



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:24 AM UTC

PDB ID : 7OPN / pdb_00007opn
Title : Human Aldehyde Oxidase SNP R1231H in complex with Raloxifene
Authors : Mota, C.; Coelho, C.; Santos Silva, T.; Romao, M.J.
Deposited on : 2021-06-01
Resolution : 2.60 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

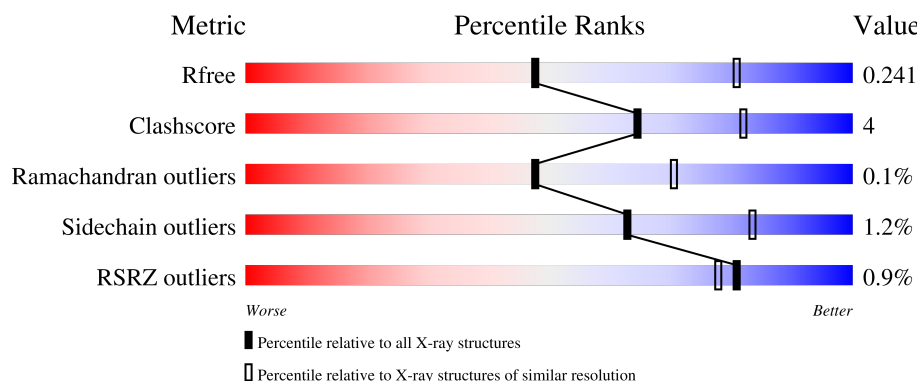
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	1338	86% 11%
1	B	1338	86% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	DMS	B	3008	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20650 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.

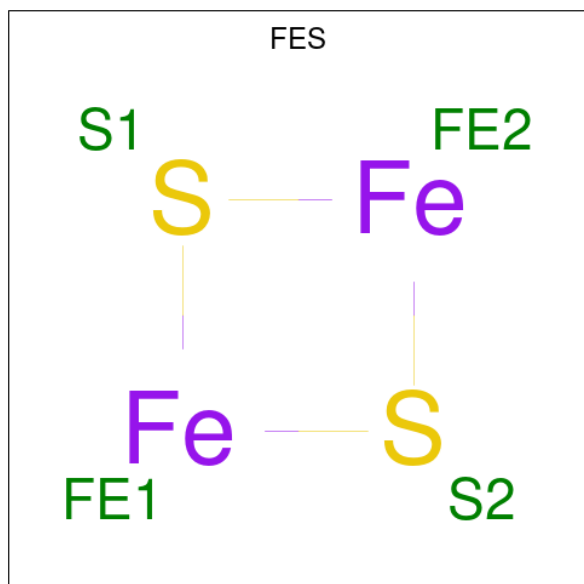
- Molecule 1 is a protein called Aldehyde oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1295	Total	C	N	O	S	0	0	0
			10055	6389	1731	1855	80			
1	B	1295	Total	C	N	O	S	0	1	0
			10064	6397	1731	1856	80			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1231	HIS	ARG	engineered mutation	UNP Q06278
B	1231	HIS	ARG	engineered mutation	UNP Q06278

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



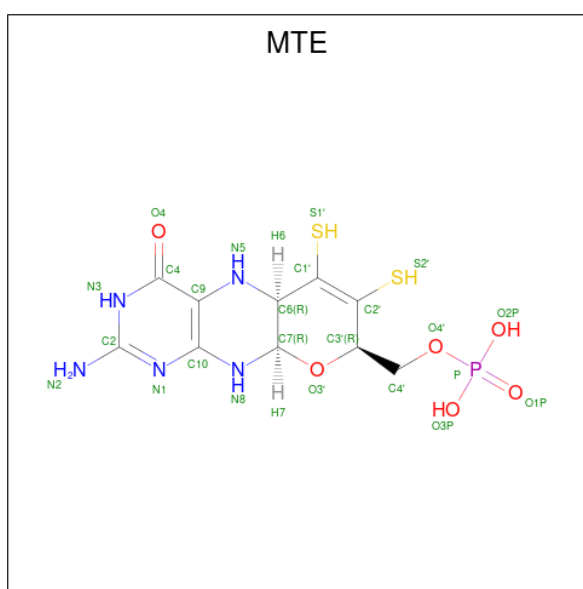
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		

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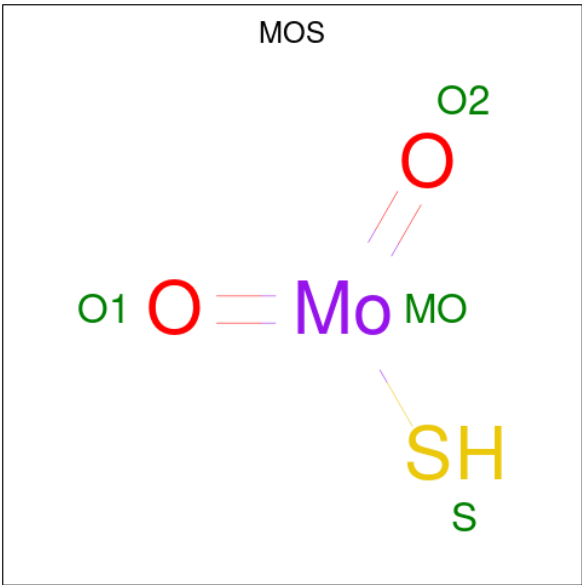
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



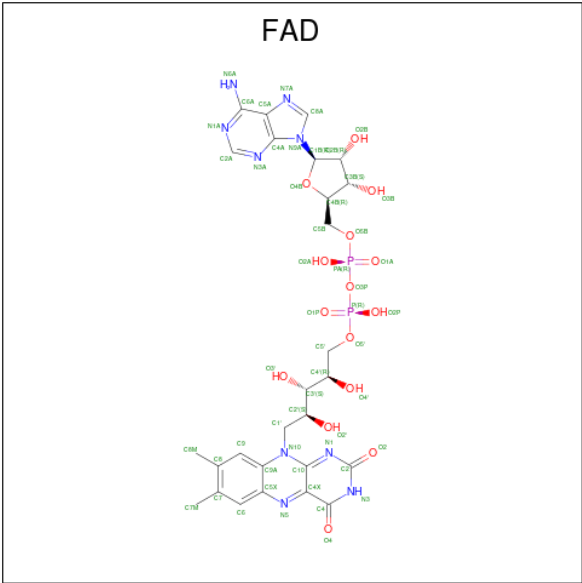
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: $HMoO_2S$).



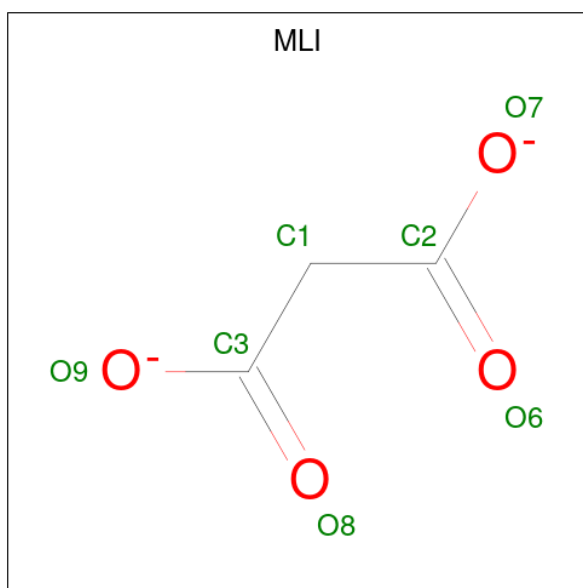
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



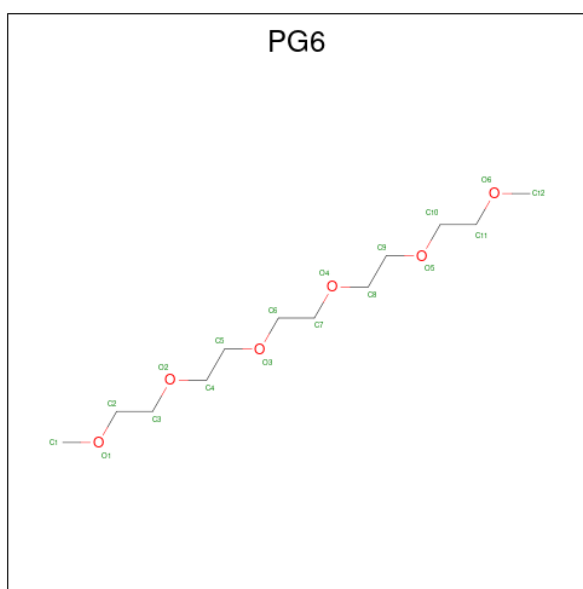
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is MALONATE ION (CCD ID: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).



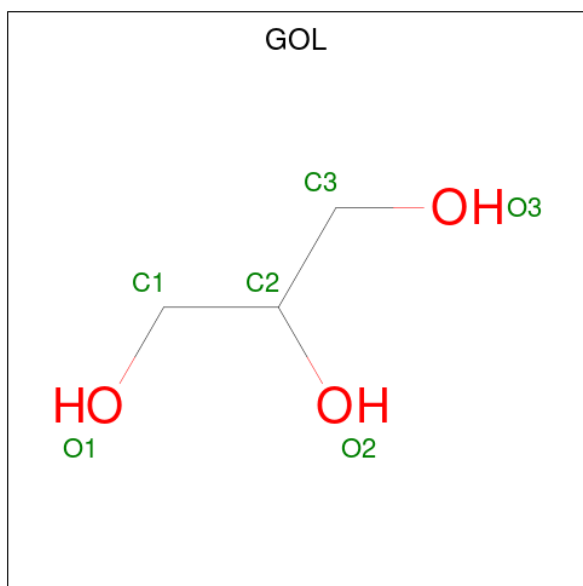
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]}-ETHANE (CCD ID: PG6) (formula: $\text{C}_{12}\text{H}_{26}\text{O}_6$).



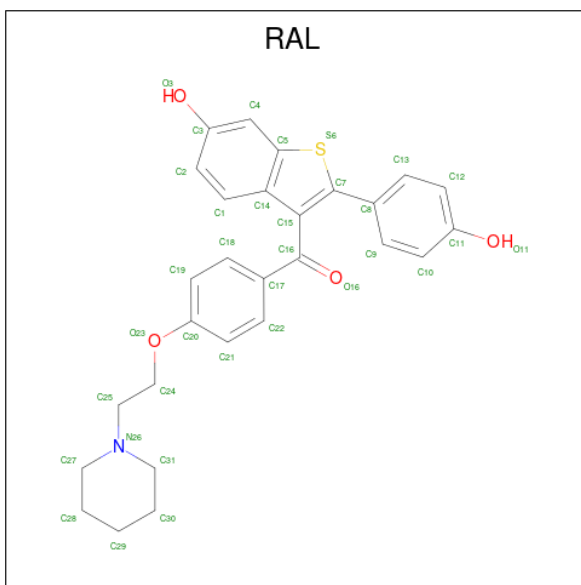
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



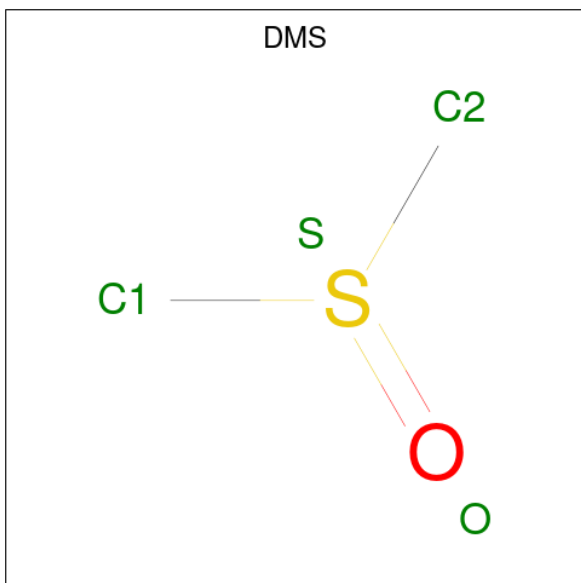
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is RALOXIFENE (CCD ID: RAL) (formula: $C_{28}H_{27}NO_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	0
			34	28	1	4	1		
9	A	1	Total	C	N	O	S	0	0
			34	28	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			34	28	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			34	28	1	4	1		

- Molecule 10 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	O	S	0	0
			4	2	1	1		

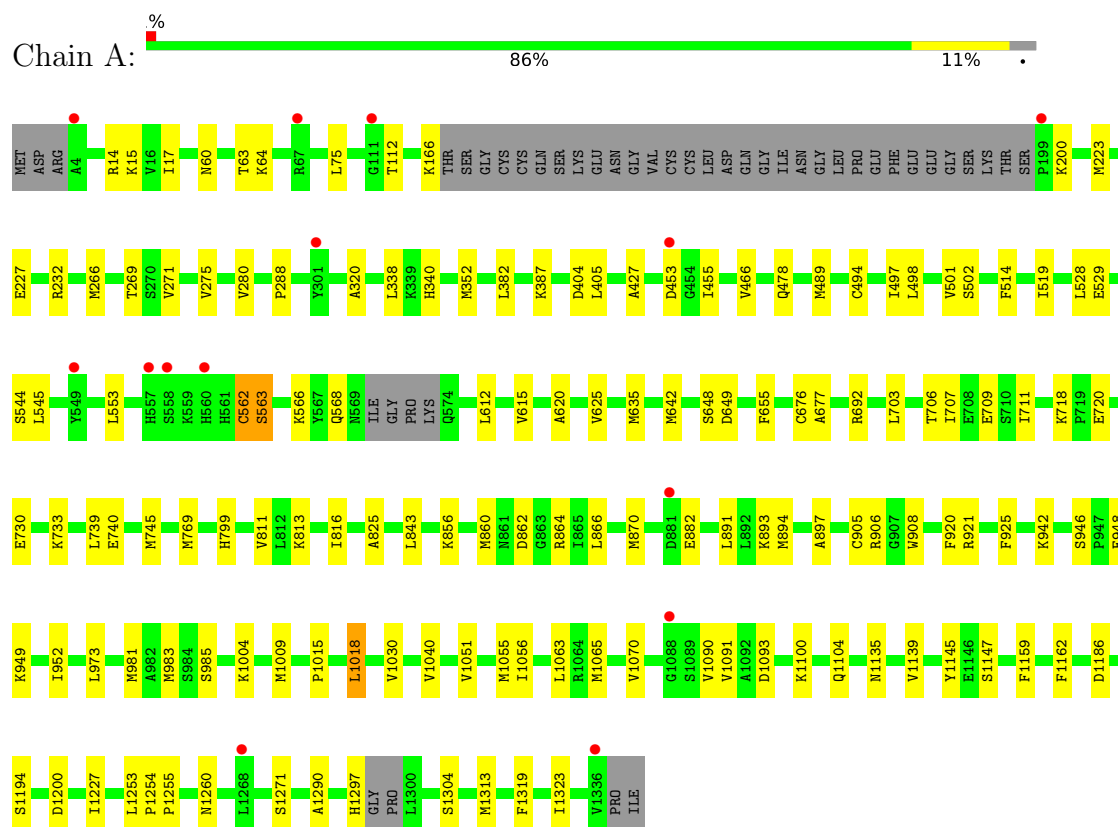
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	91	Total	O	0	0
			91	91		
11	B	72	Total	O	0	0
			72	72		

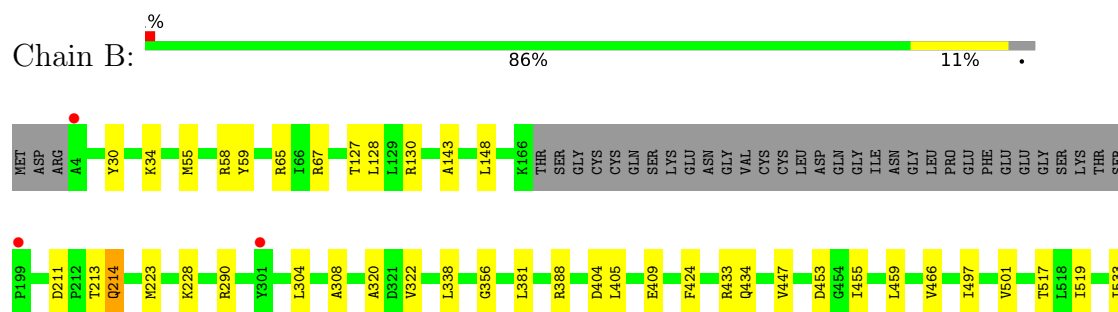
3 Residue-property plots

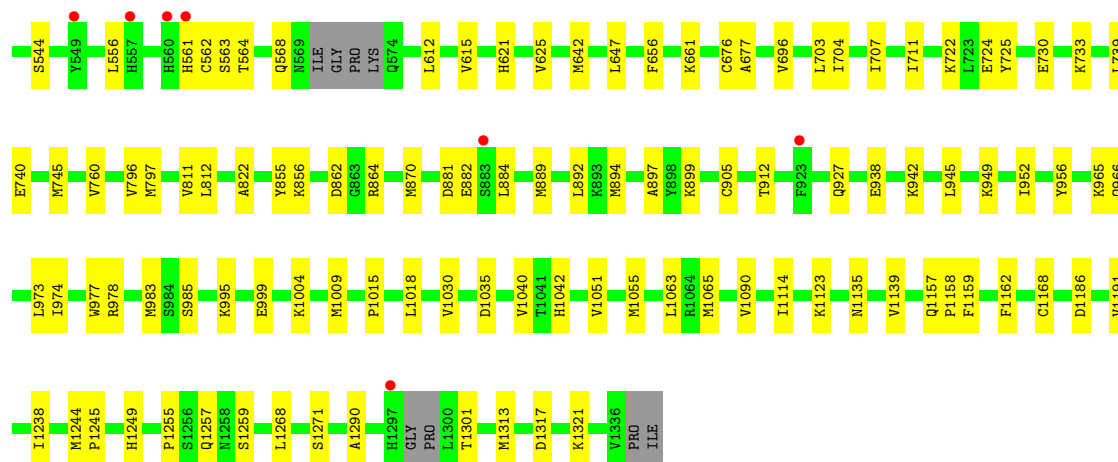
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aldehyde oxidase



• Molecule 1: Aldehyde oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.53Å 149.53Å 269.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 2.60 49.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.01-2.60) 100.0 (49.01-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.206 , 0.241 0.204 , 0.241	Depositor DCC
R_{free} test set	4735 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20650	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.52 % 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 1.7420e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, DMS, RAL, MTE, PG6, GOL, MOS, FES, FAD

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	0.13	0/10269	0.30	0/13887
1	B	0.10	0/10282	0.29	0/13905
All	All	0.11	0/20551	0.29	0/27792

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	10055	0	10093	81	0
1	B	10064	0	10102	80	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	24	0	10	0	0
3	B	24	0	10	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	0	0
6	A	7	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	7	0	2	0	0
7	A	18	0	26	2	0
8	A	12	0	16	0	0
8	B	6	0	8	1	0
9	A	68	0	52	0	0
9	B	68	0	52	1	0
10	B	4	0	6	0	0
11	A	91	0	0	0	0
11	B	72	0	0	0	0
All	All	20650	0	20441	161	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 (161) 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:B:983:MET:HE3	1:B:1186:ASP:HB3	1.62	0.81
1:B:995:LYS:NZ	1:B:999:GLU:OE2	2.24	0.70
1:B:564:THR:OG1	1:B:1249:HIS:ND1	2.27	0.67
1:B:55:MET:HE1	1:B:130:ARG:HG3	1.77	0.66
1:A:983:MET:HE3	1:A:1186:ASP:HB3	1.77	0.66
1:A:862:ASP:OD2	1:A:864:ARG:NH1	2.29	0.65
1:B:945:LEU:HD22	1:B:949:LYS:HE2	1.78	0.65
1:A:200:LYS:H	1:A:200:LYS:HD2	1.62	0.64
1:A:64:LYS:O	1:A:64:LYS:HG2	1.96	0.64
1:B:58:ARG:HH11	1:B:290:ARG:HH21	1.47	0.63
1:B:211:ASP:OD2	1:B:214:GLN:NE2	2.32	0.62
1:A:740:GLU:HG3	1:A:856:LYS:HG3	1.80	0.62
1:A:514:PHE:HA	1:A:1313:MET:HE3	1.81	0.62
1:A:612:LEU:HD11	1:A:677:ALA:HB1	1.81	0.62
1:A:15:LYS:HD3	1:A:17:ILE:HD11	1.82	0.62
1:B:739:LEU:HD12	1:B:942:LYS:HD3	1.83	0.60
1:A:453:ASP:HB2	1:A:455:ILE:HD12	1.84	0.59
1:B:1009:MET:HE2	1:B:1168:CYS:HB2	1.84	0.59
1:B:497:ILE:O	1:B:501:VAL:HG22	2.04	0.58
1:B:1257:GLN:HE22	1:B:1259:SER:HB3	1.69	0.58
1:A:1063:LEU:HB3	1:A:1065:MET:HE3	1.86	0.57
1:B:740:GLU:HG2	1:B:856:LYS:HG3	1.86	0.57
1:A:266:MET:HE1	1:A:288:PRO:HG2	1.87	0.56
1:A:648:SER:OG	1:A:649:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLN:HG3	1:A:1255:PRO:HD3	1.87	0.56
1:B:612:LEU:HD11	1:B:677:ALA:HB1	1.88	0.56
1:A:1018:LEU:HD21	1:A:1090:VAL:HG21	1.88	0.55
1:B:434:GLN:NE2	1:B:556:LEU:O	2.32	0.55
1:B:568:GLN:HG3	1:B:1255:PRO:HD3	1.87	0.54
1:B:1004:LYS:HG3	1:B:1290:ALA:HB2	1.89	0.54
1:A:1135:ASN:HD21	1:B:1139:VAL:HG11	1.73	0.54
1:B:894:MET:HE3	1:B:905:CYS:SG	2.49	0.54
1:A:799:HIS:HB3	7:A:3007:PG6:H13	1.90	0.53
1:A:497:ILE:O	1:A:501:VAL:HG22	2.08	0.53
1:A:1139:VAL:HG11	1:B:1135:ASN:HD21	1.73	0.53
1:B:447:VAL:HG12	1:B:459:LEU:HD13	1.89	0.53
1:B:1051:VAL:O	1:B:1055:MET:HG2	2.09	0.53
1:B:661:LYS:H	1:B:661:LYS:HD2	1.72	0.53
1:A:1253:LEU:HG	1:A:1254:PRO:HD2	1.89	0.53
1:B:433:ARG:NH1	1:B:1238:ILE:O	2.41	0.53
1:B:952:ILE:HD11	1:B:977:TRP:HE1	1.73	0.53
1:A:635:MET:SD	1:A:692:ARG:HD2	2.49	0.52
1:B:381:LEU:HD13	1:B:405:LEU:HG	1.92	0.52
1:A:739:LEU:HD12	1:A:942:LYS:HG3	1.91	0.52
1:B:625:VAL:HB	1:B:696:VAL:HG12	1.91	0.52
1:A:275:VAL:HG12	1:A:280:VAL:HG12	1.93	0.51
1:B:501:VAL:O	1:B:501:VAL:HG23	2.11	0.51
1:A:382:LEU:HD13	1:A:387:LYS:HG2	1.93	0.50
1:B:304:LEU:HD11	1:B:322:VAL:HG21	1.92	0.50
1:A:948:GLU:O	1:A:952:ILE:HG13	2.11	0.50
1:B:855:TYR:HB3	1:B:870:MET:SD	2.50	0.50
1:A:615:VAL:HB	1:A:676:CYS:HB2	1.94	0.50
1:A:1100:LYS:HE2	1:A:1104:GLN:NE2	2.27	0.50
1:B:974:ILE:O	1:B:978:ARG:HG3	2.11	0.49
1:B:453:ASP:HB2	1:B:455:ILE:HD13	1.94	0.49
1:B:1018:LEU:HD11	1:B:1090:VAL:HG21	1.94	0.49
1:B:561:HIS:HB3	1:B:1244:MET:HE1	1.93	0.48
1:A:1004:LYS:HG3	1:A:1290:ALA:HB2	1.95	0.48
1:B:65:ARG:HD3	1:B:67:ARG:NH2	2.27	0.48
1:A:1051:VAL:O	1:A:1055:MET:HG2	2.14	0.48
1:B:59:TYR:CE1	1:B:223:MET:HE3	2.48	0.48
1:A:894:MET:HE3	1:A:905:CYS:SG	2.54	0.48
1:A:1093:ASP:OD1	1:A:1145:TYR:OH	2.32	0.48
1:B:1015:PRO:HB3	1:B:1162:PHE:CE2	2.49	0.48
1:B:517:THR:OG1	1:B:1313:MET:HE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ALA:HB3	1:A:703:LEU:HD11	1.97	0.47
1:B:1015:PRO:HB2	1:B:1159:PHE:CG	2.50	0.47
1:B:1063:LEU:HB3	1:B:1065:MET:HE3	1.96	0.47
1:A:1015:PRO:HB3	1:A:1162:PHE:CE2	2.50	0.47
1:B:128:LEU:HD13	1:B:143:ALA:HB2	1.96	0.47
1:A:706:THR:OG1	1:A:709:GLU:HG3	2.15	0.47
1:A:733:LYS:HB2	1:A:733:LYS:HE2	1.50	0.46
1:A:769:MET:HE1	1:A:825:ALA:HB3	1.97	0.46
1:B:228:LYS:C	1:B:228:LYS:HD3	2.41	0.46
1:B:725:TYR:HE1	1:B:965:LYS:HD3	1.80	0.46
1:A:200:LYS:HD2	1:A:200:LYS:N	2.29	0.46
1:A:730:GLU:OE1	1:A:733:LYS:NZ	2.48	0.46
9:B:3009:RAL:H21	9:B:3009:RAL:H241	1.74	0.46
1:A:528:LEU:HD22	1:A:545:LEU:HD11	1.98	0.45
1:A:1015:PRO:HB2	1:A:1159:PHE:CG	2.51	0.45
1:B:760:VAL:HG11	1:B:822:ALA:HA	1.97	0.45
1:B:466:VAL:HG11	1:B:519:ILE:HD11	1.99	0.45
1:B:739:LEU:HD11	1:B:938:GLU:HB3	1.98	0.45
1:A:642:MET:HE2	1:A:642:MET:HB2	1.82	0.45
1:B:564:THR:HG1	1:B:1249:HIS:CE1	2.35	0.45
1:B:966:GLN:HG3	1:B:1157:GLN:OE1	2.16	0.45
1:B:730:GLU:HA	1:B:733:LYS:HE2	1.99	0.45
1:A:707:ILE:O	1:A:711:ILE:HG13	2.16	0.45
1:A:1030:VAL:HG22	1:A:1040:VAL:HG23	1.98	0.45
1:B:656:PHE:CE2	1:B:881:ASP:HB3	2.52	0.45
1:A:60:ASN:HB3	1:A:63:THR:HG22	1.97	0.45
1:B:55:MET:HE2	1:B:127:THR:HA	1.98	0.45
1:A:720:GLU:CD	1:A:906:ARG:HH21	2.24	0.44
1:B:704:ILE:HG22	1:B:912:THR:HG22	2.00	0.44
1:A:745:MET:HG3	1:A:1304:SER:HB3	1.99	0.44
1:B:404:ASP:OD1	1:B:405:LEU:N	2.49	0.44
1:B:308:ALA:HB1	1:B:356:GLY:HA3	1.99	0.44
1:A:1051:VAL:HG21	1:A:1091:VAL:HG12	1.98	0.44
1:B:228:LYS:HD3	1:B:228:LYS:O	2.17	0.44
1:A:946:SER:OG	1:A:949:LYS:HG3	2.16	0.44
1:A:501:VAL:HG23	1:A:501:VAL:O	2.17	0.44
1:A:860:MET:HG2	1:A:866:LEU:CD2	2.48	0.44
1:B:707:ILE:O	1:B:711:ILE:HG13	2.18	0.44
1:B:424:PHE:CE1	1:B:533:ILE:HD13	2.53	0.44
1:A:983:MET:HE2	1:A:983:MET:HB3	1.87	0.44
1:A:897:ALA:HB1	1:A:973:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:SER:OG	1:A:1200:ASP:OD2	2.30	0.43
1:B:642:MET:HE3	1:B:647:LEU:HD11	2.00	0.43
1:A:466:VAL:HG11	1:A:519:ILE:HD11	2.00	0.43
1:B:148:LEU:HD11	8:B:3006:GOL:H2	2.00	0.43
1:B:722:LYS:HE2	1:B:724:GLU:HG3	2.01	0.43
1:B:388:ARG:NH1	1:B:409:GLU:OE1	2.51	0.43
1:B:897:ALA:HB1	1:B:973:LEU:HD21	2.01	0.43
1:B:1191:VAL:HG12	1:B:1268:LEU:HD11	1.99	0.43
1:A:320:ALA:HA	1:A:338:LEU:HD11	2.01	0.43
1:A:562:CYS:SG	1:A:563:SER:N	2.92	0.43
1:B:745:MET:SD	1:B:927:GLN:HA	2.59	0.43
1:B:899:LYS:HB2	1:B:956:TYR:CD1	2.54	0.43
1:B:1191:VAL:CG1	1:B:1268:LEU:HD11	2.49	0.43
1:B:862:ASP:CG	1:B:864:ARG:HE	2.25	0.43
1:B:562:CYS:SG	1:B:563:SER:N	2.91	0.42
1:A:404:ASP:OD1	1:A:405:LEU:N	2.49	0.42
1:A:232:ARG:HH11	1:A:232:ARG:HG2	1.83	0.42
1:A:720:GLU:OE2	1:A:906:ARG:NE	2.35	0.42
1:B:621:HIS:HB3	1:B:703:LEU:HD12	2.00	0.42
1:A:223:MET:O	1:A:227:GLU:HG2	2.18	0.42
1:A:232:ARG:HG2	1:A:232:ARG:NH1	2.35	0.42
1:A:14:ARG:HE	1:A:14:ARG:HB3	1.71	0.42
1:B:320:ALA:HA	1:B:338:LEU:HD11	2.02	0.42
1:B:1317:ASP:O	1:B:1321:LYS:HD2	2.19	0.42
1:B:796:VAL:O	1:B:797:MET:HE2	2.20	0.42
1:B:1042:HIS:NE2	1:B:1055:MET:HG3	2.35	0.42
1:A:494:CYS:O	1:A:498:LEU:HD12	2.19	0.42
1:A:891:LEU:HD22	1:A:905:CYS:SG	2.60	0.41
1:B:30:TYR:CE1	1:B:34:LYS:HG2	2.55	0.41
1:B:889:MET:HE2	1:B:892:LEU:HD12	2.01	0.41
1:A:75:LEU:HB2	1:A:352:MET:HE1	2.03	0.41
1:A:1056:ILE:HG23	1:A:1070:VAL:HB	2.02	0.41
1:A:271:VAL:O	1:A:275:VAL:HG13	2.20	0.41
1:B:1244:MET:HE3	1:B:1245:PRO:O	2.20	0.41
1:A:718:LYS:HD3	1:A:908:TRP:HB3	2.03	0.41
1:A:529:GLU:HG2	1:A:553:LEU:HD22	2.01	0.41
1:A:166:LYS:HB2	1:A:166:LYS:HE2	1.71	0.41
7:A:3007:PG6:H61	7:A:3007:PG6:H81	1.87	0.41
1:B:615:VAL:HB	1:B:676:CYS:HB2	2.02	0.41
1:B:1035:ASP:HA	1:B:1123:LYS:HG3	2.02	0.41
1:A:843:LEU:HA	1:A:843:LEU:HD23	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:GLN:OE1	1:B:1158:PRO:HD2	2.21	0.41
1:B:1030:VAL:HG22	1:B:1040:VAL:HG23	2.03	0.41
1:A:655:PHE:CZ	1:A:816:ILE:HD11	2.56	0.41
1:A:870:MET:HE2	1:A:870:MET:HB2	1.93	0.41
1:A:1319:PHE:O	1:A:1323:ILE:HG23	2.21	0.41
1:A:489:MET:HE3	1:A:489:MET:HB3	1.88	0.40
1:A:860:MET:SD	1:A:866:LEU:HD23	2.61	0.40
1:A:893:LYS:HB3	1:A:925:PHE:HD1	1.86	0.40
1:A:981:MET:HE2	1:A:1009:MET:SD	2.61	0.40
1:A:340:HIS:CE1	1:A:427:ALA:HB1	2.56	0.40
1:A:920:PHE:HD1	1:A:921:ARG:N	2.19	0.40
1:B:55:MET:CE	1:B:127:THR:HA	2.50	0.40
1:A:269:THR:OG1	5:A:3005:FAD:O1P	2.33	0.40
1:A:566:LYS:HD2	1:A:566:LYS:HA	1.92	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	1287/1338 (96%)	1256 (98%)	30 (2%)	1 (0%)	48	70
1	B	1288/1338 (96%)	1258 (98%)	29 (2%)	1 (0%)	48	70
All	All	2575/2676 (96%)	2514 (98%)	59 (2%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	VAL
1	B	811	VAL

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	1100/1136 (97%)	1084 (98%)	16 (2%)	57	80
1	B	1101/1136 (97%)	1091 (99%)	10 (1%)	70	87
All	All	2201/2272 (97%)	2175 (99%)	26 (1%)	63	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	478	GLN
1	A	502	SER
1	A	544	SER
1	A	562	CYS
1	A	563	SER
1	A	625	VAL
1	A	813	LYS
1	A	882	GLU
1	A	985	SER
1	A	1018	LEU
1	A	1147	SER
1	A	1227	ILE
1	A	1260	ASN
1	A	1271	SER
1	A	1297	HIS
1	B	213	THR
1	B	214	GLN
1	B	544	SER
1	B	812	LEU
1	B	882	GLU
1	B	884	LEU
1	B	985	SER
1	B	1114	ILE
1	B	1271	SER
1	B	1301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	231	GLN
1	A	282	HIS
1	A	340	HIS
1	A	380	ASN
1	A	415	ASN
1	A	568	GLN
1	B	214	GLN
1	B	231	GLN
1	B	282	HIS
1	B	298	ASN
1	B	340	HIS
1	B	415	ASN
1	B	582	HIS
1	B	1095	ASN
1	B	1292	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](#)

21 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	$\# Z > 2$
6	MLI	A	3006	-	6,6,6	1.32	0	7,7,7	1.02	0
2	FES	A	3001	1	0,4,4	-	-	-		
7	PG6	A	3007	-	17,17,17	0.54	0	16,16,16	0.18	0
4	MOS	B	3004	3	0,3,3	-	-	-		
6	MLI	B	3007	-	6,6,6	1.34	0	7,7,7	0.98	0
10	DMS	B	3008	-	3,3,3	0.74	0	3,3,3	3.29	3 (100%)
3	MTE	B	3003	4	21,26,26	0.46	0	19,40,40	1.35	1 (5%)
2	FES	B	3001	1	0,4,4	-	-	-		
2	FES	B	3002	1	0,4,4	-	-	-		
5	FAD	A	3005	-	58,58,58	0.55	0	85,89,89	0.59	1 (1%)
9	RAL	A	3010	-	38,38,38	0.24	0	52,53,53	0.73	2 (3%)
3	MTE	A	3003	4	21,26,26	0.46	0	19,40,40	1.37	2 (10%)
9	RAL	A	3011	-	38,38,38	0.29	0	52,53,53	0.76	2 (3%)
8	GOL	A	3009	-	5,5,5	0.95	0	5,5,5	1.06	0
2	FES	A	3002	1	0,4,4	-	-	-		
8	GOL	A	3008	-	5,5,5	0.93	0	5,5,5	1.07	0
5	FAD	B	3005	-	58,58,58	0.54	0	85,89,89	0.60	1 (1%)
9	RAL	B	3010	-	38,38,38	0.33	0	52,53,53	0.82	2 (3%)
8	GOL	B	3006	-	5,5,5	0.96	0	5,5,5	1.08	0
9	RAL	B	3009	-	38,38,38	0.24	0	52,53,53	0.71	2 (3%)
4	MOS	A	3004	3	0,3,3	-	-	-		

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
5	FAD	A	3005	-	-	1/34/50/50	0/6/6/6
6	MLI	A	3006	-	-	2/4/4/4	-
9	RAL	A	3010	-	-	0/18/26/26	0/5/5/5
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
3	MTE	A	3003	4	-	1/6/34/34	0/3/3/3
6	MLI	B	3007	-	-	2/4/4/4	-
9	RAL	A	3011	-	-	0/18/26/26	0/5/5/5
8	GOL	A	3008	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	B	3005	-	-	1/34/50/50	0/6/6/6
7	PG6	A	3007	-	-	9/15/15/15	-
9	RAL	B	3010	-	-	1/18/26/26	0/5/5/5
3	MTE	B	3003	4	-	1/6/34/34	0/3/3/3
8	GOL	B	3006	-	-	2/4/4/4	-
2	FES	B	3001	1	-	-	0/1/1/1
9	RAL	B	3009	-	-	2/18/26/26	0/5/5/5
2	FES	B	3002	1	-	-	0/1/1/1
8	GOL	A	3009	-	-	2/4/4/4	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3008	DMS	C2-S-C1	4.24	120.15	98.42
3	B	3003	MTE	C2-N1-C10	3.11	118.85	113.36
3	A	3003	MTE	C2-N1-C10	3.11	118.84	113.36
9	B	3010	RAL	C17-C16-C15	3.10	124.90	119.69
9	B	3010	RAL	C5-S6-C7	3.05	92.92	90.58
9	A	3011	RAL	C5-S6-C7	2.85	92.76	90.58
9	A	3011	RAL	C17-C16-C15	2.76	124.33	119.69
10	B	3008	DMS	O-S-C2	2.71	120.08	106.49
9	A	3010	RAL	C17-C16-C15	2.66	124.16	119.69
10	B	3008	DMS	O-S-C1	2.65	119.77	106.49
9	A	3010	RAL	C5-S6-C7	2.56	92.55	90.58
9	B	3009	RAL	C5-S6-C7	2.48	92.48	90.58
9	B	3009	RAL	C17-C16-C15	2.41	123.74	119.69
3	A	3003	MTE	O3'-C7-N8	2.13	110.54	108.61
5	A	3005	FAD	C4-N3-C2	-2.09	121.93	125.64
5	B	3005	FAD	C4-N3-C2	-2.08	121.94	125.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3003	MTE	C3'-C4'-O4'-P
9	B	3009	RAL	O23-C24-C25-N26
7	A	3007	PG6	O1-C2-C3-O2
3	B	3003	MTE	C3'-C4'-O4'-P
7	A	3007	PG6	O5-C10-C11-O6

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Mol	Chain	Res	Type	Atoms
7	A	3007	PG6	O2-C4-C5-O3
7	A	3007	PG6	C2-C3-O2-C4
8	A	3008	GOL	O1-C1-C2-C3
8	A	3009	GOL	O1-C1-C2-C3
8	B	3006	GOL	O1-C1-C2-C3
8	B	3006	GOL	O1-C1-C2-O2
9	B	3009	RAL	C25-C24-O23-C20
9	B	3010	RAL	C25-C24-O23-C20
6	A	3006	MLI	C2-C1-C3-O9
6	A	3006	MLI	C2-C1-C3-O8
7	A	3007	PG6	C3-C2-O1-C1
7	A	3007	PG6	C10-C11-O6-C12
8	A	3008	GOL	O1-C1-C2-O2
7	A	3007	PG6	C11-C10-O5-C9
6	B	3007	MLI	C3-C1-C2-O6
6	B	3007	MLI	C3-C1-C2-O7
5	B	3005	FAD	C4'-C5'-O5'-P
7	A	3007	PG6	O4-C8-C9-O5
5	A	3005	FAD	C4'-C5'-O5'-P
8	A	3009	GOL	O1-C1-C2-O2
7	A	3007	PG6	C6-C7-O4-C8

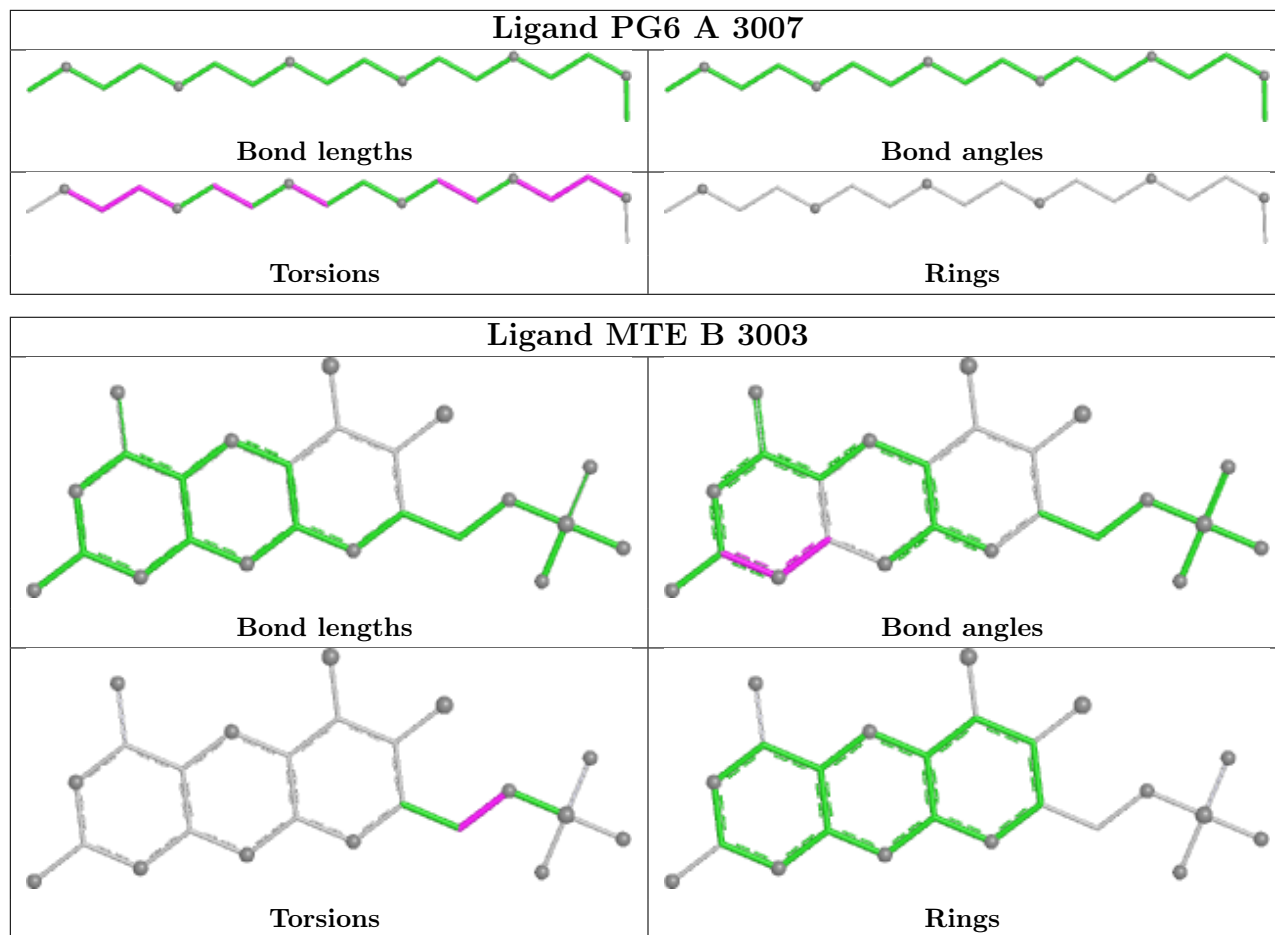
There are no ring outliers.

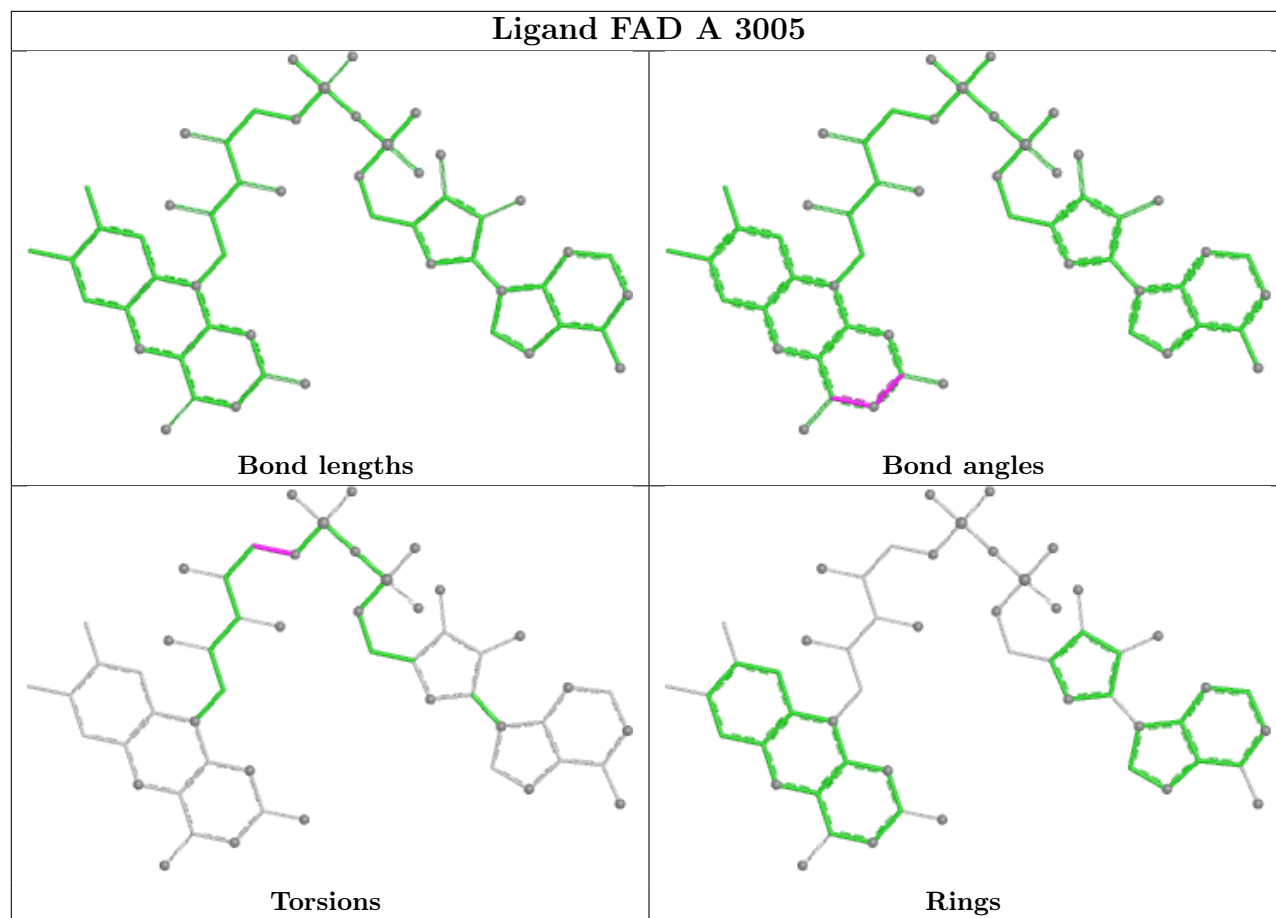
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3007	PG6	2	0
5	A	3005	FAD	1	0
8	B	3006	GOL	1	0
9	B	3009	RAL	1	0

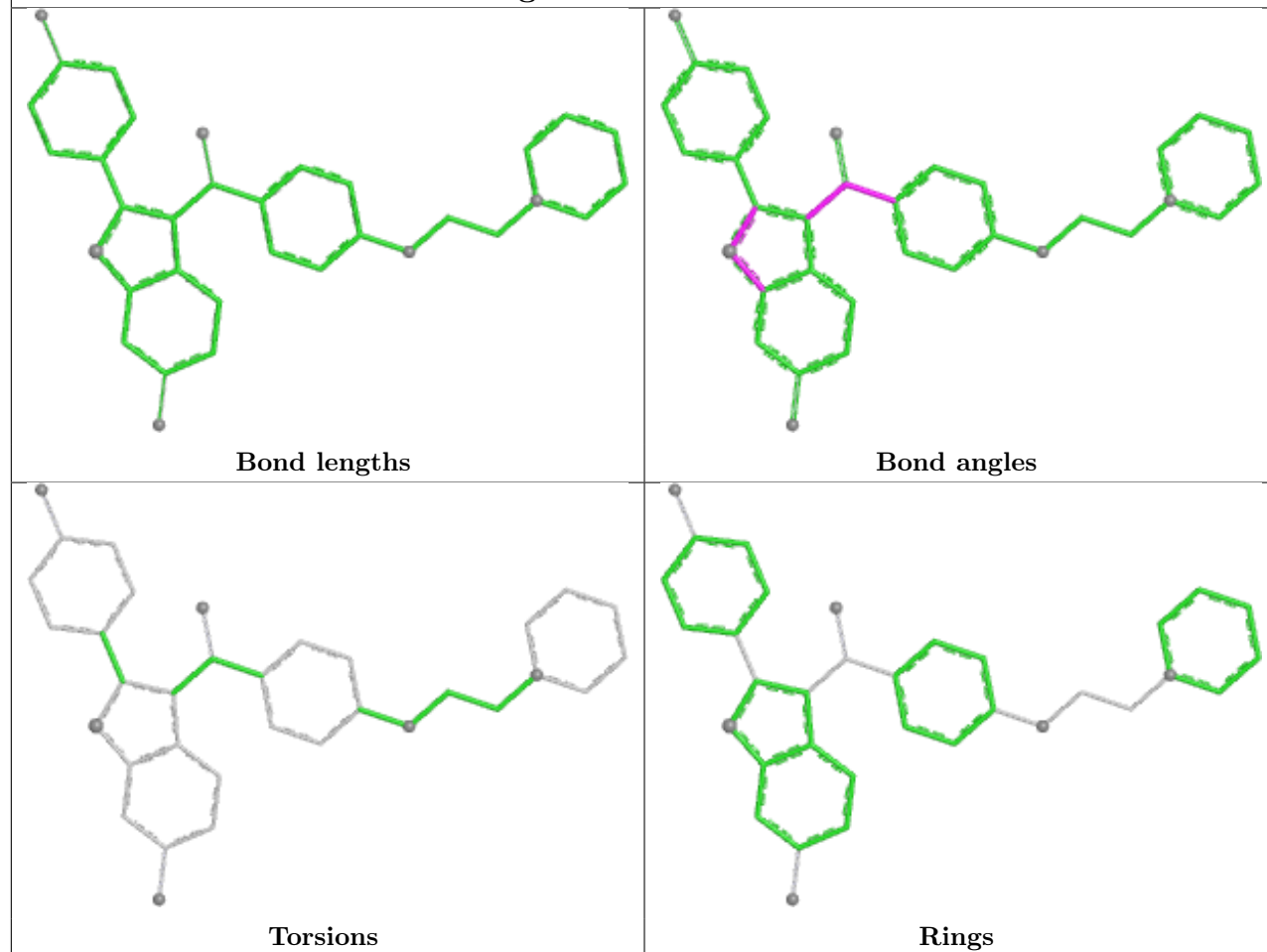
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

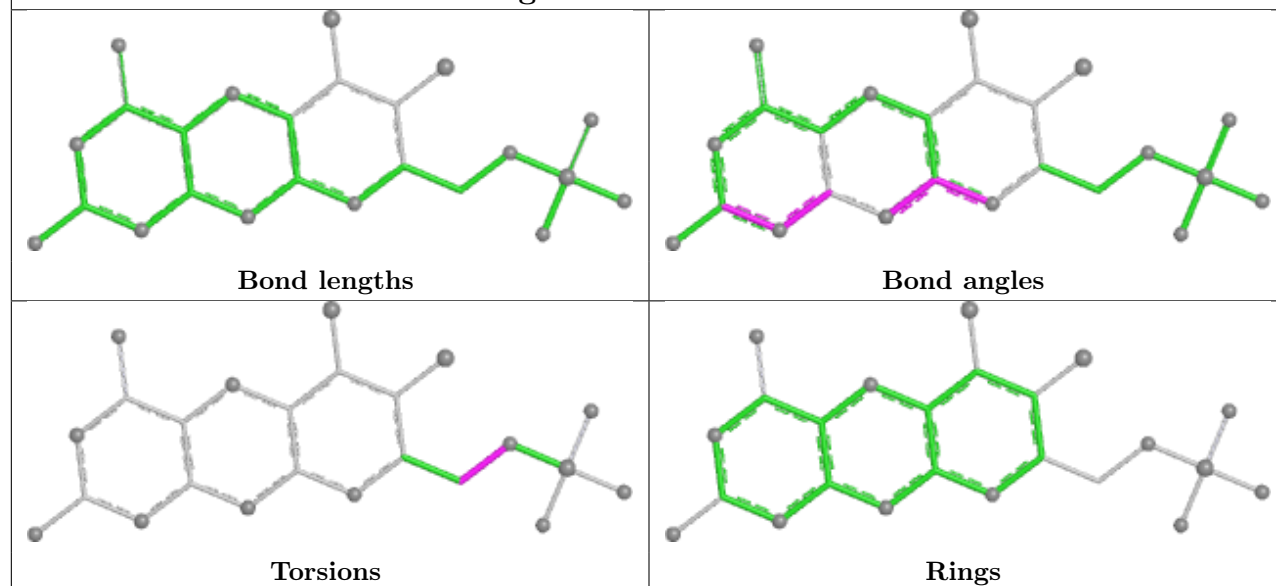


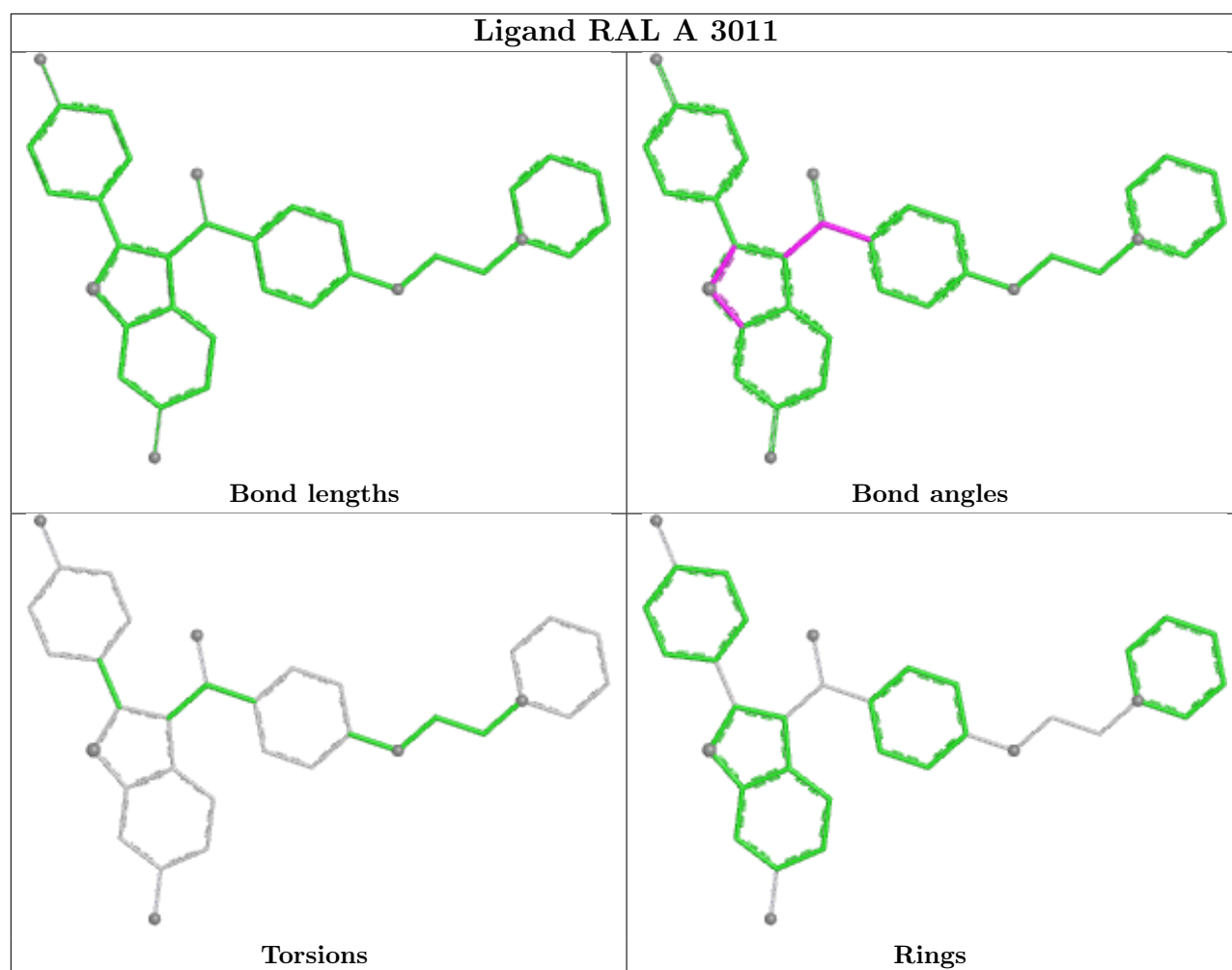


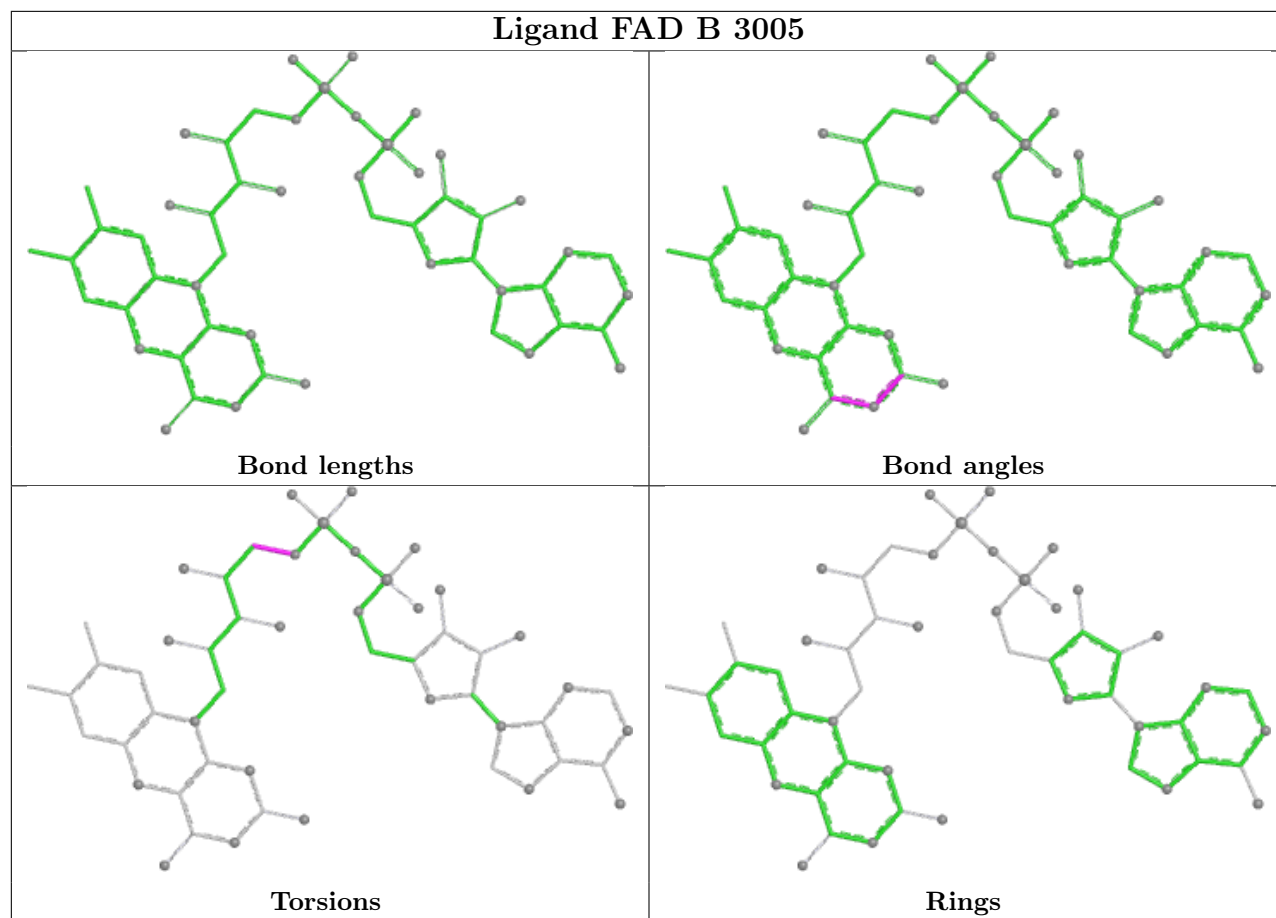
Ligand RAL A 3010

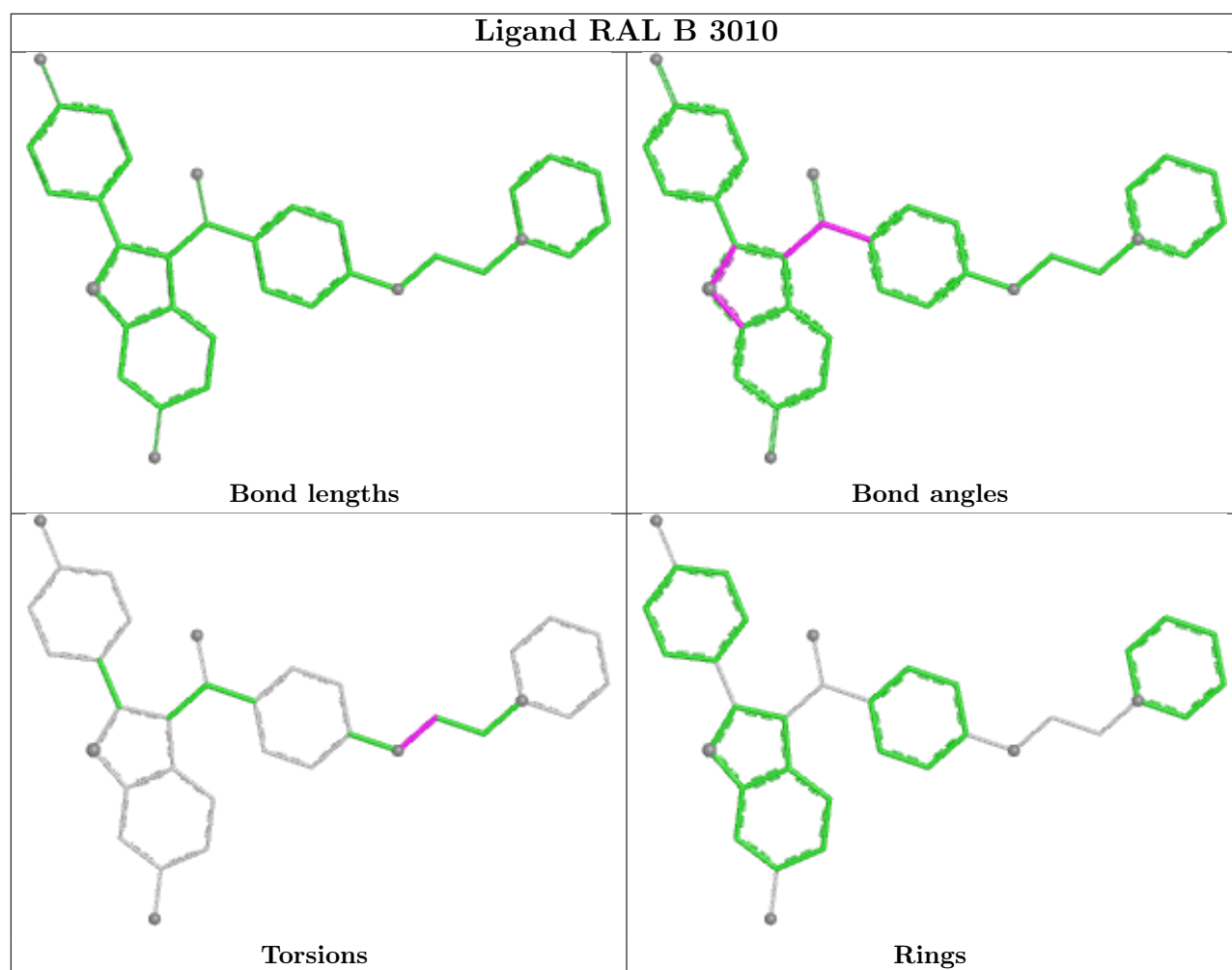


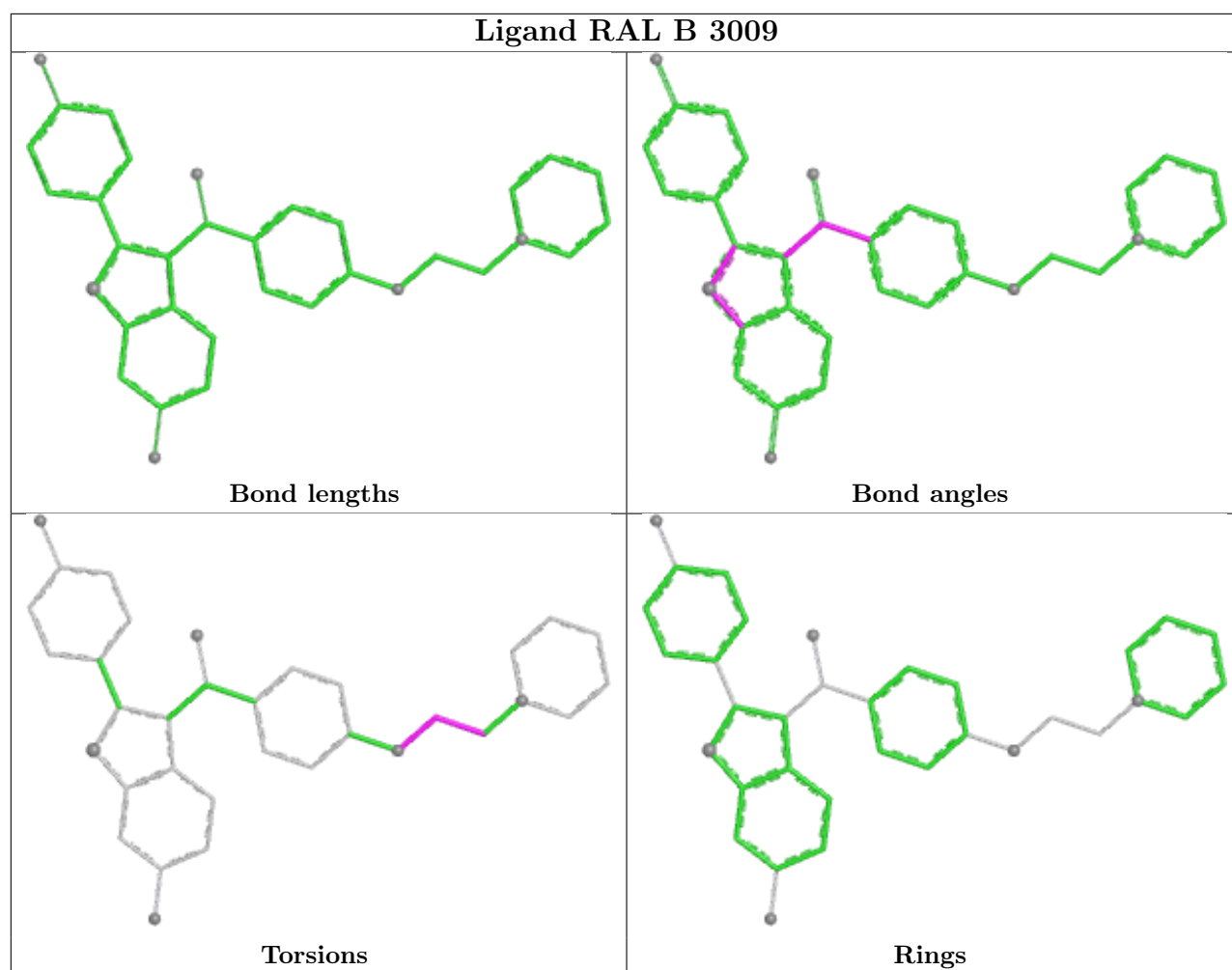
Ligand MTE A 3003











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	1295/1338 (96%)	-0.25	14 (1%) 78 74	38, 57, 80, 96	0
1	B	1295/1338 (96%)	-0.16	10 (0%) 82 80	39, 60, 82, 110	1 (0%)
All	All	2590/2676 (96%)	-0.20	24 (0%) 81 78	38, 59, 81, 110	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	PRO	3.5
1	A	560	HIS	3.0
1	B	560	HIS	3.0
1	A	557	HIS	2.5
1	A	881	ASP	2.5
1	B	1297	HIS	2.5
1	B	4	ALA	2.5
1	A	1088	GLY	2.4
1	A	453	ASP	2.4
1	B	549	TYR	2.4
1	A	4	ALA	2.4
1	A	558	SER	2.3
1	B	883	SER	2.3
1	B	301[A]	TYR	2.2
1	B	923	PHE	2.2
1	A	1268	LEU	2.2
1	B	561	HIS	2.2
1	A	301	TYR	2.2
1	A	67	ARG	2.2
1	A	1336	VAL	2.1
1	A	199	PRO	2.1
1	A	111	GLY	2.1
1	B	557	HIS	2.1
1	A	549	TYR	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](#)

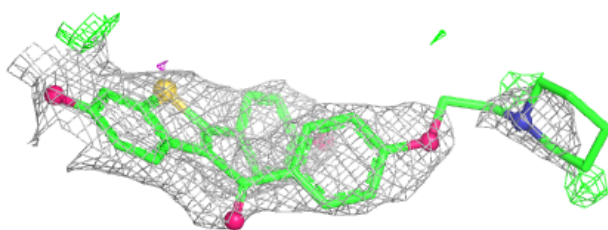
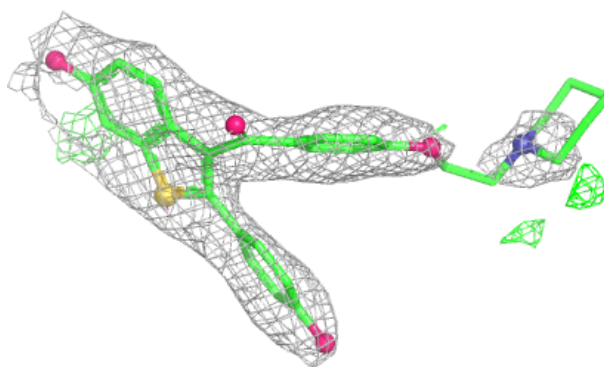
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	RAL	A	3011	34/34	0.76	0.15	77,86,100,102	0
6	MLI	A	3006	7/7	0.78	0.22	66,66,71,74	0
8	GOL	A	3009	6/6	0.79	0.12	68,71,74,76	0
8	GOL	A	3008	6/6	0.79	0.19	59,61,62,66	0
8	GOL	B	3006	6/6	0.80	0.19	53,56,58,61	6
10	DMS	B	3008	4/4	0.80	0.26	71,72,73,84	4
9	RAL	B	3009	34/34	0.81	0.16	66,75,98,102	0
9	RAL	B	3010	34/34	0.84	0.13	71,78,95,97	0
7	PG6	A	3007	18/18	0.84	0.15	39,55,60,61	0
9	RAL	A	3010	34/34	0.85	0.14	66,74,89,91	0
6	MLI	B	3007	7/7	0.91	0.08	72,74,83,84	0
3	MTE	A	3003	24/24	0.92	0.09	46,53,61,68	24
3	MTE	B	3003	24/24	0.93	0.09	47,58,66,71	24
5	FAD	B	3005	53/53	0.95	0.08	43,51,56,57	0
2	FES	B	3002	4/4	0.95	0.08	56,58,59,66	4
4	MOS	B	3004	4/4	0.95	0.11	69,70,72,76	4
4	MOS	A	3004	4/4	0.96	0.10	62,62,63,67	4
2	FES	A	3002	4/4	0.96	0.06	57,58,58,67	4
5	FAD	A	3005	53/53	0.96	0.07	44,50,54,54	0
2	FES	A	3001	4/4	0.99	0.03	36,36,43,44	0
2	FES	B	3001	4/4	0.99	0.02	40,40,45,47	0

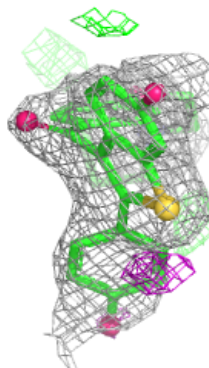
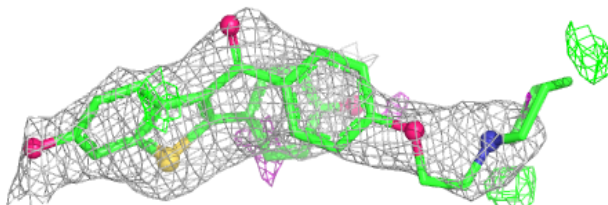
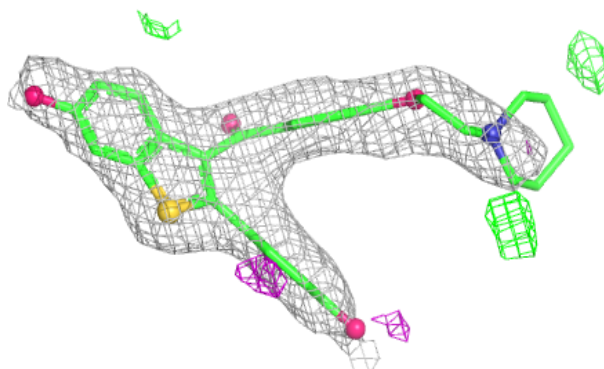
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RAL A 3011:

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

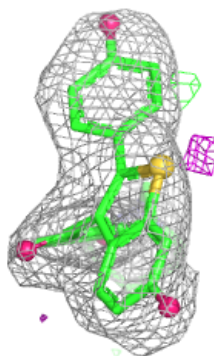
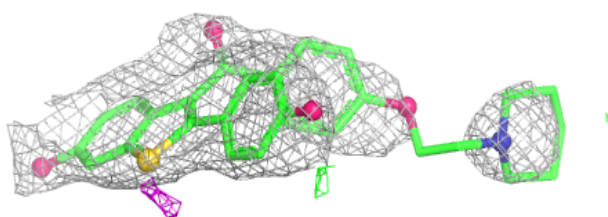
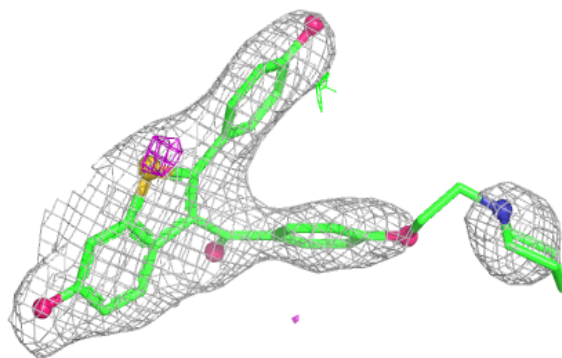
**Electron density around RAL B 3009:**

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

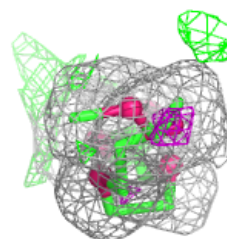
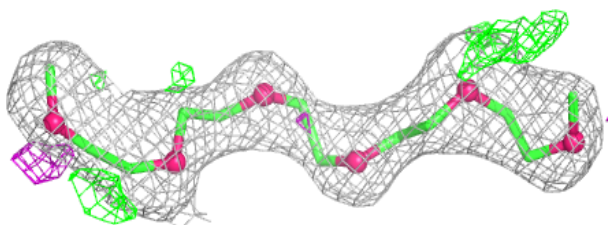
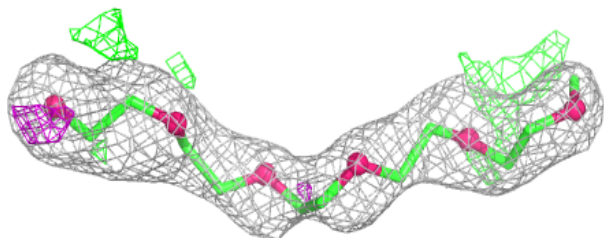


Electron density around RAL B 3010:

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

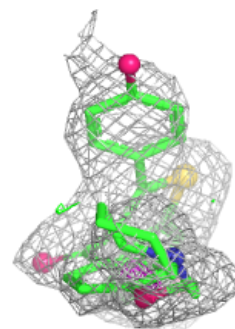
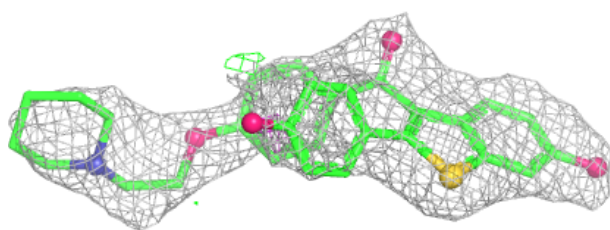
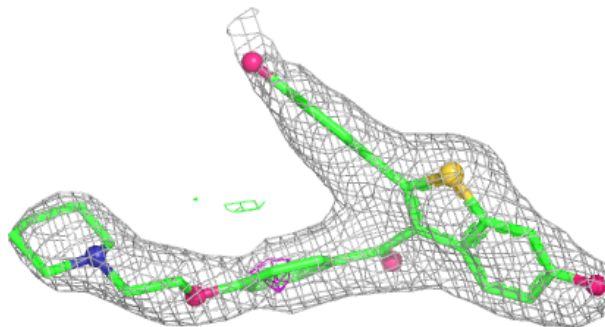
**Electron density around PG6 A 3007:**

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

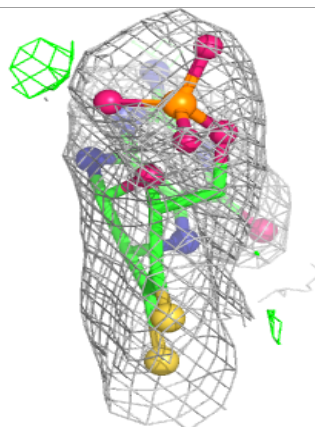
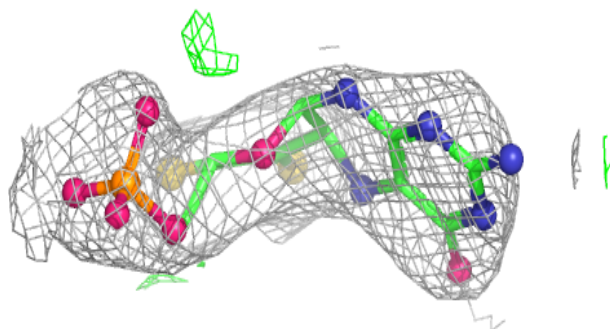
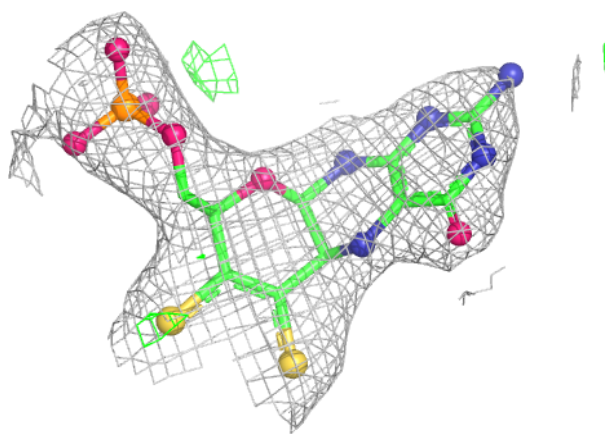


Electron density around RAL A 3010:

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

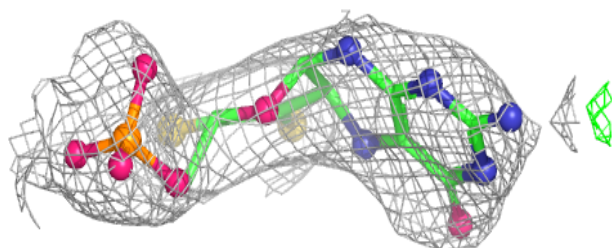
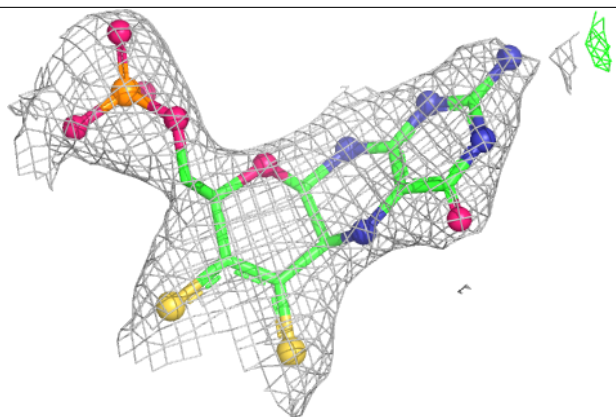
**Electron density around MTE A 3003:**

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

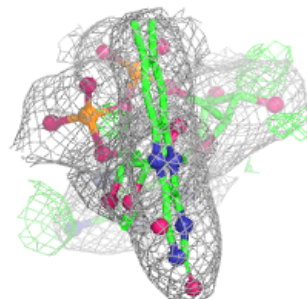
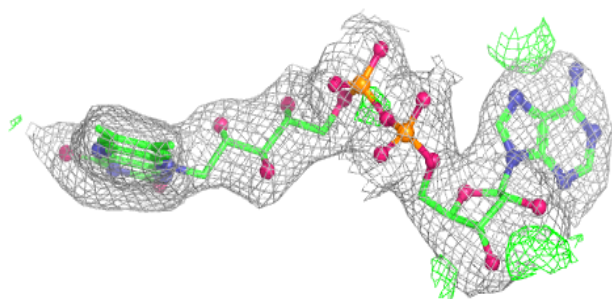
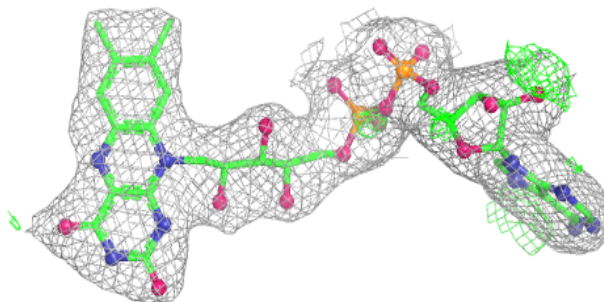


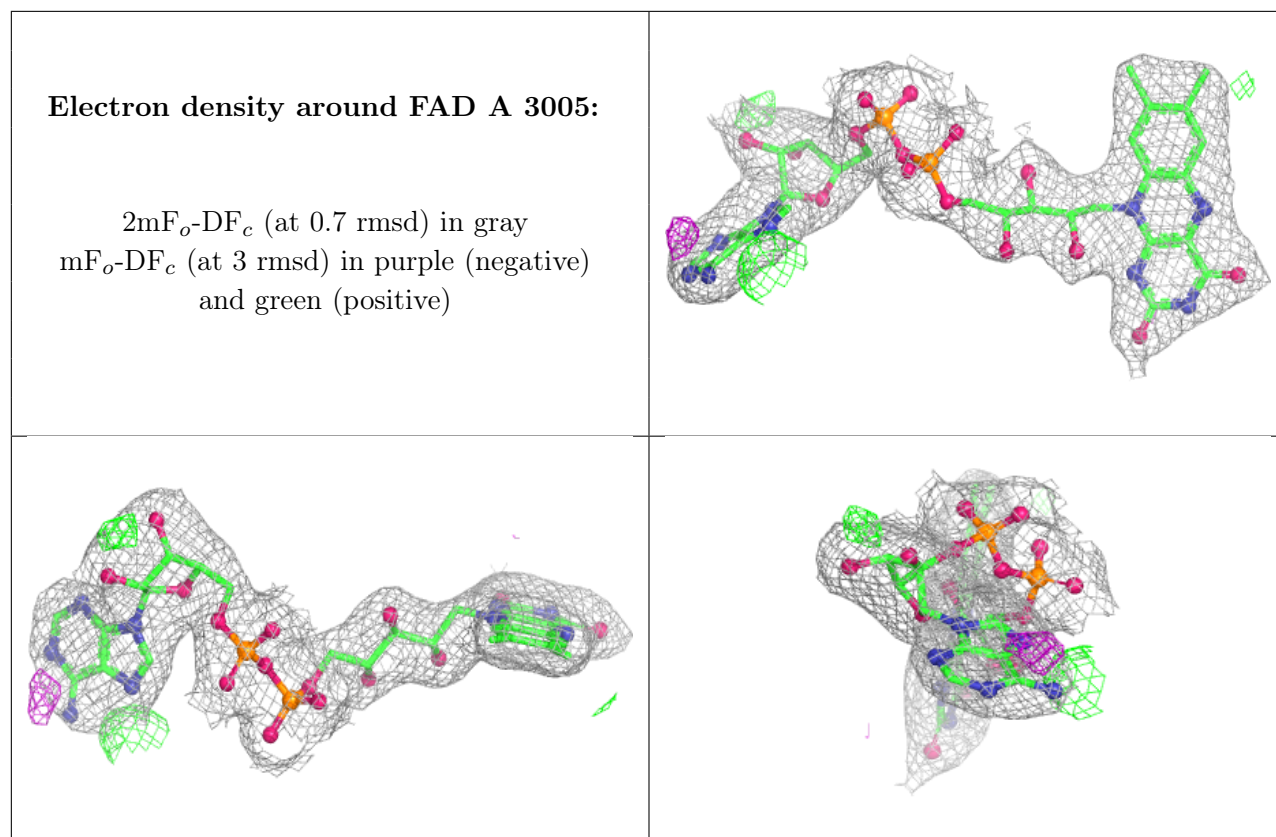
Electron density around MTE B 3003:

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

**Electron density around FAD B 3005:**

$2mF_o-DF_c$ (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.