



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:49 PM UTC

PDB ID : 4GRT / pdb_00004grt
Title : HUMAN GLUTATHIONE REDUCTASE A34E, R37W MUTANT, MIXED
DISULFIDE BETWEEN TRYPANOTHIONE AND THE ENZYME
Authors : Stoll, V.S.; Simpson, S.J.; Krauth-Siegel, R.L.; Walsh, C.T.; Pai, E.F.
Deposited on : 1997-02-12
Resolution : 2.80 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

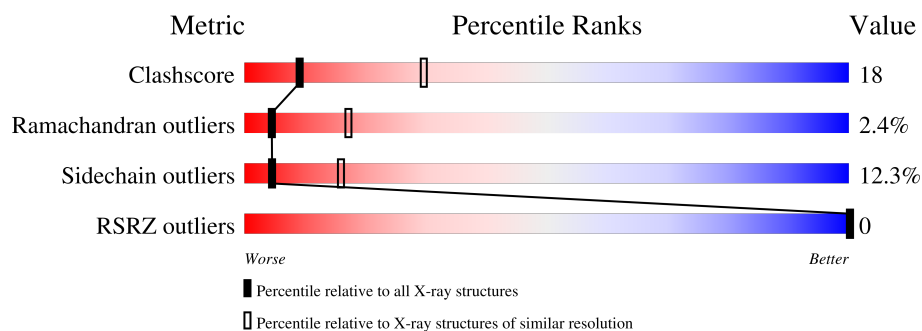
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	461	55% 36% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3607 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 GLUTATHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	461	3506	2219	601	662	24	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

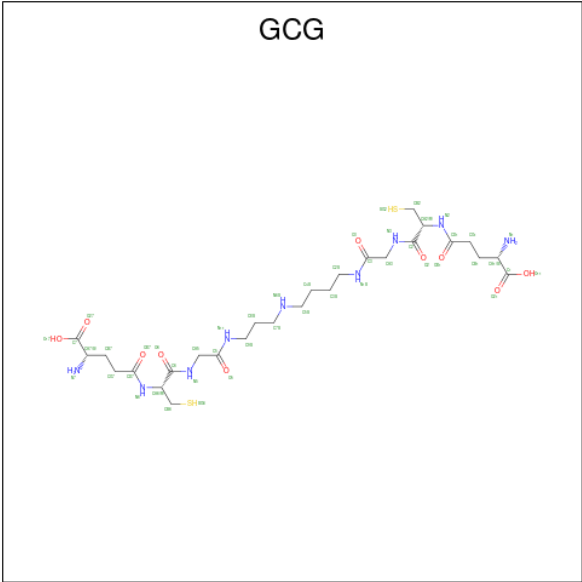
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLU	ALA	engineered mutation	UNP P00390
A	37	TRP	ARG	engineered mutation	UNP P00390

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is BIS(GAMMA-GLUTAMYL-CYSTEINYL-GLYCINYL)SPERMIDINE (CCD ID: GCG) (formula: $C_{27}H_{49}N_9O_{10}S_2$).

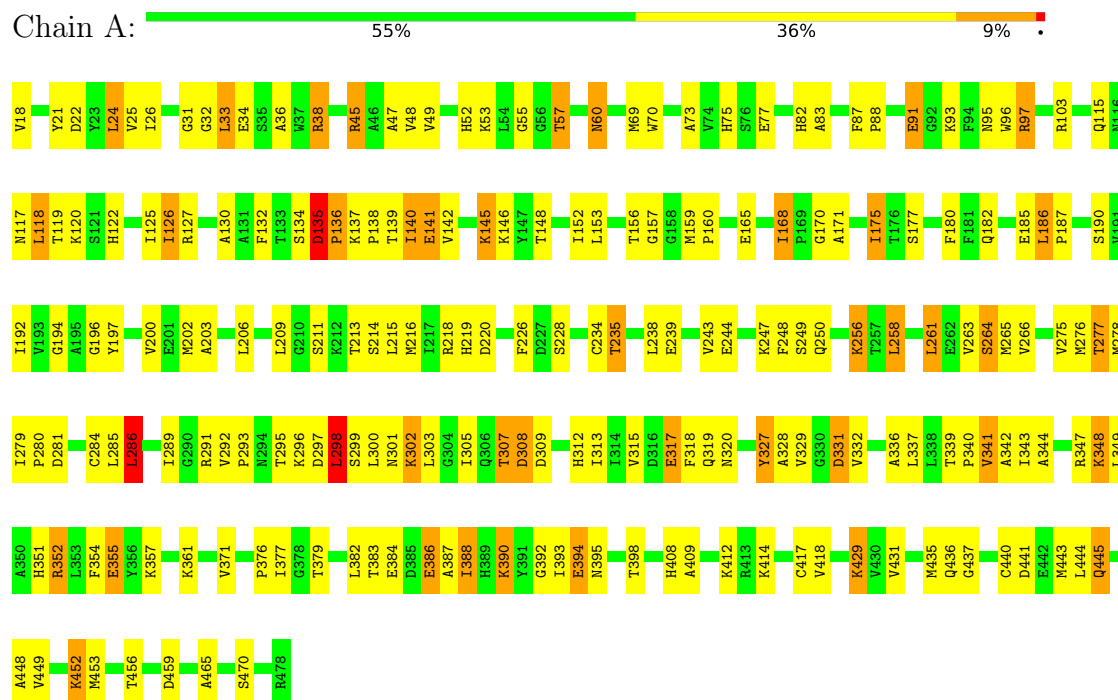


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			48	27	9	10	2		

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: GLUTATHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	119.77Å 84.98Å 63.32Å 90.00° 90.00° 58.15°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	71.7 (10.00-2.80) 70.2 (10.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , (Not available) 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 50.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3607	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: GCG, 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	0.67	0/3575	1.18	32/4838 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASN	N-CA-C	10.33	122.23	110.97
1	A	298	LEU	N-CA-C	-8.20	103.07	113.23
1	A	409	ALA	N-CA-C	-8.03	102.38	112.90
1	A	55	GLY	N-CA-C	-7.64	104.98	114.92
1	A	31	GLY	N-CA-C	-7.54	100.47	111.03
1	A	135	ASP	CA-C-N	7.29	128.95	119.84
1	A	135	ASP	C-N-CA	7.29	128.95	119.84
1	A	386	GLU	N-CA-C	-6.80	103.95	111.36
1	A	33	LEU	N-CA-C	-6.55	103.25	111.11
1	A	286	LEU	N-CA-C	6.39	119.15	108.73
1	A	470	SER	N-CA-C	-6.30	103.70	112.45
1	A	258	LEU	N-CA-C	-6.10	105.66	113.23
1	A	22	ASP	N-CA-C	-6.04	106.45	113.88
1	A	307	THR	N-CA-C	6.02	117.35	108.86
1	A	70	TRP	N-CA-C	-5.93	104.73	111.07
1	A	137	LYS	CA-C-N	5.93	127.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	LYS	C-N-CA	5.93	127.25	119.84
1	A	289	ILE	N-CA-C	5.79	118.75	112.96
1	A	168	ILE	N-CA-C	5.77	113.86	108.15
1	A	309	ASP	N-CA-C	-5.70	106.17	113.02
1	A	352	ARG	N-CA-C	-5.67	105.00	111.07
1	A	379	THR	N-CA-C	5.67	117.74	108.55
1	A	355	GLU	N-CA-C	-5.53	106.58	113.38
1	A	354	PHE	N-CA-C	5.37	119.55	112.89
1	A	465	ALA	N-CA-C	5.28	117.50	110.53
1	A	170	GLY	N-CA-C	-5.26	107.79	115.63
1	A	277	THR	N-CA-C	5.22	118.08	109.72
1	A	412	LYS	N-CA-C	-5.17	105.26	112.45
1	A	235	THR	N-CA-C	-5.17	105.73	111.36
1	A	264	SER	N-CA-C	-5.07	100.26	108.52
1	A	308	ASP	N-CA-CB	-5.05	103.46	110.38
1	A	280	PRO	N-CA-C	5.01	118.59	111.13

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	327	TYR	Sidechain

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	3506	0	3536	129	0
2	A	53	0	25	5	0
3	A	48	0	46	2	0
All	All	3607	0	3607	132	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 18.

All (132) 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:126:ILE:HD11	1:A:142:VAL:HG11	1.42	0.99
1:A:440:CYS:SG	1:A:443:MET:HE3	2.22	0.79
1:A:196:GLY:O	1:A:200:VAL:HG23	1.85	0.77
1:A:153:LEU:HD12	1:A:327:TYR:HB2	1.67	0.77
1:A:156:THR:HG21	1:A:298:LEU:HD21	1.67	0.75
1:A:118:LEU:HB3	1:A:125:ILE:HD11	1.71	0.73
1:A:218:ARG:O	1:A:248:PHE:HA	1.89	0.73
1:A:319:GLN:HG2	1:A:329:VAL:HG12	1.73	0.70
1:A:82:HIS:CD2	1:A:87:PHE:HB2	2.28	0.69
1:A:266:VAL:HG22	1:A:276:MET:HG2	1.74	0.69
1:A:293:PRO:HD3	1:A:312:HIS:CE1	2.29	0.68
1:A:126:ILE:HD11	1:A:142:VAL:CG1	2.23	0.67
1:A:256:LYS:HA	1:A:261:LEU:HD12	1.78	0.66
1:A:220:ASP:HA	1:A:247:LYS:HD3	1.77	0.65
1:A:331:ASP:HA	1:A:337:LEU:HD22	1.80	0.64
1:A:153:LEU:HD13	1:A:349:LEU:CD2	2.29	0.63
1:A:159:MET:HB2	1:A:160:PRO:HD2	1.81	0.63
1:A:175:ILE:HD13	1:A:284:CYS:SG	2.39	0.63
1:A:235:THR:O	1:A:239:GLU:HG3	1.99	0.62
1:A:34:GLU:HG2	1:A:343:ILE:HG23	1.81	0.62
1:A:383:THR:OG1	1:A:386:GLU:HG3	2.01	0.61
1:A:300:LEU:HB3	1:A:305:ILE:HB	1.81	0.61
1:A:118:LEU:CB	1:A:125:ILE:HD11	2.31	0.60
1:A:307:THR:HG22	1:A:313:ILE:HA	1.84	0.59
3:A:17:GCG:HG71	3:A:17:GCG:HA2	1.84	0.59
1:A:376:PRO:HD2	1:A:437:GLY:O	2.04	0.58
1:A:299:SER:HB3	1:A:302:LYS:HZ1	1.69	0.58
1:A:371:VAL:HB	1:A:377:ILE:HB	1.86	0.58
1:A:318:PHE:CZ	1:A:361:LYS:HD2	2.38	0.58
1:A:263:VAL:HB	1:A:279:ILE:HB	1.86	0.57
1:A:139:THR:HG23	1:A:148:THR:HB	1.87	0.57
1:A:417:CYS:HA	1:A:436:GLN:O	2.04	0.57
1:A:390:LYS:HG2	1:A:390:LYS:O	2.05	0.57
1:A:49:VAL:HG13	1:A:126:ILE:HG13	1.87	0.56
1:A:25:VAL:HG13	1:A:153:LEU:HD23	1.87	0.56
1:A:177:SER:O	1:A:180:PHE:HB3	2.06	0.56
1:A:429:LYS:HB2	1:A:429:LYS:NZ	2.21	0.55
1:A:159:MET:O	1:A:291:ARG:HA	2.07	0.55
1:A:175:ILE:CD1	1:A:284:CYS:SG	2.96	0.54
1:A:266:VAL:HG22	1:A:276:MET:CG	2.36	0.54
1:A:382:LEU:HD13	1:A:387:ALA:HB2	1.91	0.53
1:A:145:LYS:NZ	1:A:145:LYS:HB2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ALA:O	1:A:348:LYS:HB2	2.09	0.52
1:A:21:TYR:CD2	1:A:45:ARG:HD3	2.45	0.52
1:A:444:LEU:O	1:A:445:GLN:HB2	2.08	0.52
1:A:315:VAL:HG11	1:A:328:ALA:HB3	1.93	0.51
1:A:352:ARG:HA	1:A:357:LYS:O	2.10	0.51
1:A:319:GLN:O	1:A:327:TYR:HB3	2.10	0.51
1:A:449:VAL:O	1:A:453:MET:HG2	2.10	0.51
1:A:34:GLU:HG3	1:A:347:ARG:HB3	1.93	0.51
1:A:339:THR:HB	1:A:340:PRO:HD3	1.93	0.51
1:A:126:ILE:HD12	1:A:127:ARG:N	2.26	0.50
1:A:299:SER:HB3	1:A:302:LYS:NZ	2.26	0.50
1:A:440:CYS:SG	1:A:443:MET:CE	2.99	0.50
1:A:293:PRO:HG3	1:A:312:HIS:N	2.27	0.50
1:A:141:GLU:HA	1:A:145:LYS:O	2.12	0.49
1:A:153:LEU:HD13	1:A:349:LEU:HD22	1.94	0.49
1:A:73:ALA:HA	1:A:209:LEU:HD21	1.94	0.49
1:A:18:VAL:HA	1:A:146:LYS:O	2.12	0.49
1:A:156:THR:HG22	2:A:479:FAD:N7A	2.27	0.49
1:A:156:THR:HG22	2:A:479:FAD:C5A	2.43	0.49
1:A:49:VAL:HA	1:A:126:ILE:O	2.12	0.49
1:A:308:ASP:HB2	1:A:312:HIS:HB2	1.95	0.49
1:A:218:ARG:HB2	1:A:219:HIS:CD2	2.48	0.48
1:A:388:ILE:HG12	1:A:393:ILE:HA	1.94	0.48
1:A:392:GLY:O	1:A:395:ASN:N	2.46	0.48
1:A:95:ASN:OD1	1:A:97:ARG:HB2	2.13	0.48
1:A:197:TYR:HB2	1:A:371:VAL:HG13	1.96	0.48
1:A:418:VAL:O	1:A:435:MET:HA	2.13	0.48
1:A:292:VAL:CG2	1:A:293:PRO:HD2	2.44	0.48
1:A:21:TYR:CE2	1:A:47:ALA:HB2	2.48	0.48
1:A:394:GLU:H	1:A:394:GLU:CD	2.21	0.48
1:A:38:ARG:HG2	1:A:347:ARG:HB2	1.96	0.47
1:A:219:HIS:O	1:A:247:LYS:HB3	2.13	0.47
1:A:382:LEU:CD1	1:A:387:ALA:HB2	2.44	0.47
1:A:249:SER:HA	1:A:266:VAL:O	2.14	0.47
1:A:295:THR:O	1:A:298:LEU:HB2	2.14	0.47
1:A:24:LEU:O	1:A:152:ILE:HA	2.14	0.47
1:A:26:ILE:HD11	1:A:140:ILE:HG21	1.97	0.47
1:A:315:VAL:CG1	1:A:328:ALA:HB3	2.45	0.47
1:A:192:ILE:HD12	1:A:203:ALA:HA	1.97	0.47
3:A:17:GCG:HA2	3:A:17:GCG:CG7	2.44	0.47
1:A:134:SER:O	1:A:135:ASP:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:HE3	1:A:103:ARG:HE	1.80	0.46
1:A:315:VAL:HA	1:A:320:ASN:O	2.16	0.46
1:A:132:PHE:HB3	1:A:303:LEU:CD1	2.45	0.46
1:A:352:ARG:HG2	1:A:357:LYS:O	2.16	0.46
1:A:318:PHE:CE1	1:A:361:LYS:HD2	2.50	0.46
1:A:384:GLU:CD	1:A:398:THR:HG21	2.40	0.46
1:A:18:VAL:HG22	1:A:148:THR:HG22	1.98	0.46
1:A:336:ALA:HB3	1:A:341:VAL:HG11	1.98	0.46
1:A:194:GLY:O	1:A:215:LEU:HD11	2.16	0.45
1:A:408:HIS:HB3	1:A:414:LYS:HD3	1.98	0.45
1:A:351:HIS:O	1:A:355:GLU:HB3	2.15	0.45
1:A:429:LYS:HG2	1:A:431:VAL:CG1	2.46	0.45
1:A:190:SER:OG	1:A:206:LEU:HD13	2.17	0.45
1:A:168:ILE:O	1:A:171:ALA:HB2	2.17	0.45
1:A:234:CYS:O	1:A:238:LEU:HG	2.17	0.45
1:A:264:SER:HA	1:A:277:THR:O	2.16	0.45
1:A:192:ILE:HD11	1:A:206:LEU:HD12	1.97	0.45
1:A:83:ALA:HA	1:A:87:PHE:O	2.17	0.45
1:A:459:ASP:N	1:A:459:ASP:OD1	2.49	0.45
1:A:21:TYR:HA	1:A:45:ARG:CG	2.47	0.44
1:A:213:THR:HG22	1:A:214:SER:N	2.32	0.44
1:A:440:CYS:HA	1:A:443:MET:HB3	1.99	0.44
1:A:336:ALA:HB1	1:A:341:VAL:HG21	1.99	0.44
1:A:175:ILE:O	1:A:286:LEU:HA	2.17	0.44
1:A:32:GLY:O	1:A:33:LEU:C	2.59	0.44
1:A:317:GLU:H	1:A:317:GLU:CD	2.26	0.43
1:A:49:VAL:HG11	1:A:130:ALA:HB2	2.00	0.43
1:A:57:THR:HB	2:A:479:FAD:O2A	2.19	0.43
1:A:444:LEU:O	1:A:445:GLN:CB	2.67	0.43
1:A:125:ILE:O	1:A:127:ARG:HG3	2.18	0.43
1:A:187:PRO:O	1:A:211:SER:HB2	2.18	0.43
1:A:339:THR:O	1:A:342:ALA:HB3	2.19	0.42
1:A:226:PHE:CD1	1:A:226:PHE:N	2.87	0.42
1:A:120:LYS:C	1:A:122:HIS:H	2.27	0.42
1:A:115:GLN:O	1:A:119:THR:HG23	2.18	0.42
1:A:243:VAL:HG12	1:A:244:GLU:H	1.85	0.42
1:A:448:ALA:O	1:A:452:LYS:HB2	2.19	0.42
1:A:157:GLY:HA3	2:A:479:FAD:O1A	2.20	0.41
1:A:349:LEU:CD1	1:A:352:ARG:HH21	2.32	0.41
1:A:96:TRP:CE3	1:A:186:LEU:HB2	2.55	0.41
1:A:53:LYS:HD2	1:A:60:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLN:O	1:A:449:VAL:HG23	2.21	0.41
1:A:216:MET:HG3	1:A:249:SER:HB2	2.02	0.41
1:A:327:TYR:CD1	1:A:327:TYR:N	2.89	0.41
1:A:429:LYS:HB2	1:A:429:LYS:HZ2	1.86	0.41
2:A:479:FAD:O2'	2:A:479:FAD:O4'	2.33	0.41
1:A:216:MET:HE3	1:A:216:MET:HB2	1.82	0.40
1:A:25:VAL:HG21	1:A:36:ALA:HB2	2.03	0.40
1:A:377:ILE:HD12	1:A:377:ILE:N	2.36	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	459/461 (100%)	393 (86%)	55 (12%)	11 (2%)	4 17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	LYS
1	A	91	GLU
1	A	93	LYS
1	A	445	GLN
1	A	52	HIS
1	A	88	PRO
1	A	301	ASN
1	A	331	ASP
1	A	135	ASP
1	A	136	PRO
1	A	138	PRO

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	383/383 (100%)	336 (88%)	47 (12%)	4 16

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	38	ARG
1	A	45	ARG
1	A	48	VAL
1	A	57	THR
1	A	75	HIS
1	A	77	GLU
1	A	91	GLU
1	A	97	ARG
1	A	117	ASN
1	A	118	LEU
1	A	126	ILE
1	A	136	PRO
1	A	140	ILE
1	A	141	GLU
1	A	145	LYS
1	A	165	GLU
1	A	175	ILE
1	A	182	GLN
1	A	185	GLU
1	A	186	LEU
1	A	202	MET
1	A	228	SER
1	A	250	GLN
1	A	256	LYS
1	A	258	LEU
1	A	261	LEU
1	A	265	MET
1	A	275	VAL
1	A	278	MET

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Mol	Chain	Res	Type
1	A	281	ASP
1	A	285	LEU
1	A	286	LEU
1	A	297	ASP
1	A	298	LEU
1	A	302	LYS
1	A	317	GLU
1	A	332	VAL
1	A	341	VAL
1	A	348	LYS
1	A	388	ILE
1	A	390	LYS
1	A	394	GLU
1	A	429	LYS
1	A	441	ASP
1	A	452	LYS
1	A	456	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	111	ASN
1	A	117	ASN
1	A	129	HIS
1	A	167	GLN
1	A	219	HIS
1	A	233	ASN
1	A	250	GLN
1	A	312	HIS
1	A	365	ASN
1	A	425	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	GCG	A	17	1	45,47,47	0.59	0	52,58,58	1.01	1 (1%)
2	FAD	A	479	-	58,58,58	5.43	16 (27%)	85,89,89	2.38	22 (25%)

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	GCG	A	17	1	-	22/61/61/61	-
2	FAD	A	479	-	-	7/34/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	479	FAD	C7M-C7	-28.19	0.98	1.51
2	A	479	FAD	C8M-C8	-26.79	1.00	1.51
2	A	479	FAD	C4-N3	-5.08	1.29	1.38
2	A	479	FAD	C8-C7	4.53	1.51	1.40
2	A	479	FAD	C5X-N5	-4.06	1.32	1.39
2	A	479	FAD	C1B-N9A	4.03	1.57	1.46
2	A	479	FAD	C9-C8	3.94	1.45	1.39
2	A	479	FAD	C4'-C3'	-3.51	1.47	1.53
2	A	479	FAD	C9A-C5X	2.99	1.46	1.41
2	A	479	FAD	C9-C9A	2.52	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	479	FAD	C9A-N10	2.46	1.45	1.41
2	A	479	FAD	C5'-C4'	2.43	1.55	1.51
2	A	479	FAD	O4-C4	-2.35	1.19	1.23
2	A	479	FAD	O2B-C2B	-2.09	1.37	1.43
2	A	479	FAD	C4A-N9A	2.07	1.42	1.37
2	A	479	FAD	C10-N10	2.03	1.41	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	479	FAD	C4'-C3'-C2'	-10.29	96.45	113.57
2	A	479	FAD	C5'-C4'-C3'	6.62	124.70	112.22
2	A	479	FAD	O4B-C1B-C2B	-6.24	93.25	106.62
2	A	479	FAD	C3B-C2B-C1B	5.30	111.48	101.46
3	A	17	GCG	C5-CA5-N5	4.93	127.42	113.04
2	A	479	FAD	O2'-C2'-C3'	4.76	120.39	109.25
2	A	479	FAD	O4B-C4B-C5B	-4.23	95.78	109.33
2	A	479	FAD	C6-C5X-N5	-4.03	111.76	118.44
2	A	479	FAD	O2-C2-N1	3.66	127.87	121.80
2	A	479	FAD	O2-C2-N3	-3.38	112.10	118.58
2	A	479	FAD	C9-C9A-N10	3.33	126.33	121.85
2	A	479	FAD	C7M-C7-C6	-3.33	113.71	119.57
2	A	479	FAD	C6-C5X-C9A	3.31	123.60	119.05
2	A	479	FAD	O3'-C3'-C2'	3.28	116.39	108.93
2	A	479	FAD	O4'-C4'-C3'	-3.26	101.62	109.25
2	A	479	FAD	C4A-N9A-C8A	-2.93	102.66	105.74
2	A	479	FAD	C7M-C7-C8	2.90	126.67	120.76
2	A	479	FAD	O3P-PA-O1A	2.87	119.33	110.70
2	A	479	FAD	O4B-C1B-N9A	2.69	113.25	108.09
2	A	479	FAD	C5A-C6A-N1A	-2.42	111.38	117.51
2	A	479	FAD	C5X-C9A-N10	-2.20	115.98	117.97
2	A	479	FAD	C9A-C5X-N5	2.06	124.64	122.45
2	A	479	FAD	C1'-C2'-C3'	2.01	115.12	109.66

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	479	FAD	C5'-O5'-P-O1P
2	A	479	FAD	C5'-O5'-P-O2P
2	A	479	FAD	C5'-O5'-P-O3P
3	A	17	GCG	C3-CA3-N3-C2

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Mol	Chain	Res	Type	Atoms
3	A	17	GCG	C6-CA6-CB6-SG6
3	A	17	GCG	N1S-C2S-C3S-C4S
2	A	479	FAD	O2'-C2'-C3'-O3'
3	A	17	GCG	CA7-CB7-CG7-CD7
3	A	17	GCG	C3S-C4S-C5S-N6S
3	A	17	GCG	O3-C3-CA3-N3
3	A	17	GCG	C2S-C3S-C4S-C5S
3	A	17	GCG	C4S-C5S-N6S-C7S
3	A	17	GCG	N6S-C7S-C8S-C9S
2	A	479	FAD	O2'-C2'-C3'-C4'
3	A	17	GCG	C8S-C7S-N6S-C5S
3	A	17	GCG	O5-C5-N11-C9S
3	A	17	GCG	N11-C5-CA5-N5
3	A	17	GCG	O17-C7-CA7-N7
3	A	17	GCG	CB2-CA2-N2-CD1
3	A	17	GCG	N6-CA6-CB6-SG6
3	A	17	GCG	N1S-C3-CA3-N3
2	A	479	FAD	PA-O3P-P-O5'
3	A	17	GCG	C2-CA2-N2-CD1
3	A	17	GCG	C1-CA1-CB1-CG1
3	A	17	GCG	O21-C1-CA1-N1
3	A	17	GCG	O27-C7-CA7-N7
2	A	479	FAD	PA-O3P-P-O1P
3	A	17	GCG	C2-CA2-CB2-SG2
3	A	17	GCG	C5-CA5-N5-C6

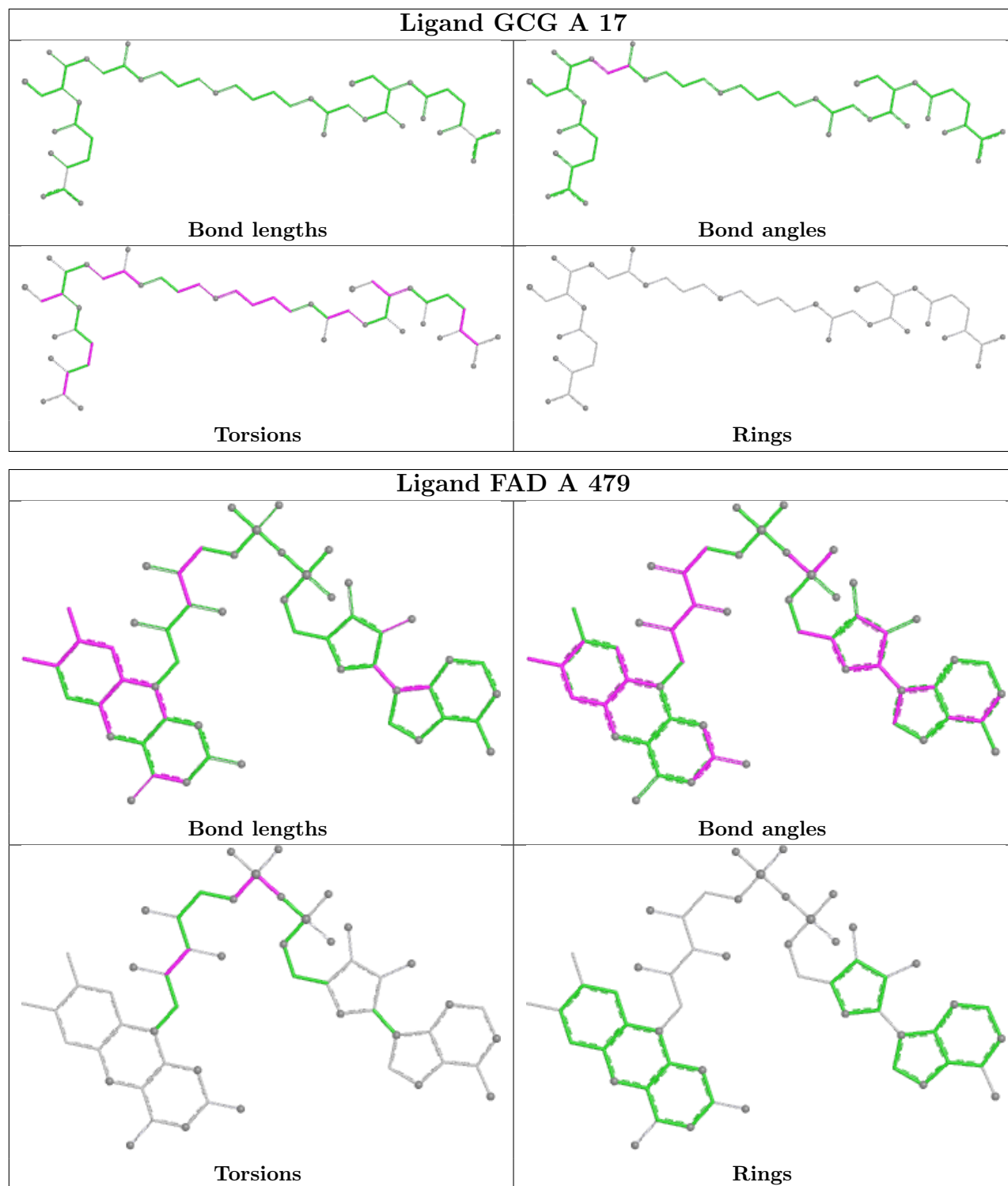
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	17	GCG	2	0
2	A	479	FAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	461/461 (100%)	-0.52	0 100 100	2, 11, 49, 77	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](#)

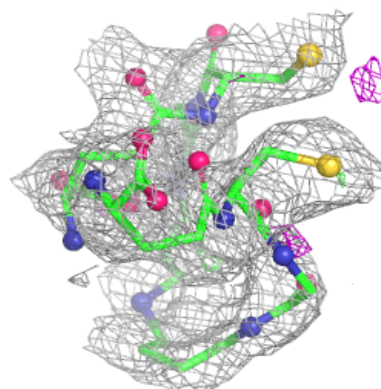
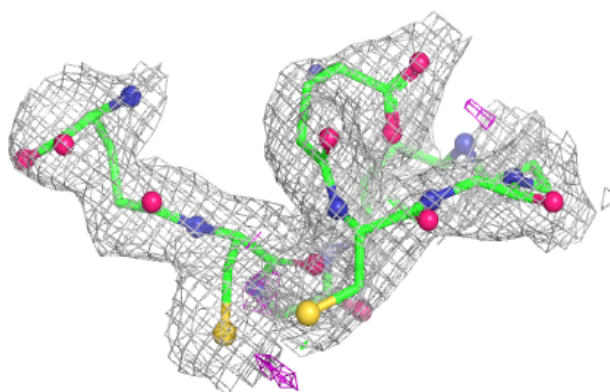
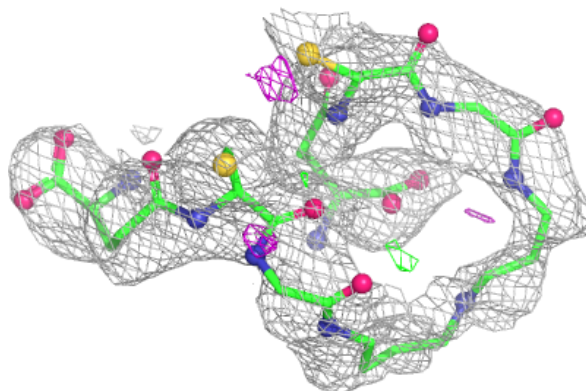
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GCG	A	17	48/48	0.86	0.11	5,40,40,40	0
2	FAD	A	479	53/53	0.97	0.06	2,4,11,12	0

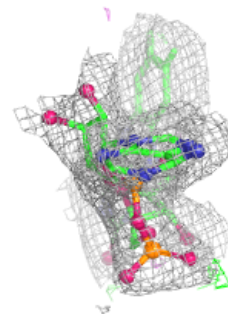
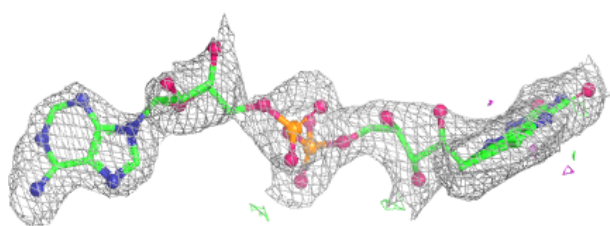
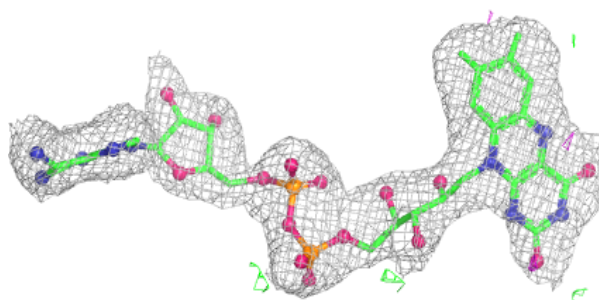
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GCG A 17:

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

**Electron density around FAD A 479:**

$2mF_o-DF_c$ (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.