



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:13 PM UTC

PDB ID : 5EPG / pdb_00005epg
Title : Human aldehyde oxidase SNP S1271L
Authors : Coelho, C.; Romao, M.J.; Santos-Silva, T.
Deposited on : 2015-11-11
Resolution : 3.39 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

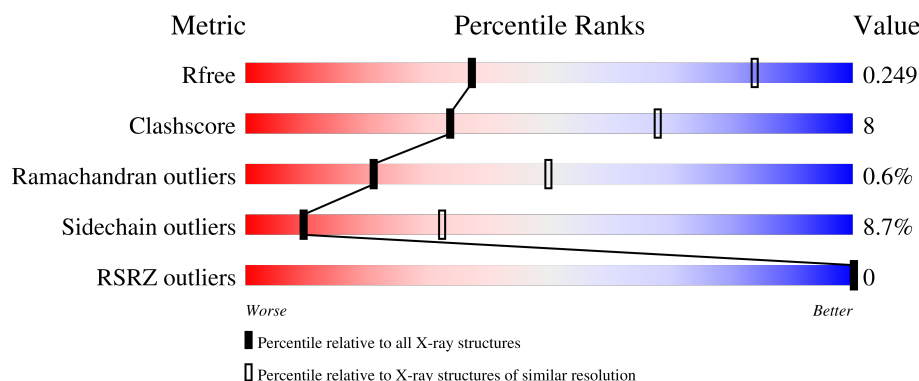
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1338	

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
5	MOS	A	3005	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10131 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.

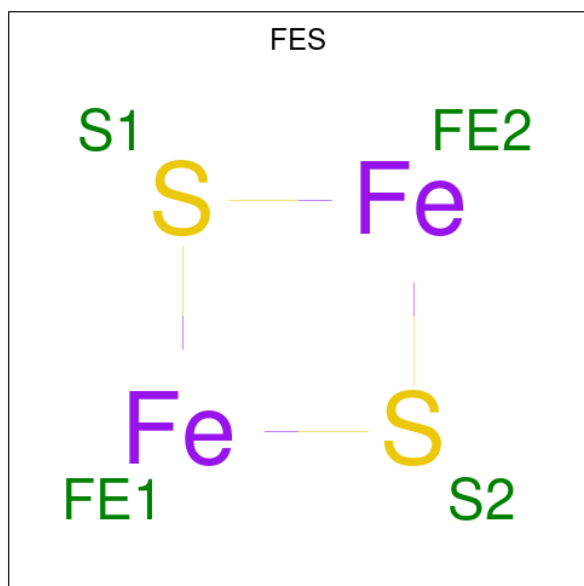
- Molecule 1 is a protein called Aldehyde oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1288	9990	6351	1722	1837	80	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	LEU	SER	engineered mutation	UNP Q06278

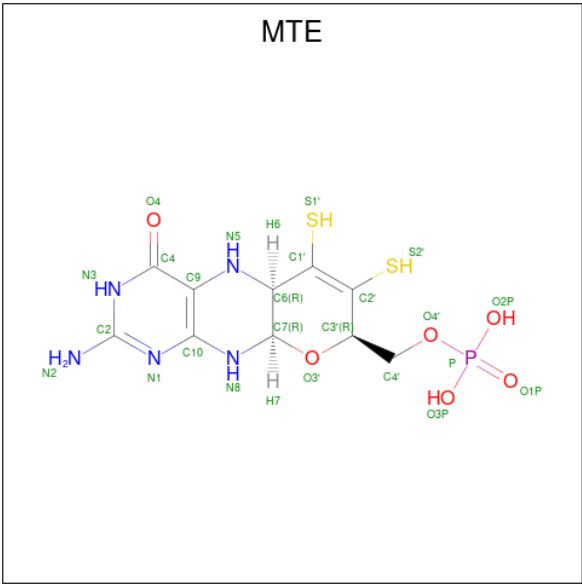
- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

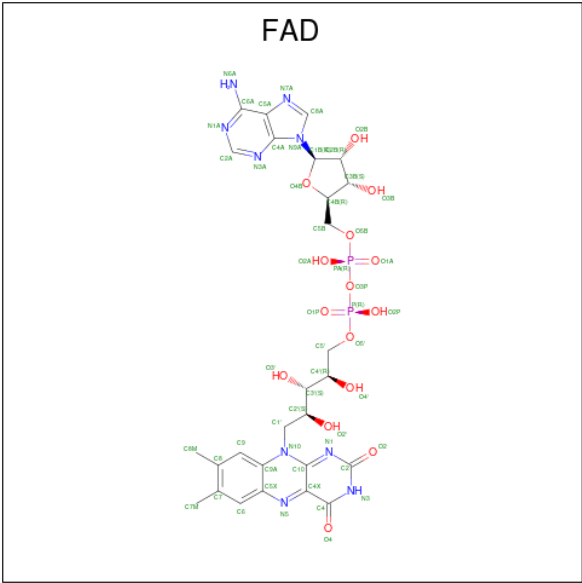
- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A,

9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL)
ESTER (CCD ID: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



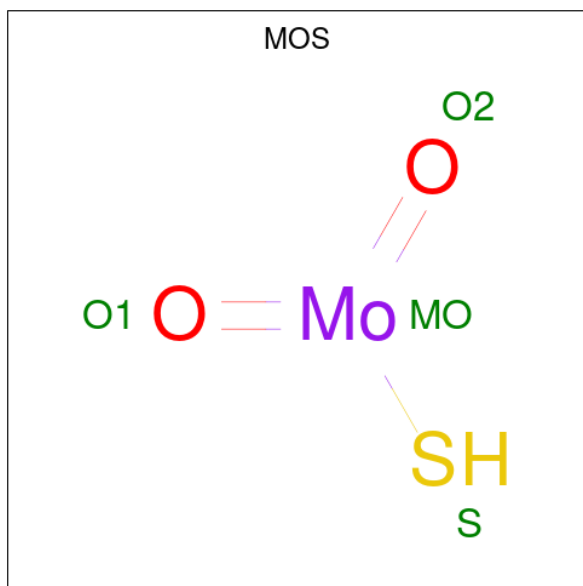
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



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

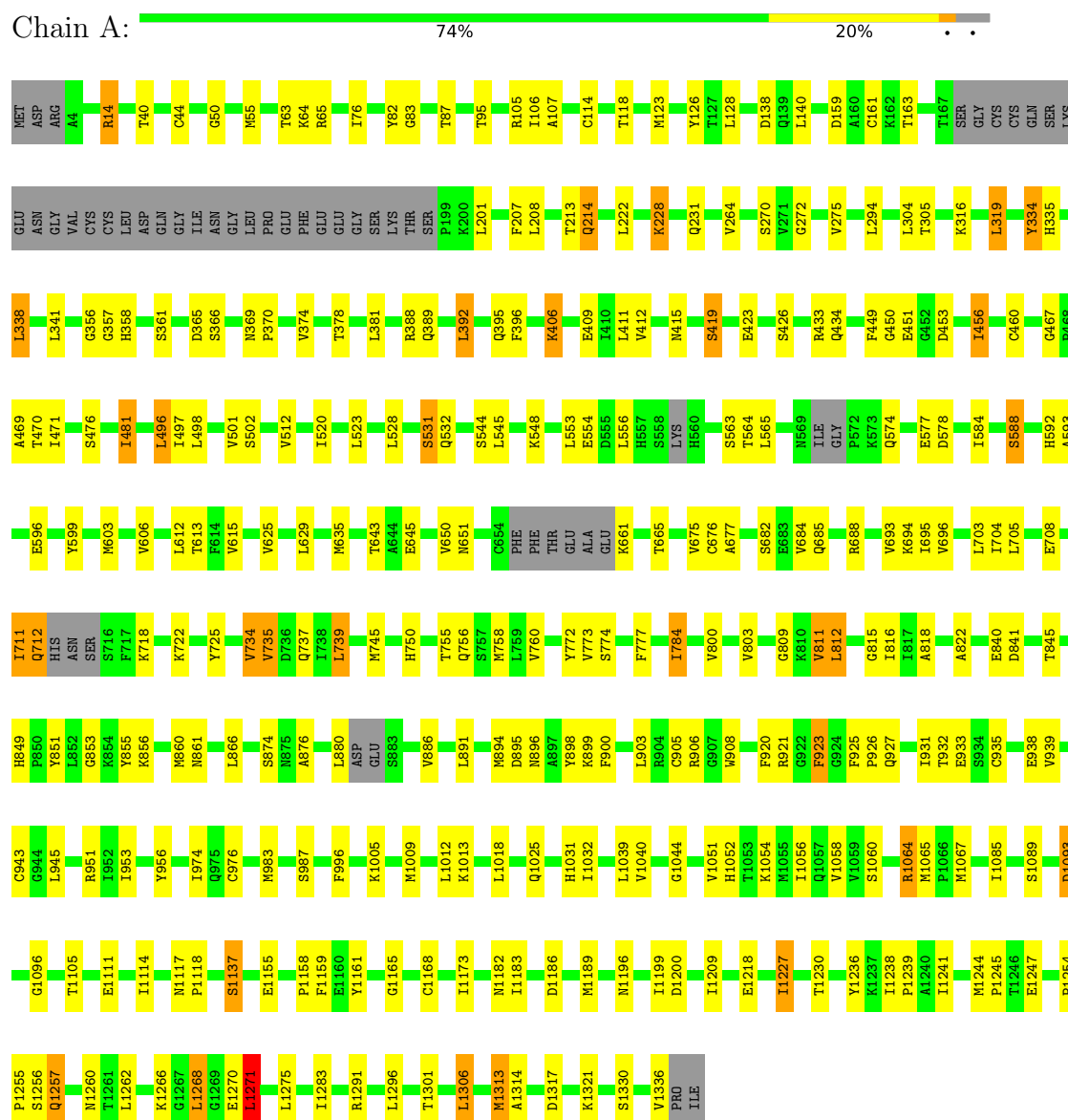
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total	O	0	0
			52	52		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	147.44Å 147.44Å 131.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 3.39 49.16 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.16-3.39) 99.2 (49.16-3.39)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.253 0.166 , 0.249	Depositor DCC
R_{free} test set	1046 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	99.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10131	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.71	0/10199	0.97	10/13788 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	GLY	CA-C-N	7.26	127.90	119.47
1	A	467	GLY	C-N-CA	7.26	127.90	119.47
1	A	1260	ASN	N-CA-C	6.46	119.14	111.71
1	A	1254	PRO	CA-C-N	6.17	126.53	119.92
1	A	1254	PRO	C-N-CA	6.17	126.53	119.92
1	A	684	VAL	CB-CA-C	-5.96	104.33	111.97
1	A	76	ILE	CB-CA-C	-5.86	104.44	110.71
1	A	1271	LEU	CB-CA-C	-5.27	102.84	110.96
1	A	1044	GLY	N-CA-C	5.10	117.80	111.93
1	A	840	GLU	CB-CA-C	-5.07	102.37	110.79

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	9990	0	10057	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	0	0	1	0
3	A	24	0	12	2	0
4	A	53	0	31	2	0
5	A	4	0	0	3	0
6	A	52	0	0	10	0
All	All	10131	0	10100	156	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 8.

All (156) 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:365:ASP:HB3	6:A:3141:HOH:O	1.60	1.00
1:A:1064:ARG:HD2	6:A:3148:HOH:O	1.77	0.85
1:A:737:GLN:NE2	1:A:861:ASN:OD1	2.11	0.83
3:A:3003:MTE:S2'	5:A:3005:MOS:O1	2.37	0.81
1:A:841:ASP:O	1:A:845:THR:HG22	1.80	0.81
1:A:1111:GLU:HG2	6:A:3147:HOH:O	1.81	0.79
1:A:388:ARG:NH1	1:A:409:GLU:OE2	2.18	0.76
1:A:305:THR:HG22	1:A:415:ASN:OD1	1.90	0.72
1:A:1268:LEU:HA	1:A:1271:LEU:HD21	1.72	0.71
1:A:140:LEU:HD13	1:A:161:CYS:HB3	1.72	0.71
1:A:584:ILE:HG21	1:A:1067:MET:HE1	1.72	0.71
1:A:711:ILE:C	1:A:712:GLN:HE21	1.97	0.71
1:A:735:VAL:HA	1:A:860:MET:HE1	1.74	0.70
1:A:433:ARG:NH1	1:A:1238:ILE:O	2.27	0.67
1:A:358:HIS:NE2	1:A:366:SER:OG	2.29	0.66
1:A:853:GLY:HA3	1:A:931:ILE:HD12	1.79	0.63
1:A:735:VAL:HA	1:A:860:MET:CE	2.27	0.62
1:A:898:TYR:HB2	1:A:900:PHE:CE1	2.35	0.62
1:A:849:HIS:CE1	6:A:3112:HOH:O	2.52	0.62
1:A:1266:LYS:O	1:A:1268:LEU:HD23	2.01	0.60
1:A:471:ILE:HD11	1:A:501:VAL:HG23	1.82	0.60
1:A:1060:SER:OG	1:A:1065:MET:O	2.16	0.60
1:A:319:LEU:HB2	1:A:338:LEU:CD1	2.30	0.60
3:A:3003:MTE:S2'	5:A:3005:MOS:O2	2.59	0.60
1:A:528:LEU:HB3	1:A:553:LEU:HD11	1.83	0.59
1:A:128:LEU:HD22	1:A:140:LEU:HD23	1.85	0.58
1:A:449:PHE:CE1	1:A:456:ILE:HG22	2.39	0.58
1:A:612:LEU:HD11	1:A:677:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HD11	1:A:481:ILE:HA	1.86	0.56
1:A:1209:ILE:HG22	1:A:1239:PRO:HG2	1.87	0.56
1:A:214:GLN:HE21	1:A:214:GLN:N	2.04	0.55
1:A:996:PHE:CD2	1:A:1005:LYS:HE3	2.42	0.55
1:A:554:GLU:OE1	1:A:554:GLU:N	2.39	0.55
1:A:319:LEU:HB2	1:A:338:LEU:HD11	1.89	0.55
1:A:896:ASN:O	1:A:1013:LYS:HE3	2.07	0.55
1:A:1227:ILE:HD12	1:A:1227:ILE:N	2.21	0.55
1:A:1031:HIS:ND1	1:A:1137:SER:OG	2.37	0.54
1:A:95:THR:HG23	1:A:596:GLU:OE2	2.07	0.54
1:A:1291:ARG:NH1	1:A:1314:ALA:O	2.41	0.53
1:A:983:MET:HE3	1:A:1186:ASP:HB3	1.90	0.53
1:A:357:GLY:O	1:A:361:SER:OG	2.23	0.53
1:A:722:LYS:HG3	1:A:906:ARG:HG2	1.89	0.53
1:A:272:GLY:O	1:A:275:VAL:HG22	2.08	0.53
1:A:1268:LEU:HB3	1:A:1271:LEU:HD11	1.90	0.53
1:A:756:GLN:HA	6:A:3125:HOH:O	2.09	0.52
1:A:635:MET:HE1	1:A:688:ARG:HB3	1.90	0.52
1:A:497:ILE:HD13	1:A:523:LEU:HD22	1.91	0.52
1:A:369:ASN:N	1:A:370:PRO:HD2	2.25	0.52
1:A:712:GLN:HE21	1:A:712:GLN:N	2.08	0.51
1:A:214:GLN:HE21	1:A:214:GLN:CA	2.23	0.51
1:A:739:LEU:C	1:A:739:LEU:HD23	2.34	0.51
1:A:908:TRP:HA	6:A:3129:HOH:O	2.10	0.51
1:A:83:GLY:O	1:A:222:LEU:HD22	2.10	0.51
1:A:63:THR:OG1	1:A:65:ARG:HG3	2.10	0.51
1:A:811:VAL:HG21	1:A:1085:ILE:HD11	1.93	0.51
1:A:925:PHE:HB3	1:A:926:PRO:HD3	1.93	0.51
1:A:615:VAL:HB	1:A:676:CYS:HB2	1.93	0.51
1:A:894:MET:O	1:A:932:THR:HG21	2.12	0.51
1:A:933:GLU:OE1	1:A:951:ARG:NE	2.43	0.50
1:A:1268:LEU:HA	1:A:1271:LEU:CD2	2.42	0.50
1:A:860:MET:HE3	1:A:866:LEU:HD12	1.94	0.50
1:A:305:THR:CG2	1:A:415:ASN:OD1	2.59	0.50
1:A:603:MET:HE1	1:A:772:TYR:HB2	1.95	0.49
1:A:891:LEU:HD22	1:A:905:CYS:SG	2.52	0.49
1:A:1200:ASP:HB3	1:A:1268:LEU:HD11	1.94	0.49
1:A:1255:PRO:HA	6:A:3127:HOH:O	2.12	0.49
1:A:711:ILE:C	1:A:712:GLN:NE2	2.67	0.49
1:A:899:LYS:HB2	1:A:956:TYR:CD1	2.48	0.49
1:A:1218:GLU:OE1	1:A:1236:TYR:OH	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TYR:CD1	1:A:334:TYR:N	2.79	0.48
1:A:855:TYR:HD2	1:A:935:CYS:HG	1.60	0.48
1:A:406:LYS:HG2	1:A:409:GLU:OE2	2.14	0.48
1:A:811:VAL:HG12	1:A:812:LEU:N	2.29	0.48
1:A:773:VAL:O	1:A:800:VAL:HG22	2.13	0.48
1:A:1012:LEU:HB2	1:A:1275:LEU:HD21	1.96	0.48
1:A:758:MET:SD	1:A:818:ALA:HA	2.54	0.48
1:A:1117:ASN:N	1:A:1118:PRO:HD3	2.29	0.48
1:A:419:SER:HA	1:A:423:GLU:OE1	2.13	0.48
1:A:316:LYS:HB2	1:A:341:LEU:HD13	1.95	0.48
1:A:381:LEU:HD23	1:A:409:GLU:OE2	2.13	0.47
1:A:264:VAL:N	4:A:3004:FAD:O2B	2.44	0.47
1:A:55:MET:HE1	1:A:126:TYR:HE2	1.77	0.47
1:A:83:GLY:C	1:A:222:LEU:HD22	2.39	0.47
1:A:264:VAL:O	4:A:3004:FAD:H2B	2.15	0.47
1:A:1196:ASN:CG	1:A:1199:ILE:HD12	2.39	0.47
1:A:356:GLY:HA2	1:A:411:LEU:HD23	1.97	0.47
1:A:734:VAL:O	1:A:734:VAL:HG23	2.13	0.47
1:A:876:ALA:HA	6:A:3112:HOH:O	2.15	0.47
1:A:629:LEU:HD23	1:A:693:VAL:HG13	1.97	0.47
1:A:1056:ILE:HG22	1:A:1067:MET:HG2	1.97	0.47
1:A:1317:ASP:O	1:A:1321:LYS:HG2	2.15	0.47
1:A:531:SER:O	1:A:545:LEU:HD11	2.15	0.47
1:A:1189:MET:HE1	1:A:1275:LEU:CD1	2.45	0.47
1:A:228:LYS:O	1:A:228:LYS:HG3	2.15	0.47
1:A:898:TYR:OH	1:A:933:GLU:OE2	2.28	0.47
1:A:774:SER:OG	1:A:803:VAL:HG13	2.14	0.46
1:A:1009:MET:HE2	1:A:1168:CYS:HB2	1.97	0.46
1:A:1227:ILE:N	1:A:1227:ILE:CD1	2.78	0.46
1:A:106:ILE:CG2	1:A:107:ALA:N	2.74	0.46
1:A:943:CYS:HB3	1:A:945:LEU:HD12	1.97	0.45
1:A:50:GLY:N	2:A:3002:FES:S1	2.89	0.45
1:A:456:ILE:CD1	1:A:481:ILE:HA	2.46	0.45
1:A:588:SER:HB2	1:A:592:HIS:CE1	2.52	0.45
1:A:849:HIS:HE1	6:A:3112:HOH:O	1.92	0.45
1:A:378:THR:CB	1:A:389:GLN:HE21	2.30	0.45
1:A:739:LEU:HD11	1:A:938:GLU:HB3	1.99	0.45
1:A:392:LEU:HD13	1:A:396:PHE:CD2	2.52	0.44
1:A:703:LEU:HD11	1:A:705:LEU:HD21	1.99	0.44
1:A:894:MET:HE1	1:A:903:LEU:HD21	1.99	0.44
1:A:87:THR:O	1:A:123:MET:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:SER:HB2	1:A:592:HIS:NE2	2.32	0.44
1:A:476:SER:OG	1:A:496:LEU:O	2.35	0.44
1:A:651:ASN:O	1:A:651:ASN:CG	2.61	0.44
1:A:750:HIS:HA	1:A:920:PHE:CZ	2.53	0.44
1:A:675:VAL:HG11	1:A:695:ILE:HD13	1.99	0.44
1:A:14:ARG:NH1	1:A:14:ARG:HB2	2.32	0.44
1:A:625:VAL:HG22	1:A:696:VAL:O	2.18	0.44
1:A:1189:MET:HE1	1:A:1275:LEU:HD11	1.99	0.44
1:A:976:CYS:SG	1:A:1165:GLY:HA2	2.58	0.43
1:A:603:MET:HE1	1:A:772:TYR:CB	2.48	0.43
1:A:1093:ASP:OD2	1:A:1161:TYR:OH	2.33	0.43
1:A:374:VAL:HG12	1:A:460:CYS:HB3	1.99	0.43
1:A:784:ILE:HD13	1:A:815:GLY:O	2.18	0.43
1:A:895:ASP:OD1	1:A:1013:LYS:NZ	2.45	0.43
1:A:114:CYS:O	1:A:599:TYR:OH	2.32	0.43
1:A:501:VAL:O	1:A:501:VAL:HG22	2.18	0.43
1:A:469:ALA:O	1:A:471:ILE:HG23	2.18	0.42
1:A:1238:ILE:HB	1:A:1239:PRO:CD	2.49	0.42
1:A:105:ARG:HG2	1:A:207:PHE:CD2	2.55	0.42
1:A:923:PHE:CE2	5:A:3005:MOS:S	3.12	0.42
1:A:1257:GLN:HE21	1:A:1257:GLN:N	2.18	0.42
1:A:118:THR:HG22	1:A:593:ALA:HA	2.02	0.42
1:A:1283:ILE:CG2	1:A:1306:LEU:HD13	2.49	0.42
1:A:528:LEU:CB	1:A:553:LEU:HD11	2.49	0.42
1:A:745:MET:SD	1:A:927:GLN:HA	2.59	0.42
1:A:1182:ASN:HB3	6:A:3107:HOH:O	2.20	0.42
1:A:1051:VAL:HG13	1:A:1052:HIS:CD2	2.55	0.42
1:A:725:TYR:HE2	1:A:899:LYS:HE3	1.85	0.41
1:A:760:VAL:HG11	1:A:822:ALA:HA	2.01	0.41
1:A:898:TYR:HB2	1:A:900:PHE:HE1	1.83	0.41
1:A:1012:LEU:HD13	1:A:1275:LEU:HD21	2.01	0.41
1:A:159:ASP:O	1:A:163:THR:HG23	2.20	0.41
1:A:750:HIS:CE1	1:A:809:GLY:CA	3.04	0.41
1:A:1244:MET:HG2	1:A:1245:PRO:HD2	2.02	0.41
1:A:777:PHE:CD2	1:A:1085:ILE:HD12	2.56	0.41
1:A:1054:LYS:O	1:A:1058:VAL:HG23	2.21	0.41
1:A:1096:GLY:HA3	1:A:1262:LEU:HD22	2.03	0.41
1:A:574:GLN:HE21	1:A:578:ASP:HB3	1.85	0.41
1:A:498:LEU:HD11	1:A:520:ILE:HD13	2.02	0.41
1:A:735:VAL:HG12	1:A:860:MET:HE3	2.02	0.41
1:A:1093:ASP:OD1	1:A:1093:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:PRO:HG2	1:A:1159:PHE:CD2	2.56	0.41
1:A:682:SER:OG	1:A:685:GLN:NE2	2.54	0.40
1:A:82:TYR:CD1	1:A:82:TYR:C	2.99	0.40
1:A:201:LEU:HD11	1:A:565:LEU:HD13	2.03	0.40
1:A:1313:MET:HA	1:A:1313:MET:HE2	2.03	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	1274/1338 (95%)	1220 (96%)	46 (4%)	8 (1%)	21 50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	LYS
1	A	451	GLU
1	A	921	ARG
1	A	1257	GLN
1	A	450	GLY
1	A	532	GLN
1	A	453	ASP
1	A	811	VAL

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	1093/1136 (96%)	998 (91%)	95 (9%)	9 32

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	40	THR
1	A	44	CYS
1	A	64	LYS
1	A	138	ASP
1	A	208	LEU
1	A	213	THR
1	A	214	GLN
1	A	231	GLN
1	A	270	SER
1	A	294	LEU
1	A	304	LEU
1	A	319	LEU
1	A	334	TYR
1	A	335	HIS
1	A	338	LEU
1	A	392	LEU
1	A	395	GLN
1	A	406	LYS
1	A	412	VAL
1	A	419	SER
1	A	426	SER
1	A	434	GLN
1	A	456	ILE
1	A	470	THR
1	A	481	ILE
1	A	496	LEU
1	A	502	SER
1	A	512	VAL
1	A	531	SER
1	A	544	SER
1	A	548	LYS
1	A	556	LEU
1	A	563	SER
1	A	564	THR
1	A	577	GLU

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Mol	Chain	Res	Type
1	A	588	SER
1	A	606	VAL
1	A	613	THR
1	A	643	THR
1	A	645	GLU
1	A	650	VAL
1	A	661	LYS
1	A	665	THR
1	A	694	LYS
1	A	704	ILE
1	A	708	GLU
1	A	711	ILE
1	A	712	GLN
1	A	718	LYS
1	A	734	VAL
1	A	735	VAL
1	A	739	LEU
1	A	755	THR
1	A	784	ILE
1	A	812	LEU
1	A	816	ILE
1	A	851	TYR
1	A	856	LYS
1	A	874	SER
1	A	880	LEU
1	A	886	VAL
1	A	923	PHE
1	A	939	VAL
1	A	953	ILE
1	A	974	ILE
1	A	987	SER
1	A	1018	LEU
1	A	1025	GLN
1	A	1032	ILE
1	A	1039	LEU
1	A	1040	VAL
1	A	1064	ARG
1	A	1089	SER
1	A	1093	ASP
1	A	1105	THR
1	A	1114	ILE
1	A	1137	SER

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Mol	Chain	Res	Type
1	A	1155	GLU
1	A	1173	ILE
1	A	1183	ILE
1	A	1227	ILE
1	A	1230	THR
1	A	1241	ILE
1	A	1247	GLU
1	A	1256	SER
1	A	1268	LEU
1	A	1270	GLU
1	A	1271	LEU
1	A	1296	LEU
1	A	1301	THR
1	A	1306	LEU
1	A	1313	MET
1	A	1330	SER
1	A	1336	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	132	HIS
1	A	147	ASN
1	A	214	GLN
1	A	229	GLN
1	A	231	GLN
1	A	268	ASN
1	A	302	ASN
1	A	332	GLN
1	A	376	ASN
1	A	389	GLN
1	A	574	GLN
1	A	685	GLN
1	A	712	GLN
1	A	975	GLN
1	A	1052	HIS
1	A	1069	ASN
1	A	1104	GLN
1	A	1150	ASN
1	A	1203	GLN
1	A	1221	ASN

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Mol	Chain	Res	Type
1	A	1225	GLN
1	A	1257	GLN
1	A	1335	ASN

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 ⓘ

5 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	$\# Z > 2$
5	MOS	A	3005	-	0,3,3	-	-	-		
2	FES	A	3001	1	0,4,4	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
3	MTE	A	3003	-	21,26,26	1.77	4 (19%)	19,40,40	2.17	7 (36%)
4	FAD	A	3004	-	58,58,58	1.50	9 (15%)	85,89,89	1.66	20 (23%)

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	FES	A	3002	1	-	-	0/1/1/1
3	MTE	A	3003	-	-	2/6/34/34	0/3/3/3
2	FES	A	3001	1	-	-	0/1/1/1
4	FAD	A	3004	-	-	0/34/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3003	MTE	C9-C10	6.18	1.49	1.38
4	A	3004	FAD	C9A-C5X	5.46	1.50	1.41
4	A	3004	FAD	C5A-C4A	4.80	1.47	1.39
4	A	3004	FAD	C8-C7	3.55	1.49	1.40
4	A	3004	FAD	C8A-N7A	2.66	1.36	1.31
4	A	3004	FAD	C4A-N9A	-2.48	1.32	1.37
4	A	3004	FAD	C5A-N7A	-2.48	1.34	1.39
3	A	3003	MTE	C9-C4	2.39	1.49	1.41
3	A	3003	MTE	C2-N1	2.30	1.38	1.33
4	A	3004	FAD	C4-N3	-2.26	1.34	1.38
4	A	3004	FAD	C5A-C6A	2.21	1.47	1.41
3	A	3003	MTE	C4'-C3'	2.17	1.54	1.51
4	A	3004	FAD	C5X-N5	-2.03	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3004	FAD	N3A-C4A-N9A	4.29	134.46	127.17
3	A	3003	MTE	C2-N1-C10	4.21	120.78	113.36
4	A	3004	FAD	C5A-C4A-N3A	-4.19	120.95	126.72
4	A	3004	FAD	N3A-C2A-N1A	-4.17	122.26	128.58
4	A	3004	FAD	C4A-N9A-C8A	4.02	109.95	105.74
3	A	3003	MTE	O3'-C7-N8	3.99	112.22	108.61
4	A	3004	FAD	O3'-C3'-C4'	-3.63	100.68	108.93
3	A	3003	MTE	O4-C4-C9	-3.53	118.75	127.26
3	A	3003	MTE	O3'-C7-C6	-3.36	106.72	108.96
4	A	3004	FAD	C2A-N3A-C4A	3.27	119.82	111.83
4	A	3004	FAD	O2-C2-N1	-3.18	116.52	121.80
4	A	3004	FAD	C4X-C10-N10	2.88	120.60	116.48
4	A	3004	FAD	C4-C4X-N5	2.86	122.16	118.21
4	A	3004	FAD	N6A-C6A-N1A	2.61	124.20	118.38
3	A	3003	MTE	O3P-P-O4'	-2.60	99.88	106.67
4	A	3004	FAD	C2A-N1A-C6A	2.60	123.00	118.73
3	A	3003	MTE	C9-C4-N3	2.54	119.11	112.13
4	A	3004	FAD	C2B-C1B-N9A	2.48	119.46	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3003	MTE	C4-C9-N5	2.28	122.48	116.27
4	A	3004	FAD	C5A-C6A-N6A	-2.24	117.74	123.29
4	A	3004	FAD	C4X-C10-N1	-2.20	119.19	124.59
4	A	3004	FAD	C9A-C5X-N5	-2.19	120.13	122.45
4	A	3004	FAD	C4A-N9A-C1B	-2.13	121.64	126.63
4	A	3004	FAD	C10-C4X-N5	-2.10	120.52	124.81
4	A	3004	FAD	N9A-C8A-N7A	-2.06	111.01	113.94
4	A	3004	FAD	O2P-P-O3P	2.05	112.82	107.27
4	A	3004	FAD	C5X-N5-C4X	2.00	121.32	118.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

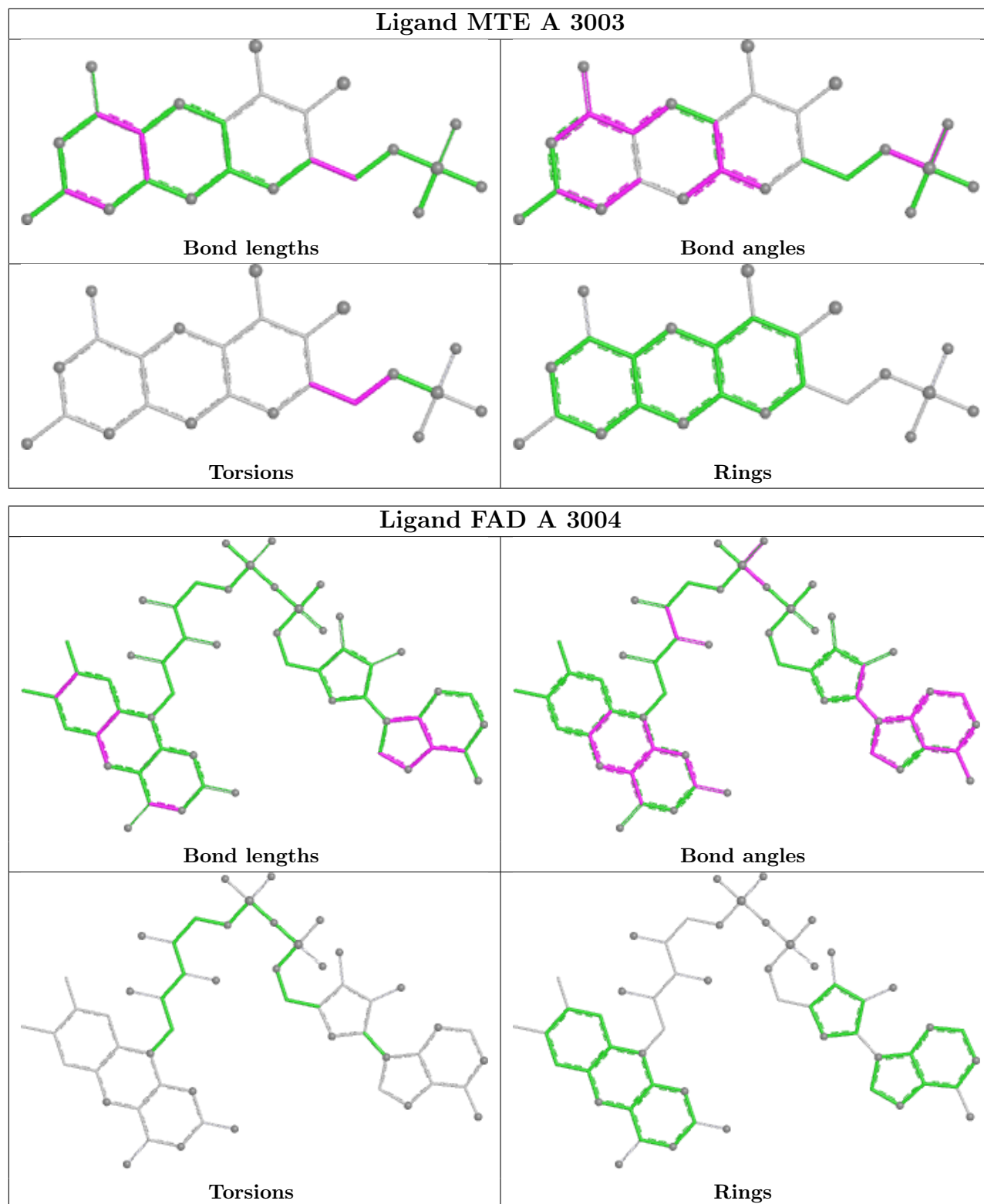
Mol	Chain	Res	Type	Atoms
3	A	3003	MTE	C3'-C4'-O4'-P
3	A	3003	MTE	O3'-C3'-C4'-O4'

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3005	MOS	3	0
2	A	3002	FES	1	0
3	A	3003	MTE	2	0
4	A	3004	FAD	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 ⓘ

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 [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	1288/1338 (96%)	-0.78	0 100 100	66, 101, 137, 169	0

There are no RSRZ outliers to report.

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](#)

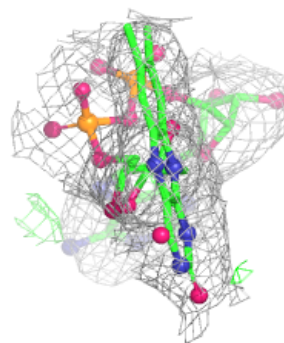
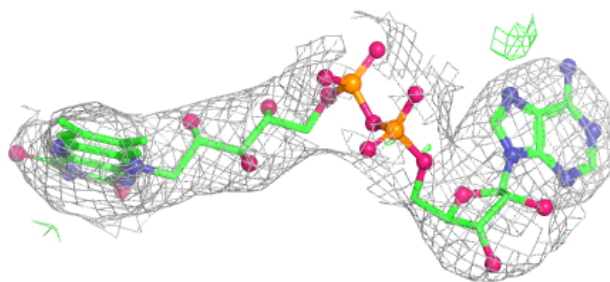
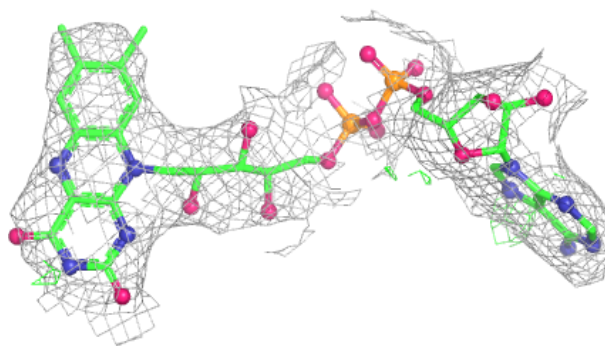
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MOS	A	3005	4/4	0.95	0.07	113,145,150,160	1
4	FAD	A	3004	53/53	0.97	0.05	67,81,101,116	0
3	MTE	A	3003	24/24	0.97	0.05	87,100,123,138	0
2	FES	A	3002	4/4	0.98	0.05	119,134,135,146	0
2	FES	A	3001	4/4	1.00	0.02	63,70,82,86	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.

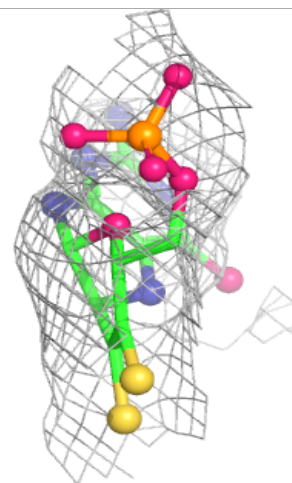
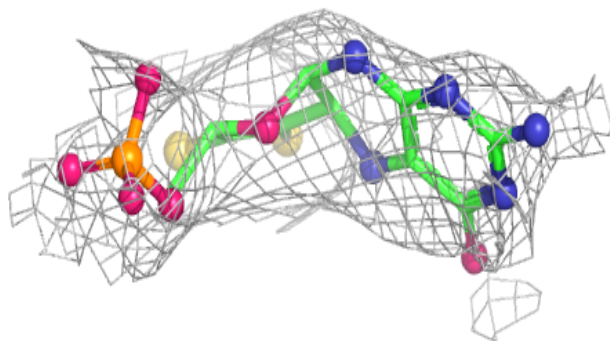
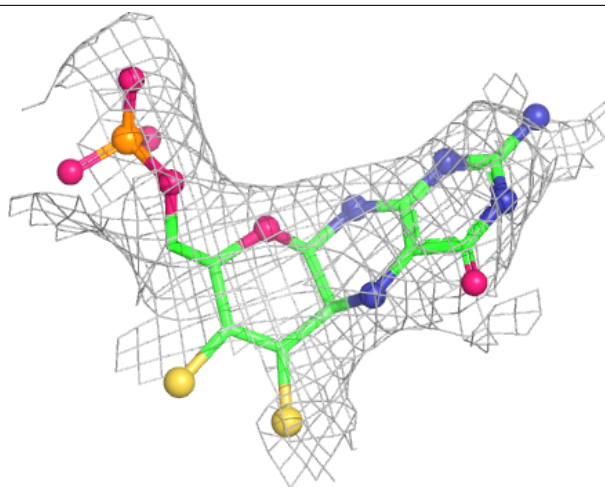
Electron density around FAD A 3004:

$2mF_o - DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.