER	-	expression tag	UNP Q0SFL8
B	-7	GLY	-	expression tag	UNP Q0SFL8
B	-6	LEU	-	expression tag	UNP Q0SFL8
B	-5	VAL	-	expression tag	UNP Q0SFL8
B	-4	PRO	-	expression tag	UNP Q0SFL8
B	-3	ARG	-	expression tag	UNP Q0SFL8
B	-2	GLY	-	expression tag	UNP Q0SFL8
B	-1	SER	-	expression tag	UNP Q0SFL8
B	0	HIS	-	expression tag	UNP Q0SFL8

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Fe 1	0	0
3	B	1	Total 1	Fe 1	0	0

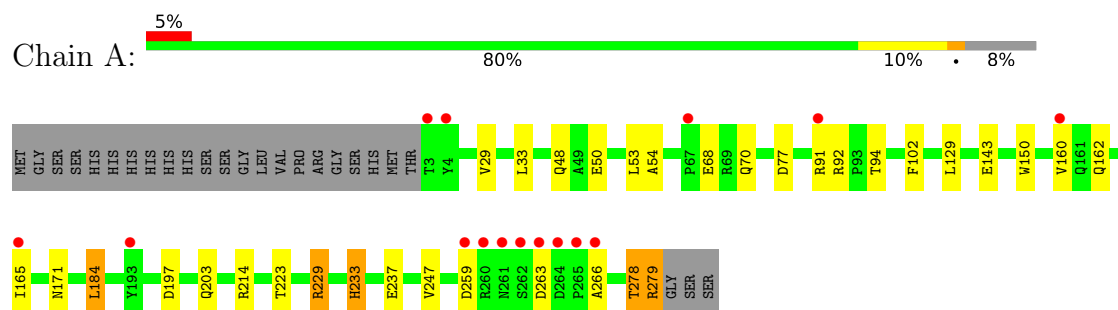
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total 188	O 188	0	0
4	B	156	Total 156	O 156	0	0

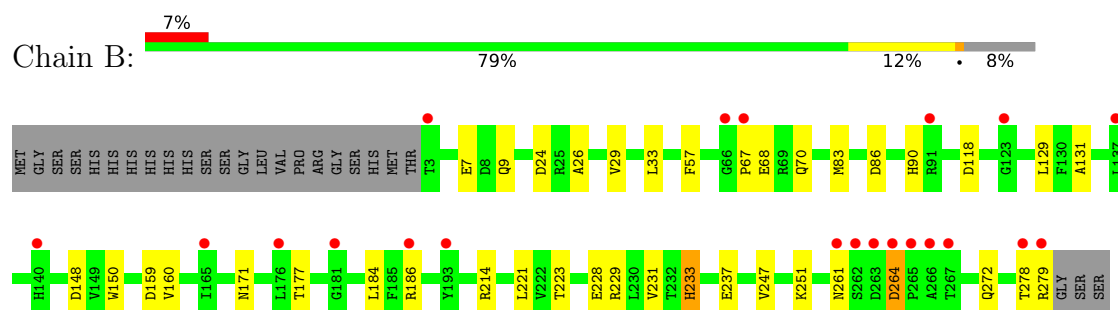
3 Residue-property plots [i](#)

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: 6-chlorohydroxyquinol-1,2-dioxygenase



- Molecule 1: 6-chlorohydroxyquinol-1,2-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.61Å 107.41Å 117.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.38 – 1.57 79.38 – 1.57	Depositor EDS
% Data completeness (in resolution range)	53.5 (79.38-1.57) 53.5 (79.38-1.57)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.182 , 0.228 0.192 , 0.234	Depositor DCC
R_{free} test set	2165 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4775	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: PTY, FE

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	0.67	0/2221	1.05	9/3021 (0.3%)
1	B	0.63	0/2218	1.00	6/3017 (0.2%)
All	All	0.65	0/4439	1.03	15/6038 (0.2%)

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	HIS	CA-CB-CG	10.32	124.12	113.80
1	A	233	HIS	CA-CB-CG	9.76	123.56	113.80
1	A	233	HIS	CB-CG-CD2	-8.96	119.56	131.20
1	B	233	HIS	CB-CG-CD2	-7.86	120.98	131.20
1	A	233	HIS	CB-CG-ND1	7.63	134.14	122.70
1	B	233	HIS	CB-CG-ND1	6.21	132.01	122.70
1	A	233	HIS	CB-CA-C	-6.06	96.74	110.07
1	B	24	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	233	HIS	CB-CA-C	-5.85	97.20	110.07
1	A	278	THR	CB-CA-C	-5.69	98.96	109.37
1	A	102	PHE	CA-CB-CG	5.63	119.43	113.80
1	B	159	ASP	CA-CB-CG	5.45	118.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CB-CA-C	5.44	118.73	109.75
1	A	48	GLN	CB-CG-CD	5.18	121.40	112.60
1	A	77	ASP	CA-CB-CG	5.16	117.76	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	ARG	Sidechain
1	A	279	ARG	Sidechain
1	A	92	ARG	Sidechain
1	B	278	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	2166	0	2047	21	0
1	B	2163	0	2046	22	0
2	A	50	0	79	5	0
2	B	50	0	79	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	188	0	0	8	1
4	B	156	0	0	2	1
All	All	4775	0	4251	42	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 5.

All (42) 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:143:GLU:OE1	4:A:401:HOH:O	1.98	0.82
1:A:29:VAL:HG11	2:B:301:PTY:H171	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NH2	1:B:7:GLU:OE2	2.19	0.74
1:A:129:LEU:HD11	1:A:184:LEU:HD11	1.72	0.70
1:A:237:GLU:HB3	4:A:527:HOH:O	1.92	0.69
1:A:223:THR:HG22	1:A:229:ARG:HG3	1.77	0.66
1:B:57:PHE:CD2	2:B:301:PTY:H332	2.31	0.66
1:B:223:THR:HG22	1:B:229:ARG:HG3	1.79	0.63
2:A:301:PTY:H121	1:B:26:ALA:HB2	1.82	0.62
1:B:86:ASP:O	1:B:90:HIS:HD2	1.83	0.61
1:B:237:GLU:OE2	4:B:401:HOH:O	2.17	0.59
1:B:129:LEU:HD11	1:B:184:LEU:HD11	1.85	0.58
2:A:301:PTY:H181	1:B:29:VAL:HG11	1.86	0.58
1:B:261:ASN:HB3	1:B:264:ASP:OD1	2.03	0.58
1:B:214:ARG:NE	1:B:247:VAL:HG22	2.19	0.57
1:B:57:PHE:CG	2:B:301:PTY:H332	2.39	0.57
1:A:54:ALA:HB2	2:A:301:PTY:H202	1.87	0.57
1:A:266:ALA:HB2	4:A:418:HOH:O	2.04	0.57
1:B:228:GLU:OE1	1:B:279:ARG:NH2	2.39	0.56
1:B:177:THR:O	4:B:402:HOH:O	2.18	0.55
1:B:33:LEU:C	1:B:33:LEU:HD23	2.33	0.53
1:A:33:LEU:C	1:A:33:LEU:HD23	2.35	0.52
1:A:50:GLU:HG2	2:A:301:PTY:H152	1.91	0.52
1:B:83:MET:HE1	1:B:251:LYS:HE3	1.92	0.52
1:A:279:ARG:NH1	4:A:405:HOH:O	2.42	0.51
1:A:94:THR:OG1	4:A:402:HOH:O	2.19	0.51
1:A:203:GLN:NE2	2:A:301:PTY:H312	2.27	0.50
1:A:214:ARG:NE	1:A:247:VAL:HG22	2.27	0.49
1:B:221:LEU:HD13	1:B:231:VAL:HG22	1.98	0.45
1:B:118:ASP:HB2	1:B:186:ARG:HH11	1.81	0.45
1:B:68:GLU:HB2	1:B:160:VAL:O	2.17	0.44
1:A:91:ARG:HG3	1:A:91:ARG:NH1	2.32	0.44
1:A:68:GLU:HB2	1:A:160:VAL:O	2.19	0.43
1:A:197:ASP:OD1	4:A:403:HOH:O	2.21	0.43
1:A:266:ALA:N	4:A:418:HOH:O	2.50	0.43
1:B:150:TRP:HA	1:B:171:ASN:O	2.20	0.42
1:A:162:GLN:HB3	1:A:165:ILE:HB	2.02	0.41
1:B:214:ARG:HE	1:B:247:VAL:HG22	1.83	0.41
1:B:148:ASP:HB3	1:B:221:LEU:HB3	2.03	0.41
1:A:68:GLU:HG2	4:A:552:HOH:O	2.20	0.41
1:B:131:ALA:O	1:B:272:GLN:HA	2.21	0.41
1:A:150:TRP:HA	1:A:171:ASN:O	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:523:HOH:O	4:B:526:HOH:O[4_545]	2.16	0.04

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	276/302 (91%)	272 (99%)	4 (1%)	0	100	100
1	B	276/302 (91%)	268 (97%)	8 (3%)	0	100	100
All	All	552/604 (91%)	540 (98%)	12 (2%)	0	100	100

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	Percentiles	
1	A	230/250 (92%)	224 (97%)	6 (3%)	40	11
1	B	230/250 (92%)	225 (98%)	5 (2%)	45	15
All	All	460/500 (92%)	449 (98%)	11 (2%)	43	13

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	70	GLN
1	A	184	LEU
1	A	233	HIS
1	A	263	ASP
1	A	278	THR
1	B	9	GLN
1	B	67	PRO
1	B	70	GLN
1	B	233	HIS
1	B	264	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	171	ASN
1	B	171	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 4 ligands modelled in this entry, 2 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	$\# Z > 2$
2	PTY	B	301	-	49,49,49	0.39	0	52,54,54	0.43	0
2	PTY	A	301	-	49,49,49	0.43	0	52,54,54	0.85	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	B	301	-	-	27/53/53/53	-
2	PTY	A	301	-	-	28/53/53/53	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	PTY	O7-C8-C11	-4.10	102.61	111.48
2	A	301	PTY	O7-C8-O10	2.63	129.85	123.70

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PTY	N1-C2-C3-O11
2	A	301	PTY	C11-C8-O7-C6
2	B	301	PTY	N1-C2-C3-O11
2	B	301	PTY	C3-O11-P1-O12
2	B	301	PTY	C3-O11-P1-O13
2	B	301	PTY	C3-O11-P1-O14
2	A	301	PTY	C8-C11-C12-C13
2	A	301	PTY	C12-C13-C14-C15
2	A	301	PTY	C30-C31-C32-C33
2	A	301	PTY	O10-C8-O7-C6
2	B	301	PTY	C32-C33-C34-C35
2	A	301	PTY	C20-C21-C22-C23
2	A	301	PTY	C16-C17-C18-C19
2	B	301	PTY	C15-C16-C17-C18
2	B	301	PTY	C21-C22-C23-C24

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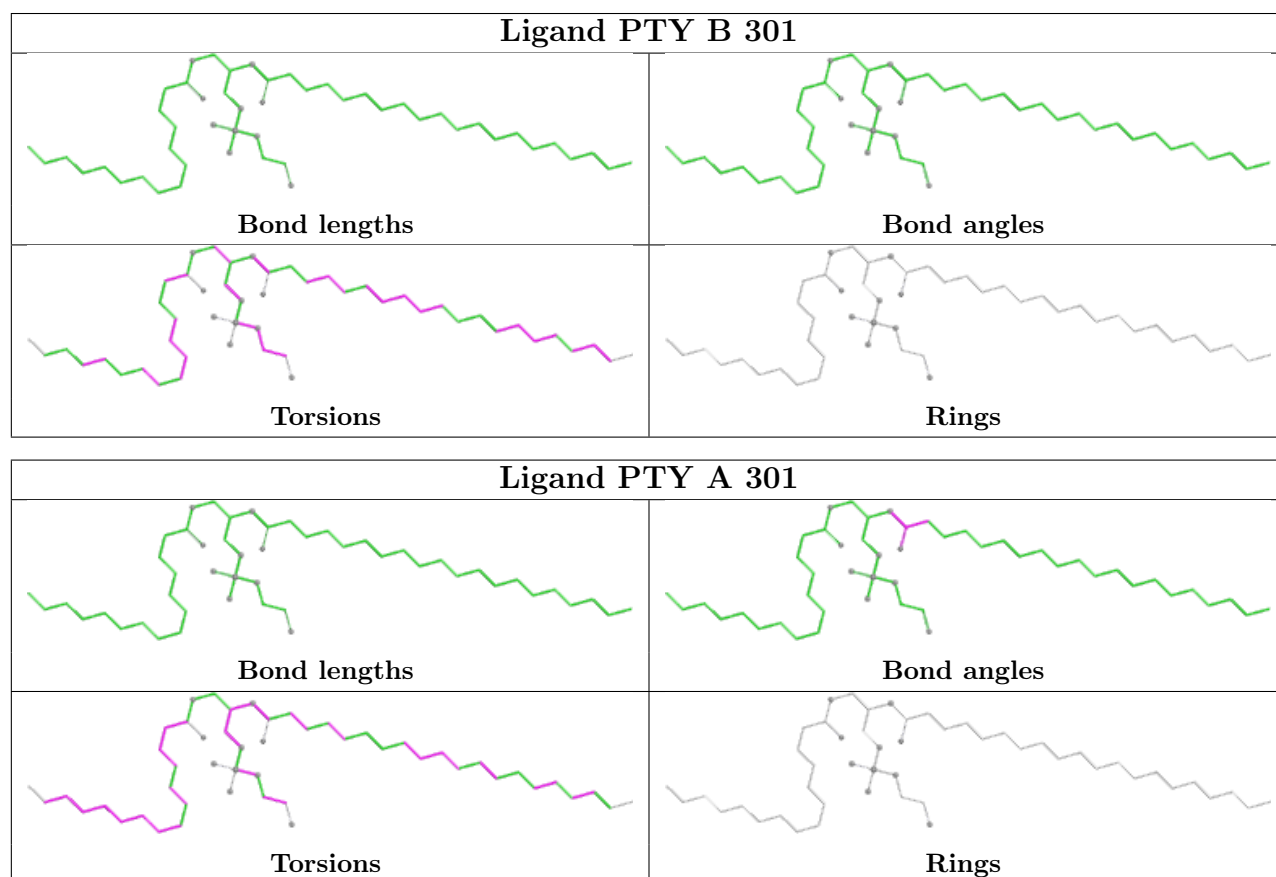
Mol	Chain	Res	Type	Atoms
2	A	301	PTY	C37-C38-C39-C40
2	B	301	PTY	C22-C23-C24-C25
2	B	301	PTY	C39-C40-C41-C42
2	B	301	PTY	C14-C15-C16-C17
2	B	301	PTY	C11-C12-C13-C14
2	A	301	PTY	C23-C24-C25-C26
2	A	301	PTY	C36-C37-C38-C39
2	B	301	PTY	C33-C34-C35-C36
2	A	301	PTY	C40-C41-C42-C43
2	A	301	PTY	C39-C40-C41-C42
2	B	301	PTY	C23-C24-C25-C26
2	A	301	PTY	C38-C39-C40-C41
2	B	301	PTY	C17-C18-C19-C20
2	A	301	PTY	C35-C36-C37-C38
2	A	301	PTY	O14-C5-C6-O7
2	A	301	PTY	C18-C19-C20-C21
2	B	301	PTY	O4-C1-C6-O7
2	B	301	PTY	C11-C8-O7-C6
2	B	301	PTY	C25-C26-C27-C28
2	A	301	PTY	O14-C5-C6-C1
2	A	301	PTY	C33-C34-C35-C36
2	A	301	PTY	C41-C42-C43-C44
2	A	301	PTY	C17-C18-C19-C20
2	B	301	PTY	C36-C37-C38-C39
2	B	301	PTY	C16-C17-C18-C19
2	B	301	PTY	O4-C1-C6-C5
2	A	301	PTY	C3-O11-P1-O12
2	A	301	PTY	C3-O11-P1-O14
2	A	301	PTY	C25-C26-C27-C28
2	A	301	PTY	C6-C5-O14-P1
2	A	301	PTY	C1-C6-O7-C8
2	A	301	PTY	C31-C32-C33-C34
2	B	301	PTY	C34-C35-C36-C37
2	B	301	PTY	C6-C5-O14-P1
2	B	301	PTY	C26-C27-C28-C29
2	A	301	PTY	O4-C30-C31-C32
2	B	301	PTY	C2-C3-O11-P1
2	B	301	PTY	C12-C13-C14-C15
2	B	301	PTY	O4-C30-C31-C32
2	B	301	PTY	O30-C30-C31-C32

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PTY	3	0
2	A	301	PTY	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/302 (91%)	0.26	15 (5%) 31 42	12, 18, 38, 116	1 (0%)
1	B	277/302 (91%)	0.62	21 (7%) 20 29	10, 23, 47, 89	1 (0%)
All	All	554/604 (91%)	0.44	36 (6%) 25 34	10, 21, 45, 116	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ALA	8.0
1	A	265	PRO	6.4
1	B	263	ASP	5.3
1	B	265	PRO	5.2
1	A	3	THR	4.2
1	A	266	ALA	4.1
1	A	264	ASP	4.0
1	B	279	ARG	4.0
1	B	267	THR	3.8
1	B	264	ASP	3.7
1	B	3	THR	3.4
1	B	165	ILE	3.4
1	A	263	ASP	3.2
1	B	193	TYR	3.2
1	A	91	ARG	3.1
1	A	262	SER	3.1
1	B	262	SER	3.0
1	A	193	TYR	3.0
1	B	67	PRO	2.9
1	A	261	ASN	2.8
1	B	278	THR	2.8
1	B	123	GLY	2.6
1	A	4	TYR	2.5
1	A	260	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	91	ARG	2.4
1	B	137	LEU	2.3
1	B	261	ASN	2.3
1	B	140	HIS	2.3
1	A	67	PRO	2.3
1	B	186	ARG	2.3
1	A	259	ASP	2.2
1	A	165	ILE	2.1
1	B	181	GLY	2.1
1	B	66	GLY	2.1
1	A	160	VAL	2.0
1	B	176	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

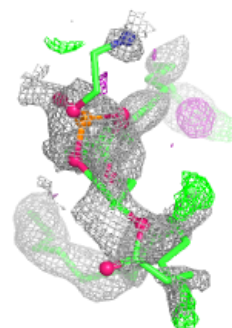
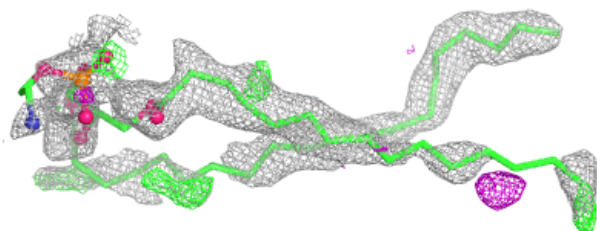
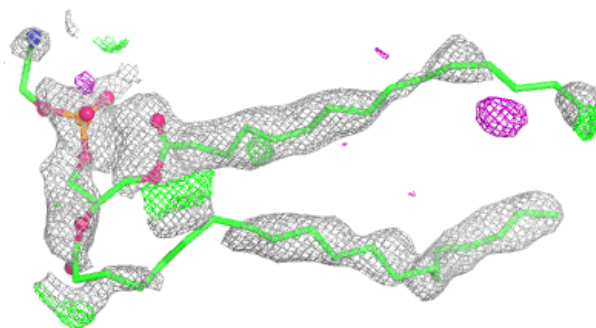
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PTY	B	301	50/50	0.76	0.22	32,52,84,96	0
2	PTY	A	301	50/50	0.78	0.21	36,49,106,132	0
3	FE	A	302	1/1	1.00	0.04	16,16,16,16	0
3	FE	B	302	1/1	1.00	0.04	19,19,19,19	0

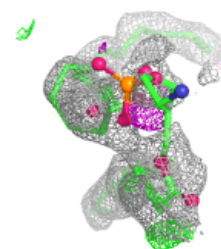
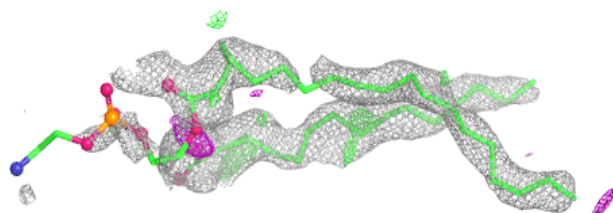
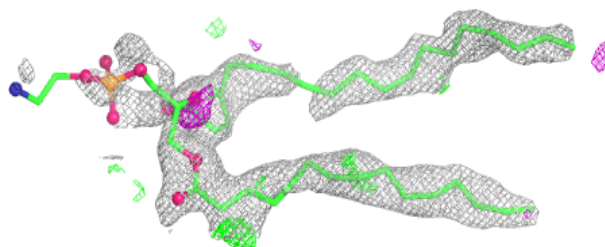
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY 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)

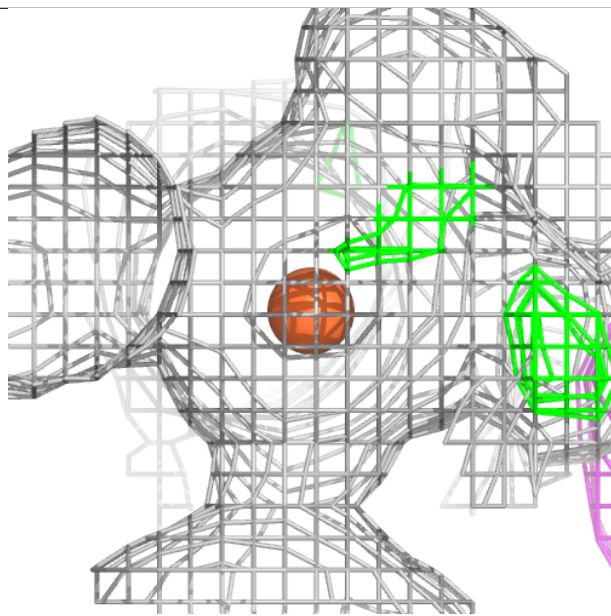
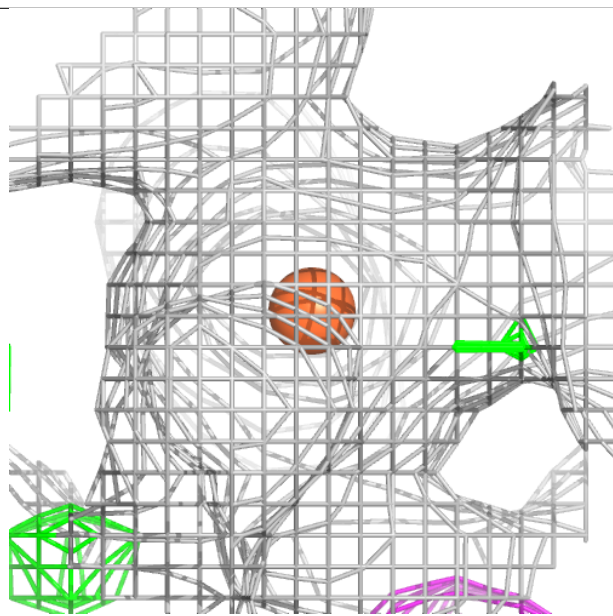
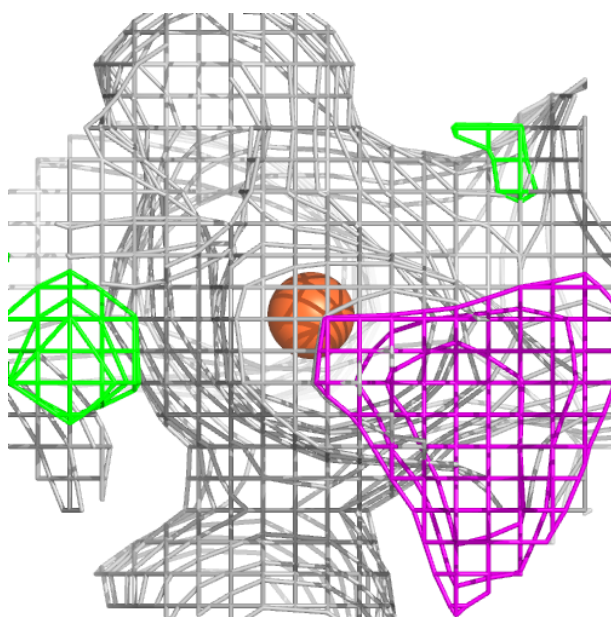
**Electron density around PTY A 301:**

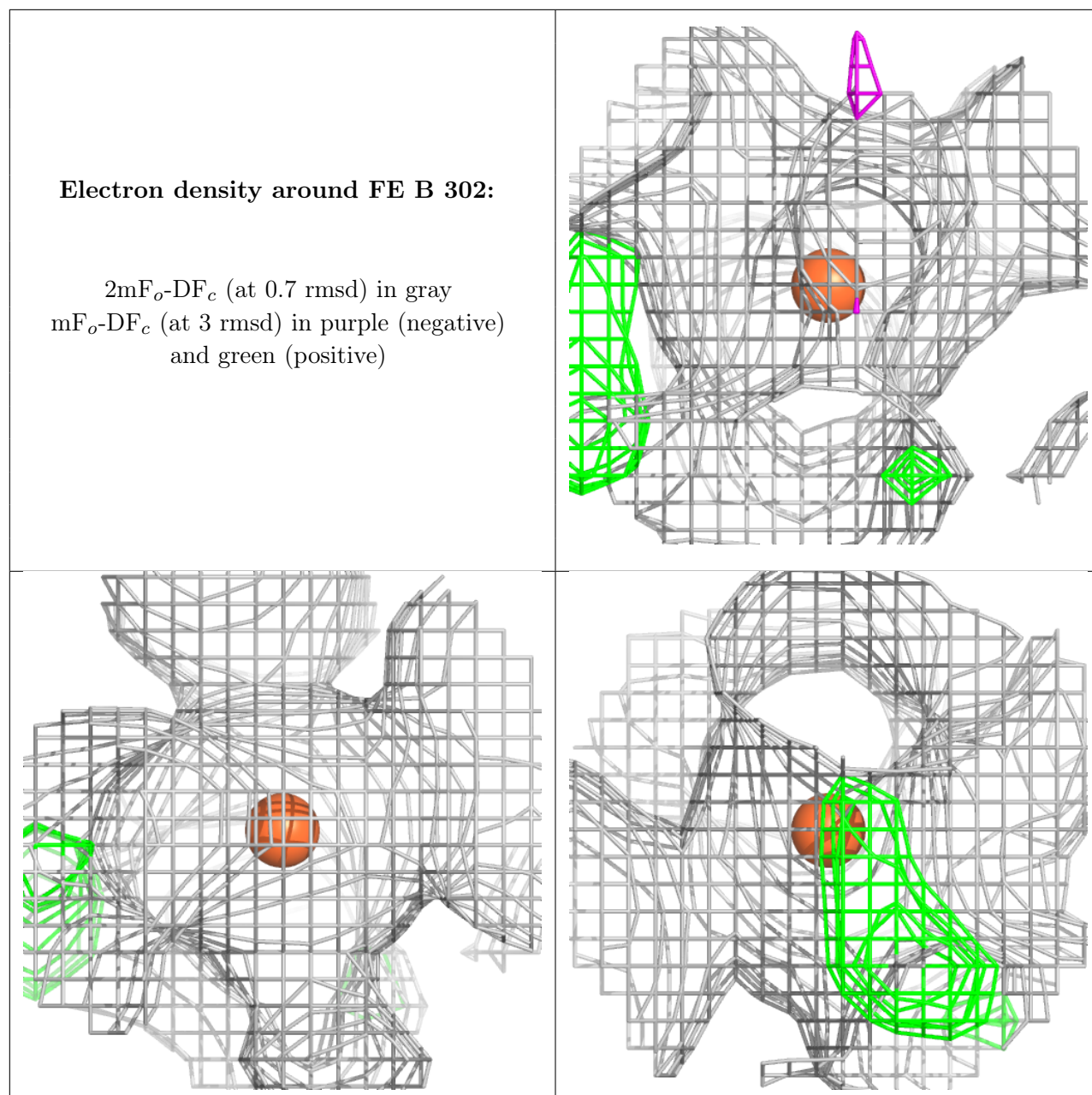
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE A 302:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.