



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:50 PM UTC

PDB ID : 2PRZ / pdb_00002prz
Title : S. cerevisiae orotate phosphoribosyltransferase complexed with OMP
Authors : Gonzalez-Segura, L.; Hurley, T.D.; McClard, R.W.
Deposited on : 2007-05-04
Resolution : 1.90 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

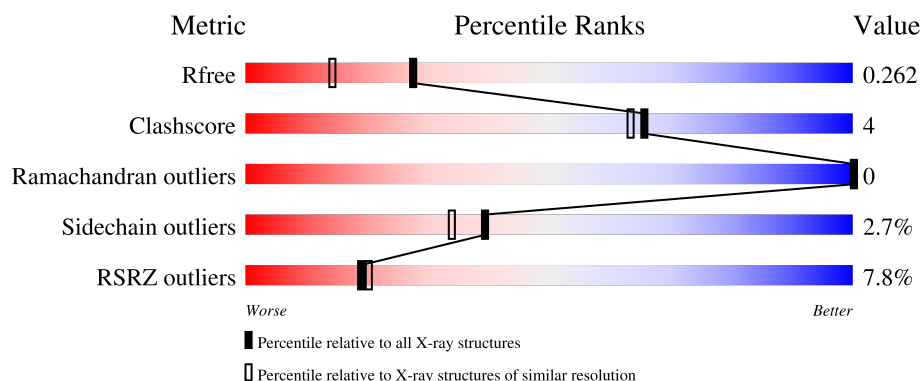
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	226	8% 87% 8% 5%
1	B	226	4% 85% 11% .
1	C	226	9% 85% 8% 5%
1	D	226	8% 90% 6% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7201 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.

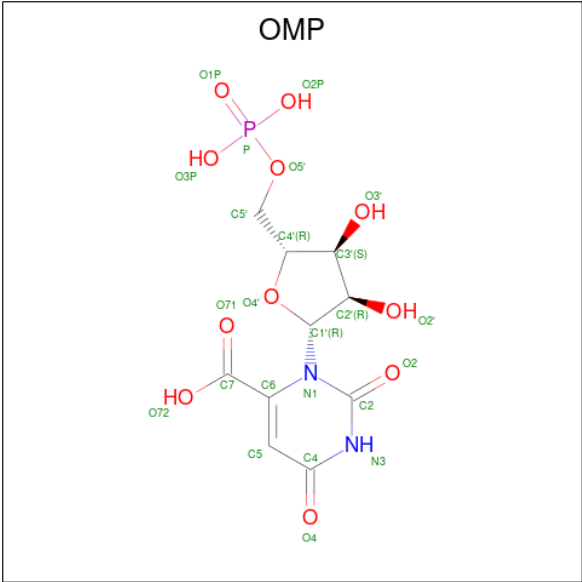
- Molecule 1 is a protein called Orotate phosphoribosyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1657	1069	270	315	3			
1	B	216	Total	C	N	O	S	0	0	0
			1669	1078	271	316	4			
1	C	215	Total	C	N	O	S	0	0	0
			1657	1069	270	315	3			
1	D	217	Total	C	N	O	S	0	0	0
			1673	1080	272	317	4			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is OROTIDINE-5'-MONOPHOSPHATE (CCD ID: OMP) (formula: C₁₀H₁₃N₂O₁₁P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	2	11	1		

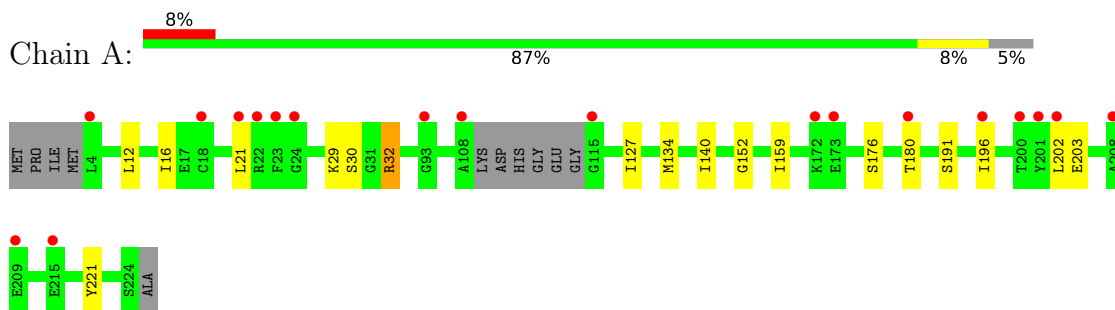
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	119	Total	O	0	0
			119	119		
4	C	89	Total	O	0	0
			89	89		
4	D	124	Total	O	0	0
			124	124		

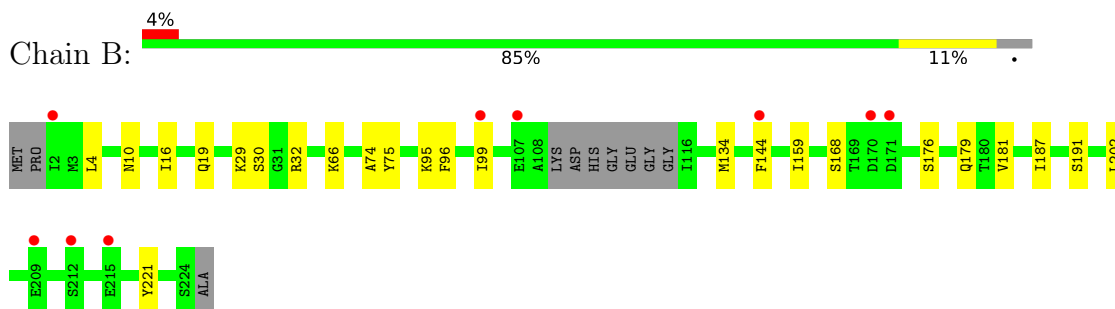
3 Residue-property plots [i](#)

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.

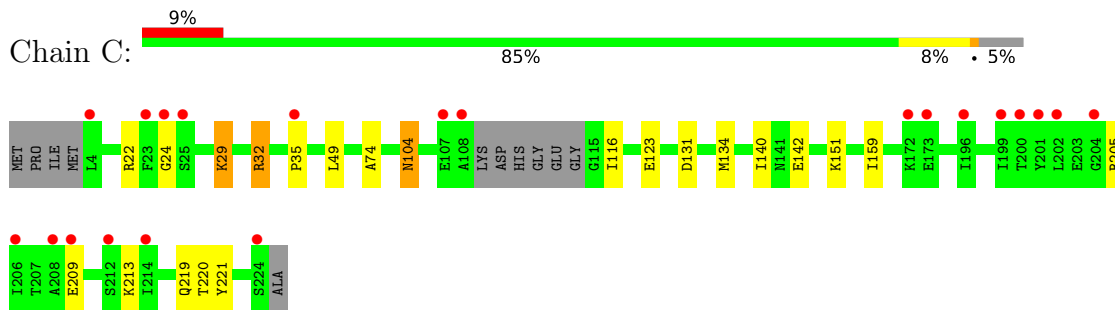
- Molecule 1: Orotate phosphoribosyltransferase 1



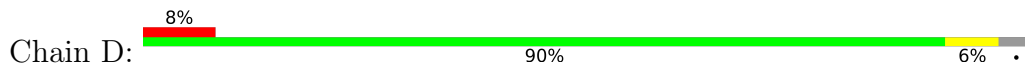
- Molecule 1: Orotate phosphoribosyltransferase 1

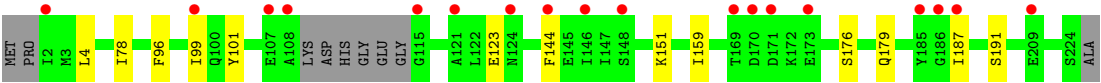


- Molecule 1: Orotate phosphoribosyltransferase 1



- Molecule 1: Orotate phosphoribosyltransferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.06Å 99.47Å 112.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-1.90) 95.8 (50.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.262 0.228 , 0.262	Depositor DCC
R_{free} test set	3715 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7201	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9674e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMP, CL

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	0.47	0/1680	0.74	0/2265
1	B	0.51	0/1692	0.76	0/2281
1	C	0.50	0/1680	0.78	0/2265
1	D	0.53	1/1696 (0.1%)	0.76	0/2286
All	All	0.50	1/6748 (0.0%)	0.76	0/9097

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	78	ILE	CA-CB	5.43	1.57	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1657	0	1705	10	0
1	B	1669	0	1722	16	0
1	C	1657	0	1705	12	0
1	D	1673	0	1725	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	10	2	0
3	B	24	0	10	3	0
3	C	24	0	10	2	0
3	D	24	0	10	2	0
4	A	113	0	0	2	0
4	B	119	0	0	2	0
4	C	89	0	0	2	0
4	D	124	0	0	0	0
All	All	7201	0	6897	52	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 4.

All (52) 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:C:134:MET:HE2	1:C:140:ILE:HG13	1.56	0.85
1:B:32:ARG:HG2	1:B:221:TYR:CZ	2.20	0.76
1:A:176:SER:O	1:A:180:THR:HG23	1.86	0.74
1:B:16:ILE:HD11	1:B:202:LEU:HD21	1.69	0.73
1:B:10:ASN:HB3	4:B:644:HOH:O	1.88	0.72
1:A:134:MET:HE2	1:A:140:ILE:HG13	1.70	0.71
1:B:134:MET:HE1	1:B:181:VAL:HG21	1.72	0.71
3:A:450:OMP:O2	3:A:450:OMP:H2'	1.98	0.63
1:C:74:ALA:H	1:C:104:ASN:HD21	1.45	0.62
3:D:750:OMP:H2'	3:D:750:OMP:O2	1.99	0.62
1:B:30:SER:OG	1:B:32:ARG:HD3	2.00	0.61
1:C:123:GLU:HG2	1:C:151:LYS:HB2	1.84	0.60
1:D:123:GLU:HG3	1:D:151:LYS:HE3	1.85	0.59
3:B:550:OMP:H2'	3:B:550:OMP:O2	2.01	0.59
1:B:176:SER:H	1:B:179:GLN:NE2	2.01	0.59
1:C:32:ARG:HD2	1:C:221:TYR:CE1	2.40	0.57
1:C:104:ASN:H	1:C:104:ASN:HD22	1.53	0.57
1:A:16:ILE:HD11	1:A:202:LEU:HD22	1.86	0.56
1:A:196:ILE:HG13	4:A:547:HOH:O	2.05	0.56
3:D:750:OMP:O4'	3:D:750:OMP:C7	2.53	0.56
1:C:49:LEU:HD11	1:D:101:TYR:CD2	2.41	0.56
1:D:96:PHE:HD2	1:D:99:ILE:HD12	1.71	0.56
3:C:650:OMP:H2'	3:C:650:OMP:O2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HD2	1:A:221:TYR:CE1	2.42	0.54
3:C:650:OMP:O4'	3:C:650:OMP:C7	2.55	0.54
3:B:550:OMP:O4'	3:B:550:OMP:C7	2.55	0.53
1:B:29:LYS:HE3	3:B:550:OMP:H4'	1.91	0.51
1:C:22:ARG:HG2	4:C:679:HOH:O	2.10	0.51
1:D:96:PHE:CD2	1:D:99:ILE:HD12	2.45	0.51
3:A:450:OMP:O4'	3:A:450:OMP:C7	2.59	0.49
1:D:176:SER:H	1:D:179:GLN:NE2	2.10	0.49
1:A:30:SER:OG	1:A:32:ARG:HG3	2.13	0.49
1:B:32:ARG:HG2	1:B:221:TYR:CE1	2.47	0.49
1:B:66:LYS:HE2	1:B:95:LYS:HE3	1.95	0.48
1:D:144:PHE:HZ	1:D:187:ILE:HD11	1.78	0.48
1:A:32:ARG:HD3	4:A:543:HOH:O	2.14	0.47
1:B:32:ARG:HD2	4:B:659:HOH:O	2.14	0.47
1:D:159:ILE:O	1:D:191:SER:HA	2.15	0.46
1:C:74:ALA:H	1:C:104:ASN:ND2	2.12	0.46
1:B:134:MET:HE1	1:B:181:VAL:CG2	2.42	0.46
1:C:24:GLY:O	1:C:35:PRO:HA	2.17	0.44
1:C:29:LYS:HE2	4:C:731:HOH:O	2.18	0.43
1:B:96:PHE:O	1:B:99:ILE:HG12	2.19	0.43
1:B:144:PHE:HZ	1:B:187:ILE:HD11	1.84	0.43
1:B:176:SER:H	1:B:179:GLN:HE21	1.65	0.42
1:B:74:ALA:HA	1:B:75:TYR:HA	1.82	0.41
1:A:16:ILE:CD1	1:A:202:LEU:HD22	2.50	0.41
1:C:104:ASN:H	1:C:104:ASN:ND2	2.16	0.41
1:A:159:ILE:O	1:A:191:SER:HA	2.21	0.41
1:C:131:ASP:O	1:C:159:ILE:HA	2.21	0.40
1:A:127:ILE:CD1	1:A:152:GLY:HA3	2.51	0.40
1:B:159:ILE:O	1:B:191:SER:HA	2.21	0.40

There are no symmetry-related clashes.

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	211/226 (93%)	208 (99%)	3 (1%)	0	100	100
1	B	212/226 (94%)	210 (99%)	2 (1%)	0	100	100
1	C	211/226 (93%)	207 (98%)	4 (2%)	0	100	100
1	D	213/226 (94%)	210 (99%)	3 (1%)	0	100	100
All	All	847/904 (94%)	835 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	177/185 (96%)	172 (97%)	5 (3%)	38	32
1	B	179/185 (97%)	176 (98%)	3 (2%)	53	52
1	C	177/185 (96%)	167 (94%)	10 (6%)	19	11
1	D	179/185 (97%)	178 (99%)	1 (1%)	78	81
All	All	712/740 (96%)	693 (97%)	19 (3%)	39	34

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	21	LEU
1	A	29	LYS
1	A	32	ARG
1	A	203	GLU
1	B	4	LEU
1	B	19	GLN
1	B	168	SER
1	C	29	LYS
1	C	32	ARG
1	C	104	ASN
1	C	116	ILE
1	C	142	GLU

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Mol	Chain	Res	Type
1	C	205	ARG
1	C	209	GLU
1	C	213	LYS
1	C	219	GLN
1	C	220	THR
1	D	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	B	51	ASN
1	B	179	GLN
1	C	10	ASN
1	C	104	ASN
1	C	124	ASN
1	C	141	ASN
1	C	153	GLN
1	C	219	GLN
1	D	10	ASN
1	D	51	ASN
1	D	141	ASN
1	D	179	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
3	OMP	B	550	-	25,25,25	1.21	1 (4%)	33,38,38	2.28	11 (33%)
3	OMP	D	750	-	25,25,25	1.18	3 (12%)	33,38,38	2.27	9 (27%)
3	OMP	C	650	-	25,25,25	1.15	2 (8%)	33,38,38	2.19	9 (27%)
3	OMP	A	450	-	25,25,25	1.21	3 (12%)	33,38,38	2.15	10 (30%)

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	OMP	B	550	-	-	5/14/30/30	0/2/2/2
3	OMP	D	750	-	-	8/14/30/30	0/2/2/2
3	OMP	C	650	-	-	9/14/30/30	0/2/2/2
3	OMP	A	450	-	-	8/14/30/30	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	OMP	C4-N3	-2.40	1.34	1.38
3	B	550	OMP	C4-N3	-2.38	1.34	1.38
3	C	650	OMP	C4-N3	-2.34	1.34	1.38
3	D	750	OMP	C4-N3	-2.20	1.34	1.38
3	D	750	OMP	O72-C7	-2.13	1.24	1.30
3	A	450	OMP	C2-N1	2.09	1.43	1.38
3	A	450	OMP	O72-C7	-2.06	1.25	1.30
3	C	650	OMP	O72-C7	-2.05	1.25	1.30
3	D	750	OMP	C2-N1	2.03	1.43	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	OMP	O72-C7-C6	7.38	123.34	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	OMP	O72-C7-C6	6.34	121.80	112.41
3	D	750	OMP	O72-C7-C6	6.32	121.77	112.41
3	C	650	OMP	O72-C7-C6	6.22	121.61	112.41
3	D	750	OMP	N3-C2-N1	4.24	121.03	115.66
3	C	650	OMP	N3-C2-N1	4.19	120.96	115.66
3	D	750	OMP	O4-C4-C5	-4.15	119.73	125.46
3	B	550	OMP	O71-C7-C6	-4.13	115.20	123.66
3	C	650	OMP	C5-C4-N3	4.09	120.33	115.24
3	C	650	OMP	O4-C4-C5	-4.09	119.81	125.46
3	C	650	OMP	C1'-N1-C2	4.08	124.00	117.29
3	A	450	OMP	C5-C4-N3	3.97	120.18	115.24
3	B	550	OMP	N3-C2-N1	3.97	120.68	115.66
3	B	550	OMP	C5-C4-N3	3.94	120.14	115.24
3	A	450	OMP	N3-C2-N1	3.90	120.60	115.66
3	D	750	OMP	C5-C4-N3	3.88	120.07	115.24
3	D	750	OMP	O71-C7-C6	-3.84	115.79	123.66
3	A	450	OMP	O71-C7-C6	-3.83	115.80	123.66
3	D	750	OMP	C1'-N1-C2	3.79	123.52	117.29
3	A	450	OMP	O4-C4-C5	-3.76	120.27	125.46
3	C	650	OMP	O71-C7-C6	-3.62	116.24	123.66
3	B	550	OMP	O4-C4-C5	-3.56	120.55	125.46
3	C	650	OMP	C4-N3-C2	-3.50	122.27	126.61
3	D	750	OMP	C4-N3-C2	-3.45	122.33	126.61
3	B	550	OMP	C1'-N1-C2	3.36	122.82	117.29
3	A	450	OMP	C1'-N1-C2	3.27	122.68	117.29
3	B	550	OMP	C4-N3-C2	-3.08	122.79	126.61
3	A	450	OMP	C4-N3-C2	-3.04	122.83	126.61
3	B	550	OMP	O4'-C1'-C2'	-2.63	100.99	106.62
3	A	450	OMP	O4'-C1'-C2'	-2.60	101.06	106.62
3	C	650	OMP	O4'-C1'-C2'	-2.28	101.74	106.62
3	D	750	OMP	O4'-C1'-C2'	-2.19	101.93	106.62
3	C	650	OMP	O2-C2-N3	-2.18	117.46	121.49
3	B	550	OMP	C4'-O4'-C1'	2.18	114.27	109.47
3	B	550	OMP	C3'-C2'-C1'	2.12	105.46	101.46
3	A	450	OMP	O2-C2-N3	-2.08	117.66	121.49
3	D	750	OMP	O2-C2-N3	-2.06	117.69	121.49
3	A	450	OMP	C3'-C2'-C1'	2.02	105.28	101.46
3	B	550	OMP	O2-C2-N3	-2.02	117.77	121.49

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	450	OMP	O4'-C1'-N1-C6
3	A	450	OMP	N1-C6-C7-O71
3	B	550	OMP	O4'-C1'-N1-C6
3	C	650	OMP	O4'-C1'-N1-C6
3	D	750	OMP	O4'-C1'-N1-C2
3	D	750	OMP	O4'-C1'-N1-C6
3	C	650	OMP	N1-C6-C7-O71
3	C	650	OMP	C2'-C1'-N1-C6
3	A	450	OMP	O4'-C1'-N1-C2
3	A	450	OMP	C2'-C1'-N1-C2
3	B	550	OMP	O4'-C1'-N1-C2
3	B	550	OMP	C2'-C1'-N1-C2
3	C	650	OMP	O4'-C1'-N1-C2
3	C	650	OMP	C2'-C1'-N1-C2
3	D	750	OMP	C2'-C1'-N1-C2
3	A	450	OMP	N1-C6-C7-O72
3	C	650	OMP	N1-C6-C7-O72
3	D	750	OMP	N1-C6-C7-O72
3	A	450	OMP	C4'-C5'-O5'-P
3	A	450	OMP	C5-C6-C7-O71
3	A	450	OMP	C5-C6-C7-O72
3	B	550	OMP	C5-C6-C7-O71
3	B	550	OMP	C5-C6-C7-O72
3	C	650	OMP	C5-C6-C7-O71
3	C	650	OMP	C5-C6-C7-O72
3	D	750	OMP	C5-C6-C7-O71
3	D	750	OMP	C5-C6-C7-O72
3	C	650	OMP	C4'-C5'-O5'-P
3	D	750	OMP	C5'-O5'-P-O2P
3	D	750	OMP	N1-C6-C7-O71

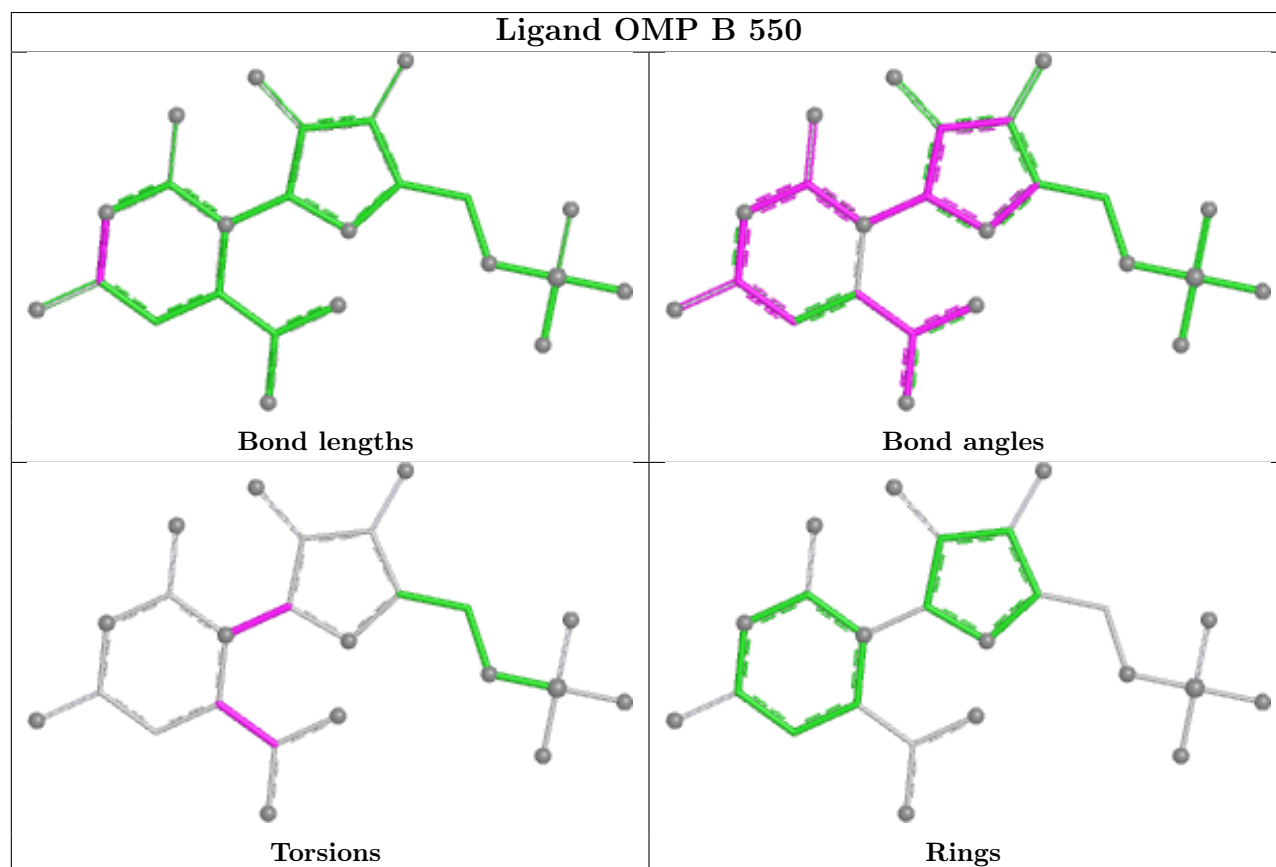
There are no ring outliers.

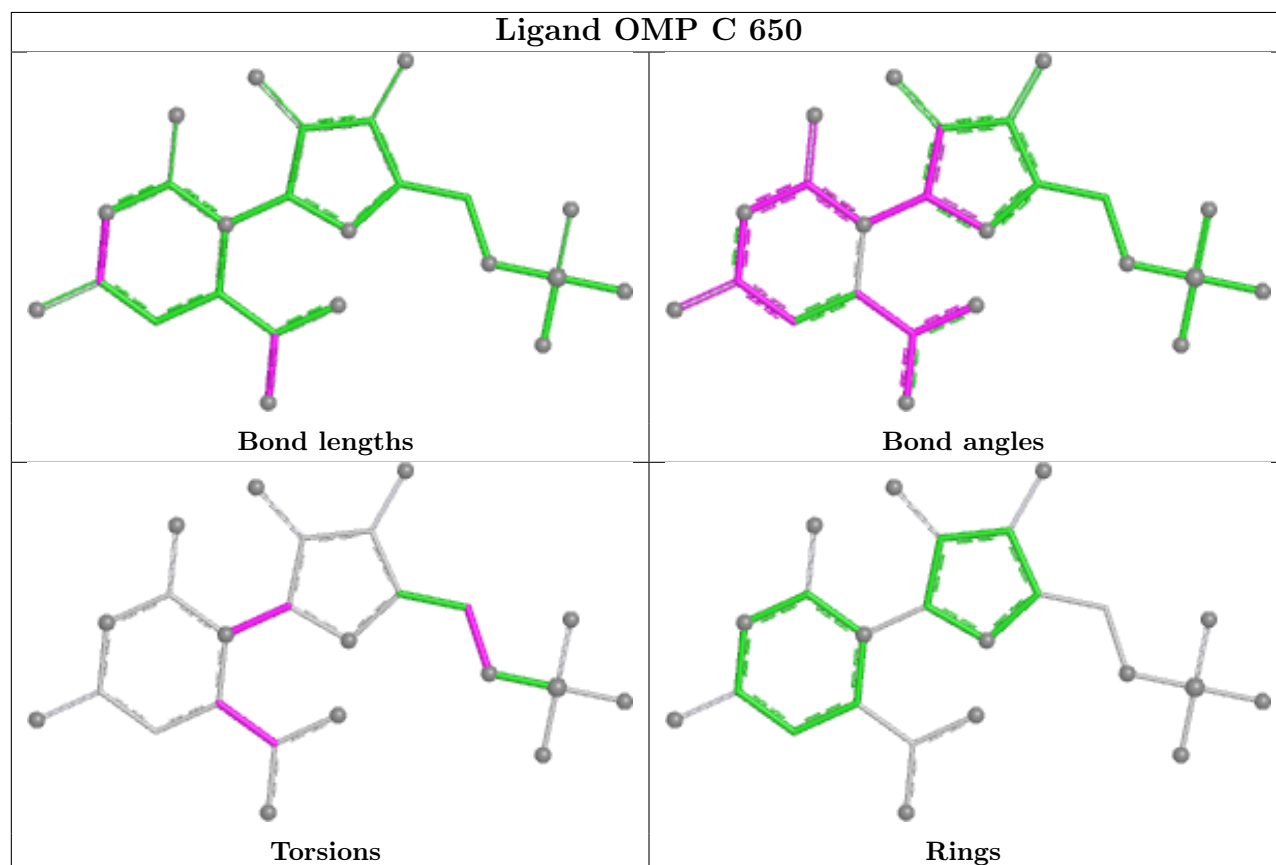
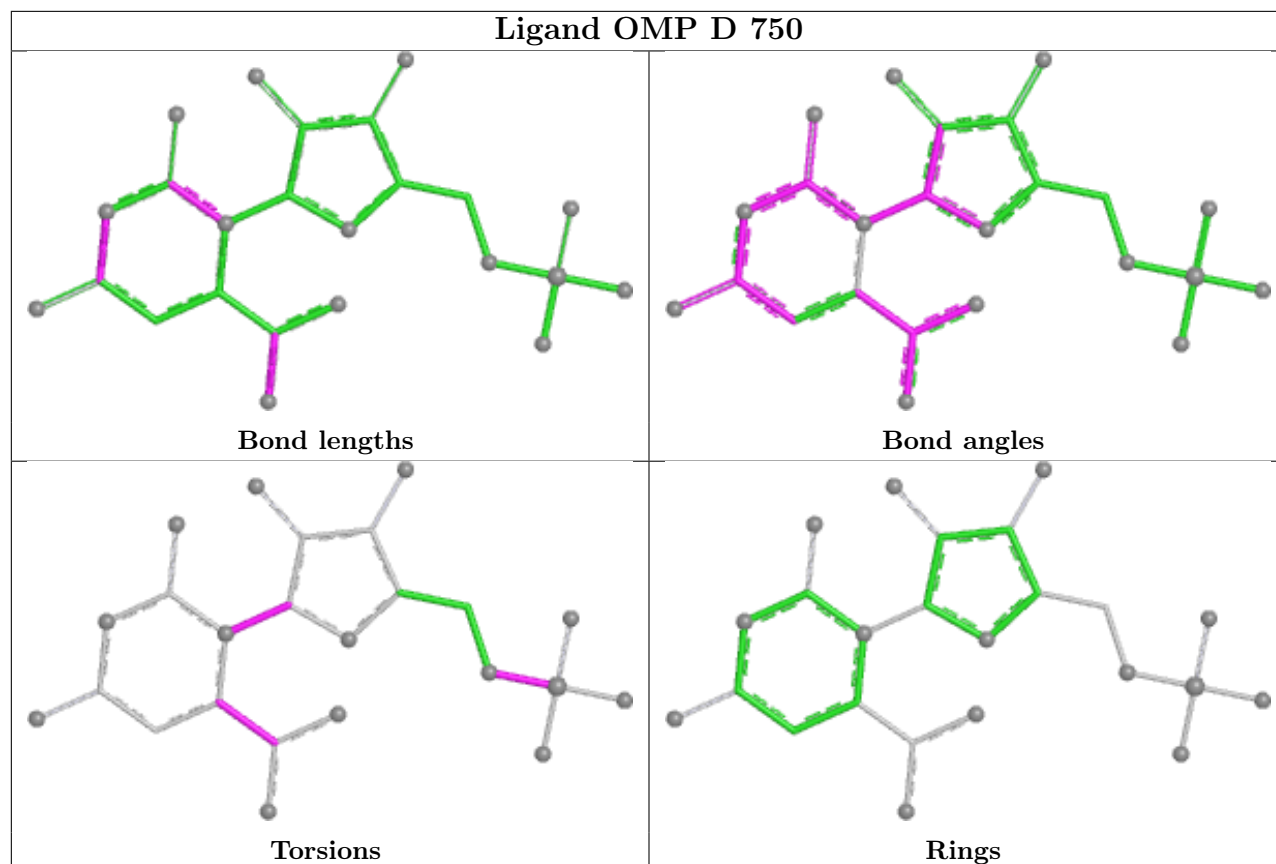
4 monomers are involved in 9 short contacts:

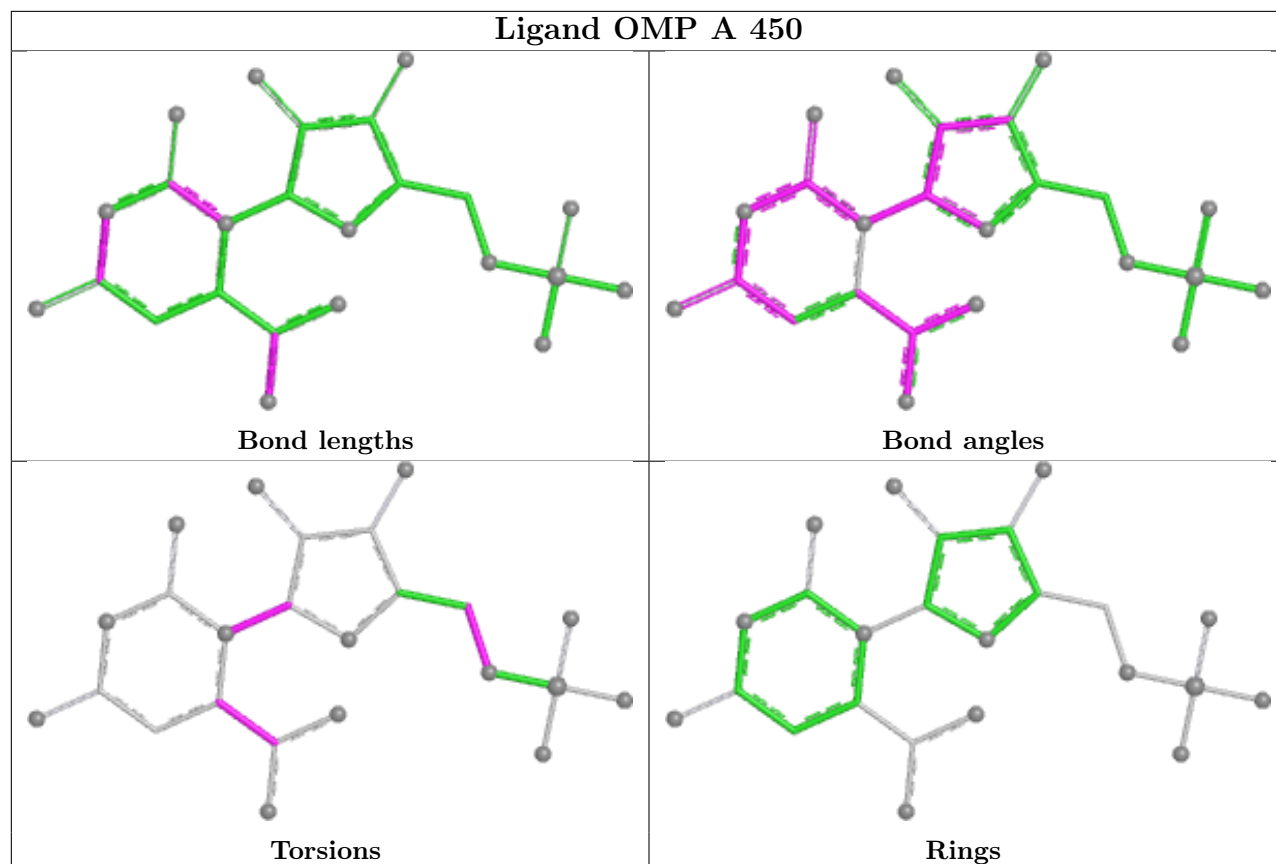
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	550	OMP	3	0
3	D	750	OMP	2	0
3	C	650	OMP	2	0
3	A	450	OMP	2	0

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	215/226 (95%)	0.59	19 (8%) 15 16	18, 28, 49, 55	0
1	B	216/226 (95%)	0.39	9 (4%) 40 43	17, 27, 38, 45	0
1	C	215/226 (95%)	0.82	21 (9%) 13 13	19, 31, 51, 61	0
1	D	217/226 (96%)	0.45	18 (8%) 17 18	17, 27, 40, 44	0
All	All	863/904 (95%)	0.56	67 (7%) 19 20	17, 28, 44, 61	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202	LEU	4.2
1	D	148	SER	4.0
1	D	185	TYR	3.8
1	C	23	PHE	3.7
1	C	201	TYR	3.5
1	A	200	THR	3.5
1	C	4	LEU	3.4
1	D	169	THR	3.4
1	A	201	TYR	3.2
1	A	202	LEU	3.2
1	C	212	SER	3.1
1	D	170	ASP	3.1
1	D	2	ILE	3.1
1	A	208	ALA	3.0
1	B	2	ILE	3.0
1	C	199	ILE	3.0
1	C	25	SER	3.0
1	C	224	SER	2.9
1	A	4	LEU	2.9
1	D	171	ASP	2.9
1	A	23	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	144	PHE	2.8
1	A	93	GLY	2.7
1	A	209	GLU	2.7
1	D	108	ALA	2.7
1	A	108	ALA	2.6
1	D	186	GLY	2.6
1	B	171	ASP	2.6
1	D	107	GLU	2.6
1	C	108	ALA	2.5
1	C	209	GLU	2.5
1	C	200	THR	2.5
1	C	196	ILE	2.4
1	C	214	ILE	2.4
1	D	121	ALA	2.4
1	B	144	PHE	2.4
1	C	206	ILE	2.4
1	B	107	GLU	2.4
1	C	172	LYS	2.3
1	A	115	GLY	2.3
1	C	35	PRO	2.3
1	B	170	ASP	2.3
1	A	18	CYS	2.3
1	A	21	LEU	2.3
1	A	215	GLU	2.2
1	A	24	GLY	2.2
1	B	212	SER	2.2
1	B	209	GLU	2.2
1	B	215	GLU	2.2
1	C	24	GLY	2.2
1	C	208	ALA	2.2
1	A	22	ARG	2.2
1	D	209	GLU	2.1
1	A	196	ILE	2.1
1	B	99	ILE	2.1
1	C	204	GLY	2.1
1	D	115	GLY	2.1
1	D	99	ILE	2.1
1	A	173	GLU	2.1
1	D	173	GLU	2.1
1	C	173	GLU	2.0
1	D	146	ILE	2.0
1	D	187	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	180	THR	2.0
1	D	124	ASN	2.0
1	C	107	GLU	2.0
1	A	172	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](#)

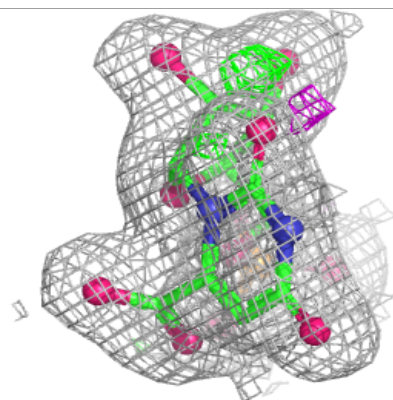
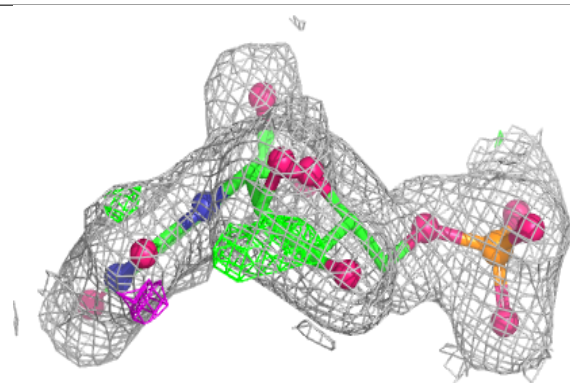
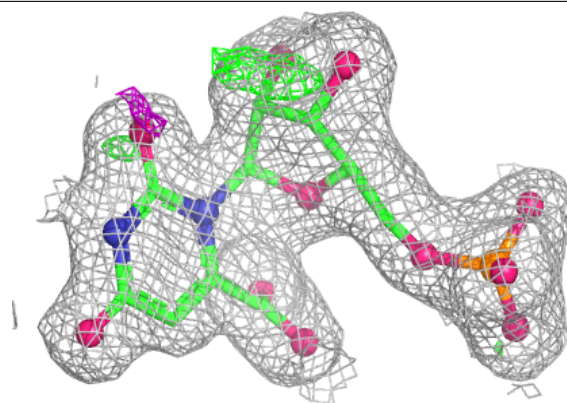
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	225	1/1	0.93	0.09	38,38,38,38	0
3	OMP	D	750	24/24	0.93	0.08	23,26,28,29	0
3	OMP	B	550	24/24	0.95	0.07	22,23,27,29	0
3	OMP	C	650	24/24	0.95	0.07	23,26,27,27	0
2	CL	D	225	1/1	0.95	0.08	40,40,40,40	0
3	OMP	A	450	24/24	0.96	0.06	20,23,25,27	0
2	CL	C	2	1/1	0.98	0.04	36,36,36,36	0
2	CL	A	1	1/1	0.99	0.04	34,34,34,34	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.

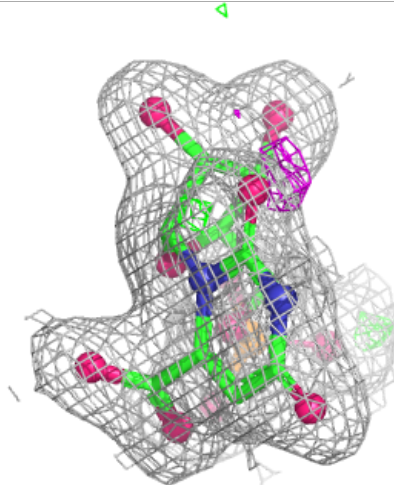
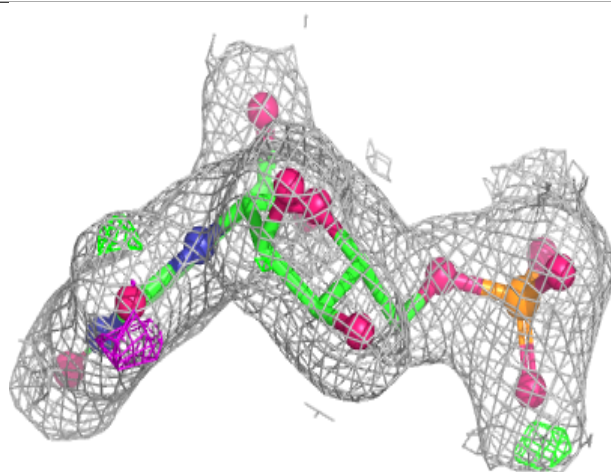
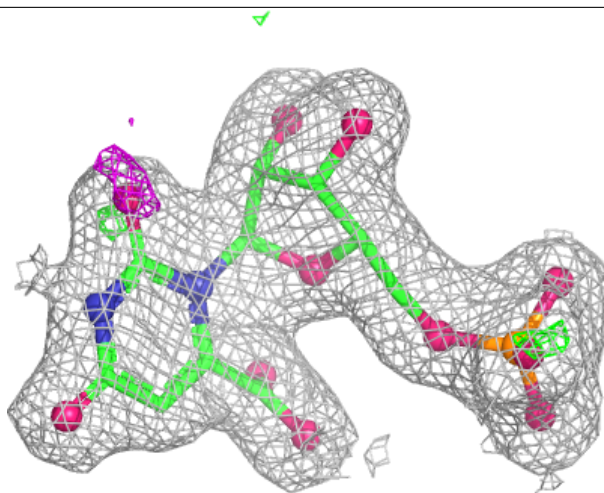
Electron density around OMP D 750:

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



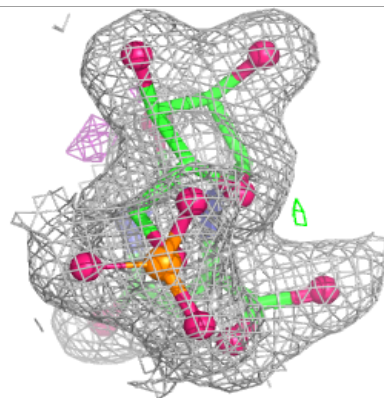
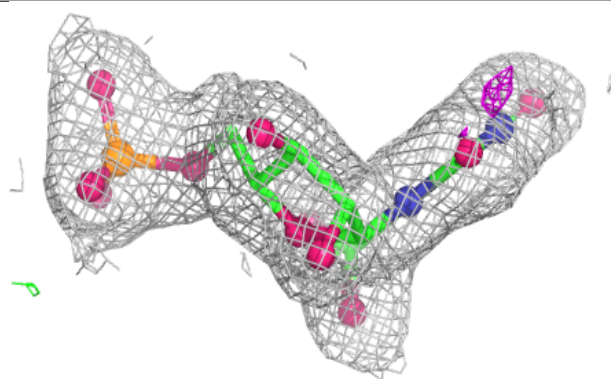
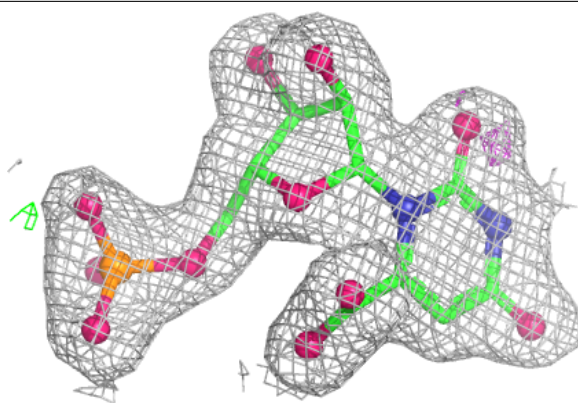
Electron density around OMP B 550:

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

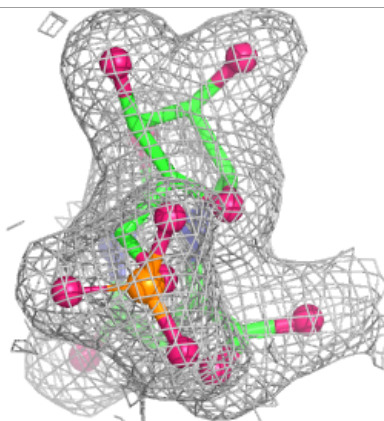
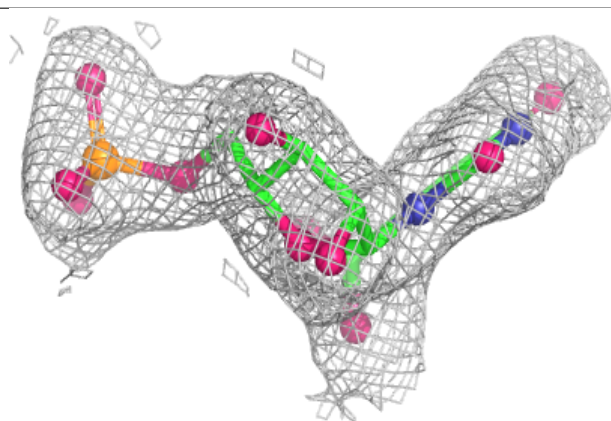
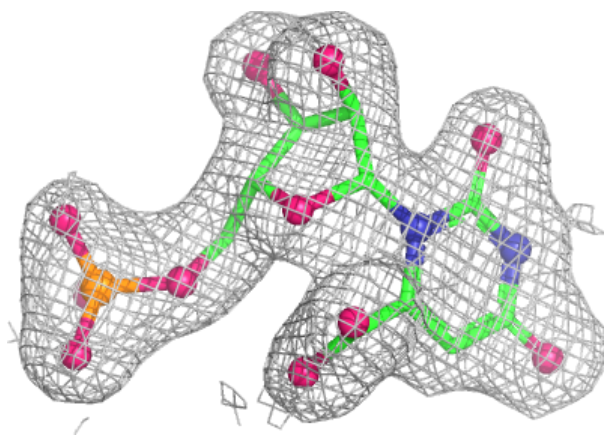


Electron density around OMP C 650:

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

**Electron density around OMP A 450:**

$2mF_o-DF_c$ (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.