



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 30, 2025 – 01:08 pm BST

PDB ID : 9R0Q / pdb_00009r0q
Title : Paraoxonase-1 in complex with terbium(III) and 2-hydroxyquinoline
Authors : Smerkolj, J.; Pavsic, M.; Golicnik, M.
Deposited on : 2025-04-24
Resolution : 2.35 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

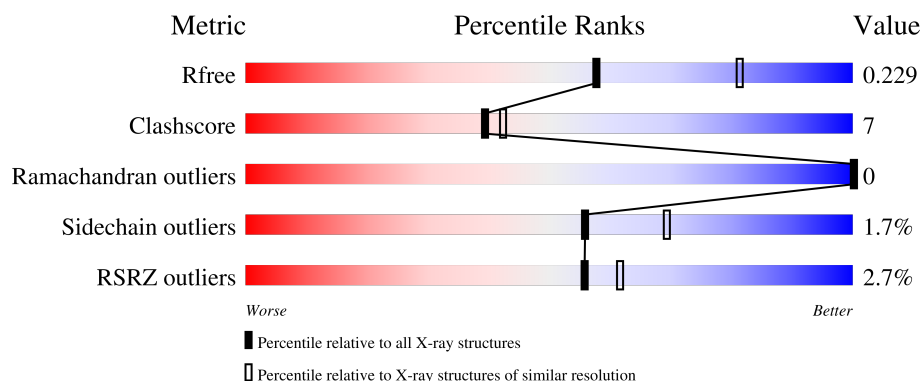
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	360	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2765 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 Serum paraoxonase/arylesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	1	0
			2677	1724	435	510	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ASP	-	expression tag	UNP P27170
A	-3	ASP	-	expression tag	UNP P27170
A	-2	ASP	-	expression tag	UNP P27170
A	-1	LYS	-	expression tag	UNP P27170
A	0	ALA	-	expression tag	UNP P27170
A	12	MET	LEU	conflict	UNP P27170
A	19	ARG	GLY	conflict	UNP P27170
A	67	SER	ALA	conflict	UNP P27170
A	82	SER	PRO	variant	UNP P27170
A	94	GLU	ASP	conflict	UNP P27170
A	96	ALA	VAL	conflict	UNP P27170
A	98	SER	LEU	conflict	UNP P27170
A	101	GLU	SER	conflict	UNP P27170
A	103	ILE	THR	conflict	UNP P27170
A	105	ASN	SER	conflict	UNP P27170
A	107	LEU	PHE	conflict	UNP P27170
A	109	ILE	LEU	conflict	UNP P27170
A	121	ILE	THR	conflict	UNP P27170
A	123	ASP	GLU	conflict	UNP P27170
A	126	THR	ILE	conflict	UNP P27170
A	130	LEU	MET	conflict	UNP P27170
A	136	GLY	ASP	conflict	UNP P27170
A	138	SER	LYS	conflict	UNP P27170
A	143	VAL	LEU	conflict	UNP P27170
A	149	GLU	LYS	conflict	UNP P27170
A	260	ARG	LYS	conflict	UNP P27170
A	261	VAL	SER	conflict	UNP P27170

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Chain	Residue	Modelled	Actual	Comment	Reference
A	263	SER	ASP	conflict	UNP P27170
A	265	ASP	ASN	conflict	UNP P27170
A	293	PHE	TYR	conflict	UNP P27170
A	296	ALA	PRO	conflict	UNP P27170
A	297	GLU	LYS	conflict	UNP P27170
A	301	GLY	ALA	conflict	UNP P27170
A	313	GLU	LYS	conflict	UNP P27170
A	320	VAL	ALA	conflict	UNP P27170
A	341	LEU	MET	conflict	UNP P27170
A	343	ILE	VAL	conflict	UNP P27170
A	354	ASP	GLU	conflict	UNP P27170

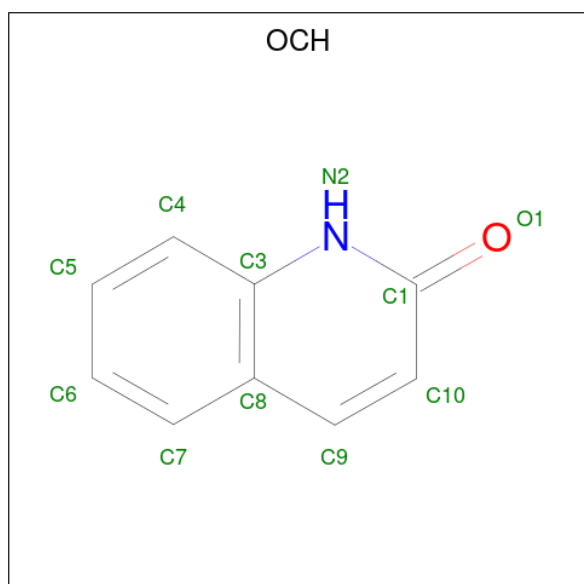
- Molecule 2 is TERBIUM(III) ION (CCD ID: TB) (formula: Tb) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Tb 2 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0

- Molecule 4 is QUINOLIN-2(1H)-ONE (CCD ID: OCH) (formula: C₉H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	9	1	1		
4	A	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 5 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Br	0	0
			2	2		

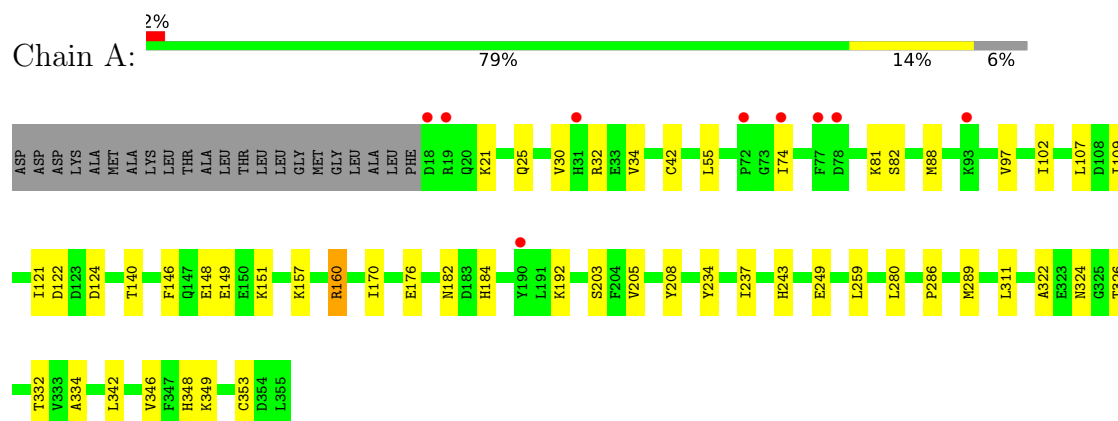
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total	O	0	0
			60	60		

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: Serum paraoxonase/arylesterase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.06Å 98.06Å 138.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.82 – 2.35 19.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.82-2.35) 99.7 (19.82-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.35Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.190 , 0.229 0.191 , 0.229	Depositor DCC
R_{free} test set	1387 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2765	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: TB, OCH, CA, BR

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	0.36	0/2750	0.54	0/3747

There are no bond length outliers.

There are no bond angle outliers.

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	2677	0	2618	35	0
2	A	2	0	0	0	0
3	A	2	0	0	0	0
4	A	22	0	14	1	0
5	A	2	0	0	0	0
6	A	60	0	0	3	0
All	All	2765	0	2632	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (35) 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:102:ILE:HG21	1:A:109:ILE:HD11	1.65	0.77
1:A:205:VAL:HG21	1:A:237:ILE:HD13	1.66	0.76
1:A:324:ASN:OD1	1:A:326:THR:HG23	1.87	0.74
1:A:149:GLU:H	1:A:149:GLU:CD	1.95	0.73
1:A:182:ASN:O	1:A:203:SER:HB2	1.97	0.65
1:A:148:GLU:O	1:A:151:LYS:HD3	1.96	0.65
1:A:140:THR:HG22	1:A:160:ARG:HG3	1.83	0.61
1:A:184:HIS:CD2	1:A:192:LYS:HB2	2.40	0.57
1:A:122:ASP:HB3	1:A:124:ASP:OD2	2.09	0.52
1:A:102:ILE:CG2	1:A:109:ILE:HD11	2.37	0.50
1:A:88:MET:CG	1:A:97:VAL:HG12	2.42	0.50
1:A:25:GLN:HG2	1:A:30:VAL:HG21	1.94	0.49
1:A:249:GLU:HG3	1:A:259:LEU:HD22	1.94	0.48
1:A:349:LYS:HB3	6:A:513:HOH:O	2.14	0.48
1:A:234:TYR:CZ	1:A:311:LEU:HD11	2.49	0.47
1:A:348:HIS:CE1	1:A:349:LYS:HG3	2.52	0.45
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.73	0.45
1:A:311:LEU:HB2	6:A:524:HOH:O	2.16	0.44
1:A:42:CYS:SG	1:A:353[B]:CYS:SG	3.13	0.44
1:A:32:ARG:NH1	1:A:286:PRO:HB3	2.34	0.43
1:A:81:LYS:HG2	1:A:82:SER:N	2.32	0.43
1:A:21:LYS:HD2	1:A:21:LYS:HA	1.64	0.43
1:A:280:LEU:HD12	1:A:280:LEU:N	2.35	0.42
1:A:107:LEU:HD23	1:A:109:ILE:CD1	2.49	0.42
1:A:157:LYS:HE2	6:A:512:HOH:O	2.18	0.42
1:A:234:TYR:CE1	1:A:311:LEU:HD11	2.54	0.42
1:A:334:ALA:HA	1:A:342:LEU:O	2.20	0.42
1:A:74:ILE:HG13	4:A:405:OCH:H7	2.01	0.42
1:A:34:VAL:CG2	1:A:322:ALA:HB1	2.50	0.41
1:A:332:THR:CG2	1:A:346:VAL:HG22	2.50	0.41
1:A:88:MET:HG3	1:A:97:VAL:HG12	2.01	0.41
1:A:208:TYR:CD1	1:A:208:TYR:C	2.99	0.41
1:A:146:PHE:CZ	1:A:148:GLU:HA	2.55	0.40
1:A:30:VAL:HG13	1:A:289:MET:HG3	2.02	0.40
1:A:55:LEU:HD12	1:A:55:LEU:C	2.47	0.40

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.

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	337/360 (94%)	321 (95%)	16 (5%)	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	302/317 (95%)	297 (98%)	5 (2%)	56	69

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ILE
1	A	160	ARG
1	A	170	ILE
1	A	176	GLU
1	A	243	HIS

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	329	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 ⓘ

Of 8 ligands modelled in this entry, 6 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
4	OCH	A	406	-	11,12,12	1.30	1 (9%)	14,16,16	2.15	3 (21%)
4	OCH	A	405	2,3	11,12,12	1.15	1 (9%)	14,16,16	1.69	2 (14%)

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	OCH	A	406	-	-	-	0/2/2/2
4	OCH	A	405	2,3	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	OCH	C1-N2	3.20	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	OCH	C1-N2	2.27	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	OCH	C3-N2-C1	5.77	125.98	117.86
4	A	405	OCH	C3-N2-C1	4.14	123.69	117.86
4	A	406	OCH	C10-C1-N2	-4.05	114.39	123.31
4	A	405	OCH	C10-C1-N2	-3.27	116.11	123.31
4	A	406	OCH	C8-C3-N2	-2.64	118.79	122.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	OCH	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/360 (93%)	-0.14	9 (2%) 56 62	28, 44, 73, 104	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ASP	3.9
1	A	190	TYR	3.5
1	A	31	HIS	3.5
1	A	72	PRO	3.4
1	A	19	ARG	2.3
1	A	78	ASP	2.3
1	A	77	PHE	2.2
1	A	74	ILE	2.1
1	A	93	LYS	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](#)

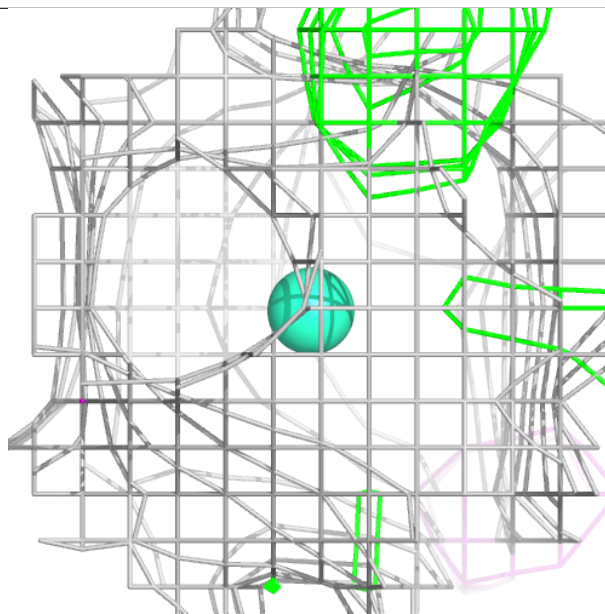
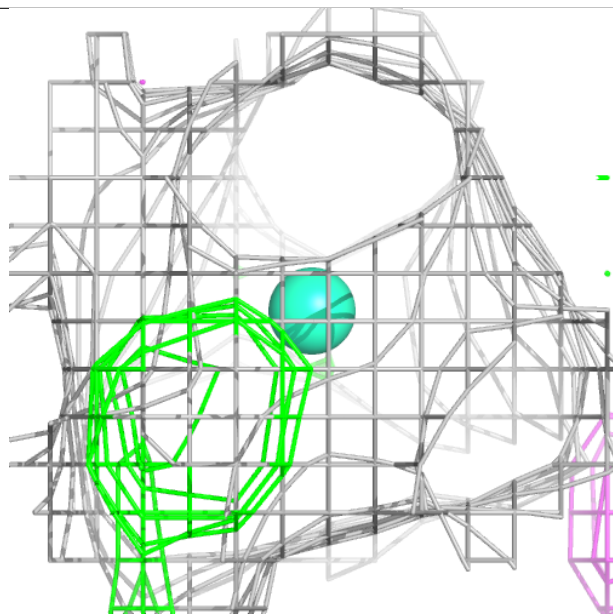
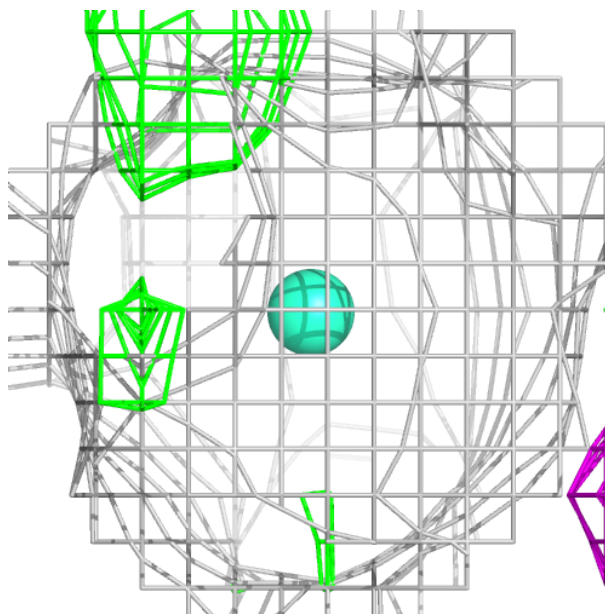
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OCH	A	406	11/11	0.67	0.23	73,79,86,89	0
4	OCH	A	405	11/11	0.89	0.19	41,55,61,61	11
5	BR	A	407	1/1	0.96	0.07	59,59,59,59	1
5	BR	A	408	1/1	0.96	0.06	65,65,65,65	1
2	TB	A	401	1/1	1.00	0.01	38,38,38,38	1
2	TB	A	402	1/1	1.00	0.03	35,35,35,35	1
3	CA	A	403	1/1	1.00	0.01	38,38,38,38	1
3	CA	A	404	1/1	1.00	0.03	35,35,35,35	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.

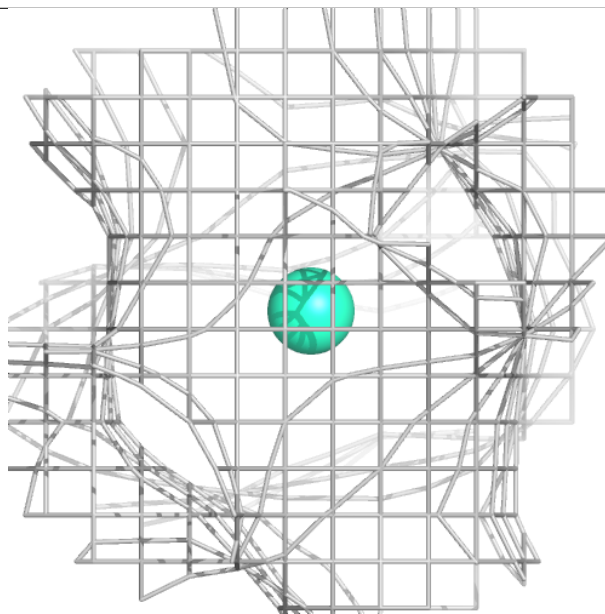
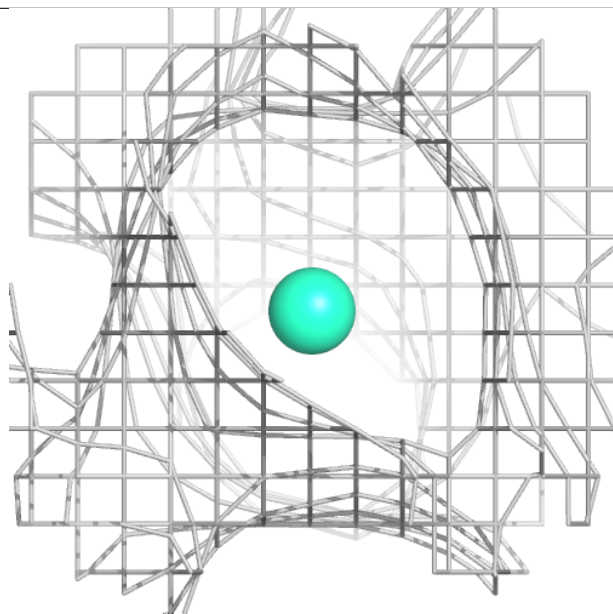
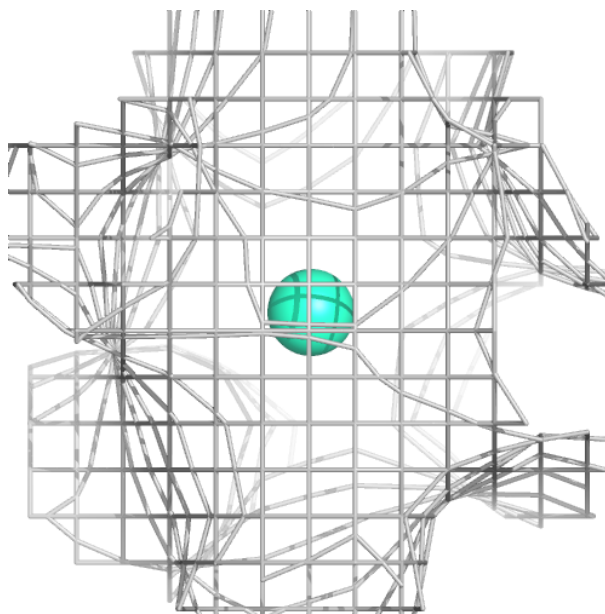
Electron density around TB A 401:

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



Electron density around TB A 402:

$2mF_o-DF_c$ (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.