



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:13 PM UTC

PDB ID : 6X9A / pdb_00006x9a
Title : Structure of proline utilization A with trans-4-hydroxy-D-proline bound in the L-glutamate-gamma-semialdehyde dehydrogenase active site
Authors : Tanner, J.J.; Campbell, A.C.
Deposited on : 2020-06-02
Resolution : 1.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

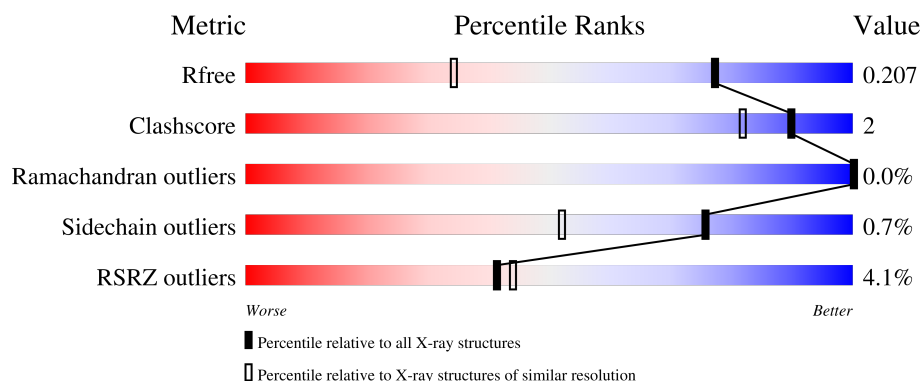
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	1235	3% 94% • •
1	B	1235	5% 93% 5% •

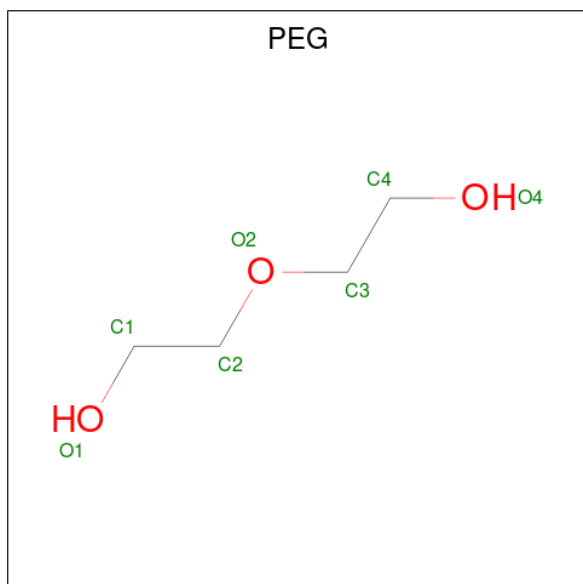
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



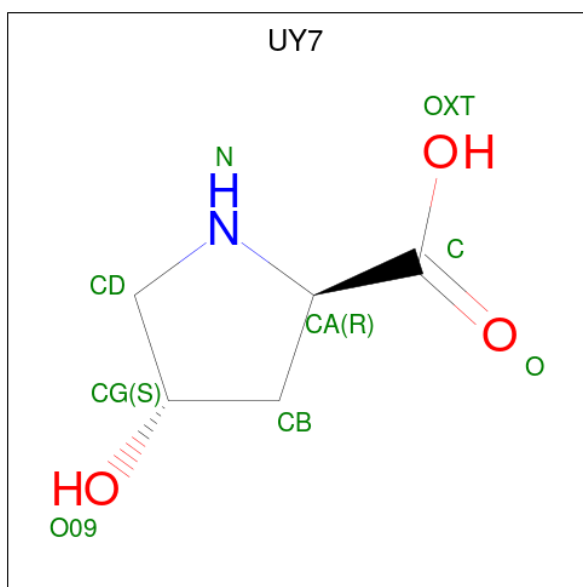
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



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

- Molecule 5 is (4S)-4-hydroxy-D-proline (CCD ID: UY7) (formula: C₅H₉NO₃) (labeled as "Ligand of Interest" by depositor).



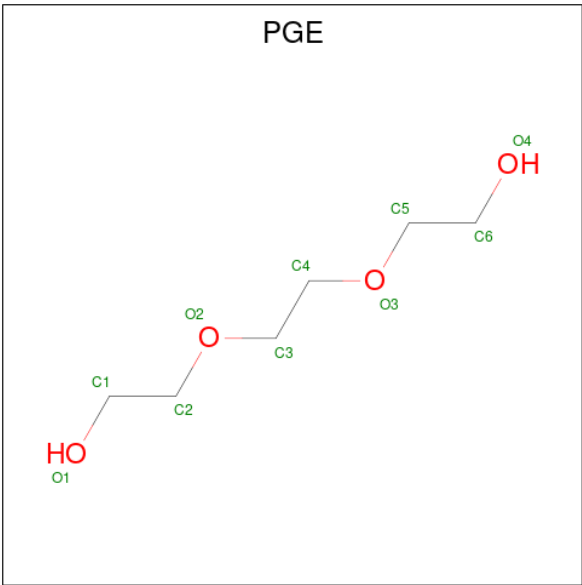
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	5	1	3		
5	A	1	Total	C	N	O	0	0
			9	5	1	3		
5	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

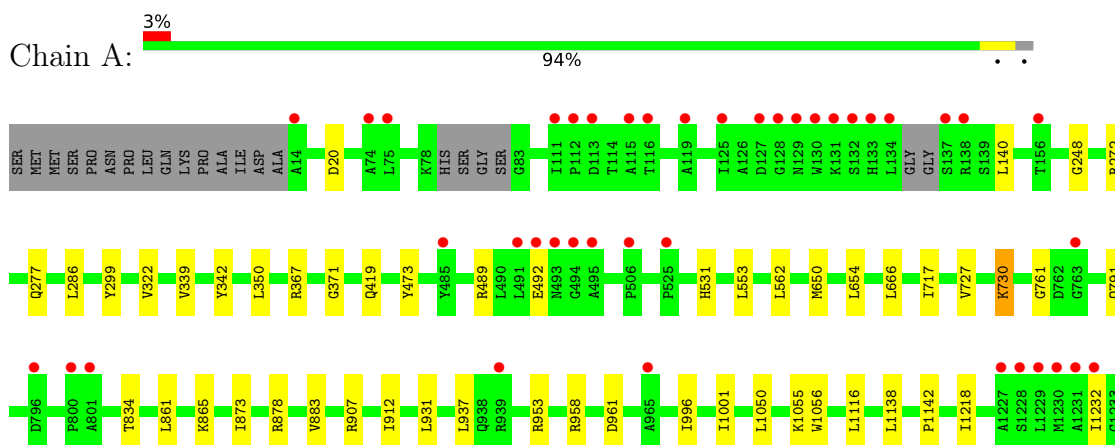
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1263	Total	O	0	0
			1263	1263		
8	B	1258	Total	O	0	0
			1258	1258		

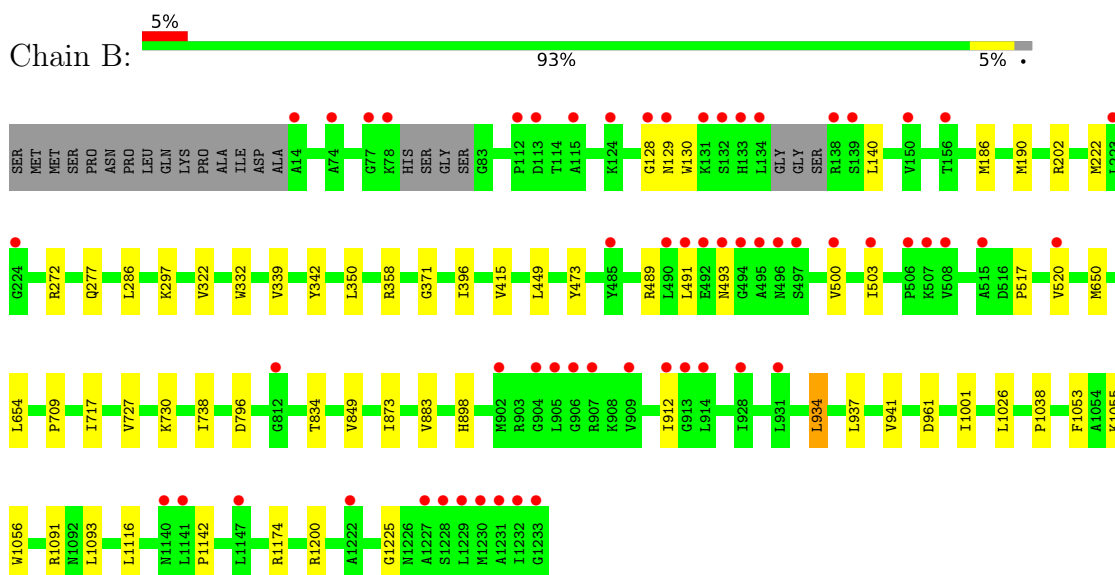
3 Residue-property plots

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: Bifunctional protein PutA



• Molecule 1: Bifunctional protein PutA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.15Å 102.00Å 126.75Å 90.00° 106.45° 90.00°	Depositor
Resolution (Å)	45.98 – 1.41 45.98 – 1.41	Depositor EDS
% Data completeness (in resolution range)	96.1 (45.98-1.41) 96.1 (45.98-1.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.41Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.175 , 0.199 0.185 , 0.207	Depositor DCC
R_{free} test set	22768 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20837	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UY7, PEG, PGE, SO4, FMT, 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	0.23	0/9243	0.46	0/12577
1	B	0.23	0/9266	0.47	0/12608
All	All	0.23	0/18509	0.46	0/25185

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	9046	0	9111	29	0
1	B	9058	0	9132	34	0
2	A	53	0	31	4	0
2	B	53	0	31	4	0
3	A	3	0	1	0	0
4	A	14	0	20	0	0
4	B	7	0	10	0	0
5	A	18	0	0	0	0
5	B	9	0	0	0	0
6	A	25	0	0	0	0
6	B	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	0	14	0	0
8	A	1263	0	0	2	0
8	B	1258	0	0	3	0
All	All	20837	0	18350	64	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 2.

All (64) 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:202:ARG:NH1	6:B:2006:SO4:O1	2.21	0.72
1:B:473:TYR:HB2	2:B:2001:FAD:HM71	1.78	0.66
1:B:1174[A]:ARG:NH1	8:B:2102:HOH:O	2.30	0.64
1:B:873:ILE:HG13	1:B:883:VAL:HB	1.80	0.63
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.82	0.61
1:A:473:TYR:HB2	2:A:2001:FAD:HM71	1.85	0.58
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.86	0.56
1:B:834:THR:HG22	1:B:1001:ILE:HD11	1.86	0.56
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.87	0.56
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.88	0.56
1:A:730[B]:LYS:NZ	1:A:761:GLY:O	2.32	0.54
1:B:339[A]:VAL:HG21	1:B:350:LEU:HD21	1.89	0.54
1:B:849:VAL:HG11	1:B:934:LEU:HD13	1.89	0.53
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.91	0.52
1:B:128:GLY:O	1:B:130:TRP:N	2.38	0.52
1:B:873:ILE:HD13	1:B:912:ILE:HG21	1.92	0.52
1:B:371:GLY:N	2:B:2001:FAD:O2'	2.42	0.51
1:B:449:LEU:HD21	1:B:489:ARG:HD2	1.92	0.51
1:B:796:ASP:OD1	1:B:1174[A]:ARG:NH2	2.44	0.50
1:A:473:TYR:HE2	1:A:489:ARG:HH12	1.59	0.50
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.47	0.49
1:B:650:MET:O	1:B:654:LEU:HG	2.13	0.49
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.40	0.48
1:A:562:LEU:HD11	1:A:654:LEU:HD12	1.95	0.47
1:B:449:LEU:CD2	1:B:489:ARG:HD2	2.45	0.47
1:A:1055:LYS:NZ	1:B:961:ASP:OD2	2.48	0.46
1:A:371:GLY:N	2:A:2001:FAD:O2'	2.43	0.46
1:B:222:MET:HG2	8:B:2132:HOH:O	2.15	0.46
1:A:791:GLN:NE2	8:A:2117:HOH:O	2.46	0.46
1:A:1116[B]:LEU:HD11	1:A:1138:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:ARG:HD3	8:A:2124:HOH:O	2.16	0.45
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.52	0.45
1:A:650:MET:O	1:A:654:LEU:HG	2.16	0.45
1:A:717:ILE:HG12	1:A:727:VAL:HG11	1.98	0.45
1:A:492:GLU:HB3	2:A:2001:FAD:H4'	1.99	0.45
1:B:272:ARG:HB3	1:B:277:GLN:HG3	2.00	0.44
1:B:849:VAL:HG21	1:B:934:LEU:HD11	1.99	0.44
1:A:531:HIS:CE1	1:A:1232:ILE:HG23	2.52	0.43
1:A:20:ASP:OD2	1:A:878:ARG:NH1	2.52	0.43
1:B:297:LYS:HG3	1:B:332:TRP:HB2	2.00	0.43
1:A:834:THR:HG22	1:A:1001:ILE:HD11	2.00	0.43
2:A:2001:FAD:HM81	2:A:2001:FAD:HM73	1.85	0.43
1:B:493:ASN:HB3	1:B:500:VAL:HB	2.01	0.43
1:A:958:ARG:O	1:A:961:ASP:HB2	2.19	0.42
1:B:186:MET:O	1:B:190:MET:HG3	2.19	0.42
1:B:1053:PHE:CE1	1:B:1116[B]:LEU:HD23	2.54	0.42
1:A:861:LEU:HG	1:A:865:LYS:HE3	2.00	0.42
1:B:396:ILE:HD11	1:B:517:PRO:HA	2.01	0.42
1:A:272:ARG:HB3	1:A:277:GLN:HG3	2.00	0.42
1:B:709:PRO:HB2	1:B:738:ILE:CG2	2.50	0.42
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	2.00	0.42
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.02	0.42
2:B:2001:FAD:HM73	2:B:2001:FAD:HM81	1.79	0.41
2:B:2001:FAD:H8A	8:B:2725:HOH:O	2.20	0.41
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.45	0.41
1:B:1091:ARG:HG2	1:B:1093:LEU:HD21	2.02	0.41
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.55	0.41
1:B:898:HIS:CD2	1:B:941:VAL:HG21	2.56	0.41
1:B:358:ARG:HG2	1:B:415:VAL:HG11	2.02	0.41
1:B:396:ILE:HD11	1:B:520:VAL:HB	2.02	0.41
1:B:491:LEU:HD11	1:B:1225:GLY:HA3	2.03	0.40
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.04	0.40
1:A:907:ARG:HD2	1:A:931:LEU:HD23	2.02	0.40
1:A:553:LEU:HD12	1:A:666:LEU:HD13	2.02	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	1221/1235 (99%)	1204 (99%)	17 (1%)	0	100	100
1	B	1224/1235 (99%)	1204 (98%)	19 (2%)	1 (0%)	48	22
All	All	2445/2470 (99%)	2408 (98%)	36 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ASN

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	912/951 (96%)	906 (99%)	6 (1%)	76	52
1	B	915/951 (96%)	907 (99%)	8 (1%)	70	43
All	All	1827/1902 (96%)	1813 (99%)	14 (1%)	76	47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	342	TYR
1	A	730[A]	LYS
1	A	730[B]	LYS
1	A	912	ILE

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Mol	Chain	Res	Type
1	A	937	LEU
1	B	140	LEU
1	B	342	TYR
1	B	503	ILE
1	B	730	LYS
1	B	934	LEU
1	B	937	LEU
1	B	1200[A]	ARG
1	B	1200[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	501	HIS
1	A	685	GLN
1	A	1114	HIS
1	B	304	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 ⓘ

19 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	SO4	A	2010	-	4,4,4	0.25	0	6,6,6	0.23	0
3	FMT	A	2002	-	2,2,2	0.65	0	1,1,1	0.19	0
5	UY7	A	2005	-	9,9,9	0.99	0	10,12,12	1.29	2 (20%)
6	SO4	B	2008	-	4,4,4	0.23	0	6,6,6	0.11	0
6	SO4	B	2006	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	B	2007	-	4,4,4	0.24	0	6,6,6	0.09	0
2	FAD	A	2001	-	58,58,58	2.17	12 (20%)	85,89,89	1.62	17 (20%)
4	PEG	A	2003	-	6,6,6	0.50	0	5,5,5	0.31	0
6	SO4	A	2008	-	4,4,4	0.22	0	6,6,6	0.16	0
7	PGE	B	2002	-	9,9,9	0.52	0	8,8,8	0.18	0
2	FAD	B	2001	-	58,58,58	2.09	13 (22%)	85,89,89	1.62	16 (18%)
4	PEG	B	2003	-	6,6,6	0.49	0	5,5,5	0.31	0
6	SO4	A	2007	-	4,4,4	0.19	0	6,6,6	0.23	0
5	UY7	B	2004	-	9,9,9	0.99	0	10,12,12	1.02	0
4	PEG	A	2006	-	6,6,6	0.50	0	5,5,5	0.18	0
5	UY7	A	2004	-	9,9,9	0.92	0	10,12,12	1.24	1 (10%)
6	SO4	B	2005	-	4,4,4	0.27	0	6,6,6	0.14	0
6	SO4	A	2011	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	A	2009	-	4,4,4	0.24	0	6,6,6	0.06	0

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	UY7	A	2005	-	-	0/4/13/13	0/1/1/1
5	UY7	B	2004	-	-	0/4/13/13	0/1/1/1
4	PEG	A	2006	-	-	0/4/4/4	-
7	PGE	B	2002	-	-	1/7/7/7	-
2	FAD	A	2001	-	-	5/34/50/50	0/6/6/6
4	PEG	A	2003	-	-	1/4/4/4	-
2	FAD	B	2001	-	-	5/34/50/50	0/6/6/6
5	UY7	A	2004	-	-	0/4/13/13	0/1/1/1
4	PEG	B	2003	-	-	1/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	PA-O3P	-8.16	1.50	1.59
2	B	2001	FAD	O4-C4	7.08	1.37	1.23
2	B	2001	FAD	PA-O3P	-6.98	1.52	1.59
2	A	2001	FAD	O4-C4	6.92	1.36	1.23
2	A	2001	FAD	O2-C2	4.80	1.33	1.24
2	B	2001	FAD	O2-C2	4.74	1.33	1.24
2	B	2001	FAD	C6A-N6A	4.25	1.45	1.34
2	A	2001	FAD	C6A-N6A	4.12	1.44	1.34
2	A	2001	FAD	C4X-N5	4.11	1.39	1.30
2	B	2001	FAD	C4X-N5	3.99	1.39	1.30
2	A	2001	FAD	P-O3P	3.65	1.63	1.59
2	A	2001	FAD	C2-N1	3.15	1.43	1.36
2	B	2001	FAD	C2-N1	3.09	1.43	1.36
2	A	2001	FAD	O2'-C2'	-3.07	1.36	1.43
2	B	2001	FAD	O2'-C2'	-2.95	1.37	1.43
2	B	2001	FAD	P-O3P	2.61	1.62	1.59
2	A	2001	FAD	PA-O5B	-2.44	1.49	1.59
2	B	2001	FAD	O4'-C4'	-2.41	1.38	1.43
2	A	2001	FAD	O4B-C4B	-2.33	1.39	1.45
2	B	2001	FAD	C10-N1	2.33	1.37	1.33
2	A	2001	FAD	O4'-C4'	-2.27	1.38	1.43
2	B	2001	FAD	PA-O5B	-2.25	1.50	1.59
2	B	2001	FAD	PA-O2A	-2.15	1.45	1.55
2	A	2001	FAD	C10-N1	2.13	1.37	1.33
2	B	2001	FAD	O4B-C4B	-2.12	1.40	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	FAD	N3A-C2A-N1A	-5.88	119.69	128.58
2	A	2001	FAD	N3A-C2A-N1A	-5.13	120.82	128.58
2	A	2001	FAD	C5A-C4A-N3A	-4.27	120.84	126.72
2	A	2001	FAD	C4-C4X-N5	3.97	123.70	118.21
2	B	2001	FAD	C5A-C4A-N3A	-3.83	121.44	126.72
2	A	2001	FAD	C5A-N7A-C8A	3.74	109.33	103.45
2	A	2001	FAD	N3A-C4A-N9A	3.60	133.29	127.17
2	B	2001	FAD	C5A-N7A-C8A	3.50	108.94	103.45
2	B	2001	FAD	C2A-N3A-C4A	3.22	119.69	111.83
2	A	2001	FAD	N9A-C8A-N7A	-3.21	109.39	113.94
2	B	2001	FAD	C4A-C5A-N7A	-3.11	107.02	110.58
2	A	2001	FAD	C2A-N3A-C4A	3.00	119.15	111.83
2	B	2001	FAD	O2P-P-O3P	-2.96	99.28	107.27
2	B	2001	FAD	N9A-C8A-N7A	-2.93	109.78	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	FAD	N3A-C4A-N9A	2.88	132.07	127.17
2	B	2001	FAD	C9-C9A-N10	-2.79	118.10	121.85
2	B	2001	FAD	C4-C4X-N5	2.74	121.99	118.21
2	A	2001	FAD	C4A-C5A-N7A	-2.70	107.50	110.58
2	B	2001	FAD	C4-N3-C2	-2.66	120.93	125.64
2	B	2001	FAD	C2A-N1A-C6A	2.51	122.85	118.73
2	A	2001	FAD	C4-N3-C2	-2.50	121.21	125.64
2	A	2001	FAD	C4X-C4-N3	2.49	119.58	113.25
2	B	2001	FAD	C4X-C10-N10	2.43	119.97	116.48
2	A	2001	FAD	C10-C4X-N5	-2.42	119.86	124.81
2	A	2001	FAD	C9-C9A-N10	-2.41	118.61	121.85
2	A	2001	FAD	O2P-P-O3P	-2.40	100.79	107.27
2	A	2001	FAD	O2A-PA-O3P	-2.38	100.84	107.27
2	A	2001	FAD	C4X-C10-N10	2.36	119.86	116.48
2	B	2001	FAD	C10-C4X-N5	-2.33	120.04	124.81
5	A	2004	UY7	CG-CB-CA	2.14	106.22	103.75
5	A	2005	UY7	O-C-CA	-2.13	115.38	122.26
5	A	2005	UY7	O09-CG-CD	-2.11	105.98	110.30
2	B	2001	FAD	C4X-C4-N3	2.09	118.58	113.25
2	A	2001	FAD	C4A-N9A-C8A	2.07	107.91	105.74
2	B	2001	FAD	O3P-P-O1P	2.05	116.87	110.70
2	A	2001	FAD	C5X-C9A-N10	2.03	119.80	117.97

There are no chirality outliers.

All (13) torsion outliers are listed below:

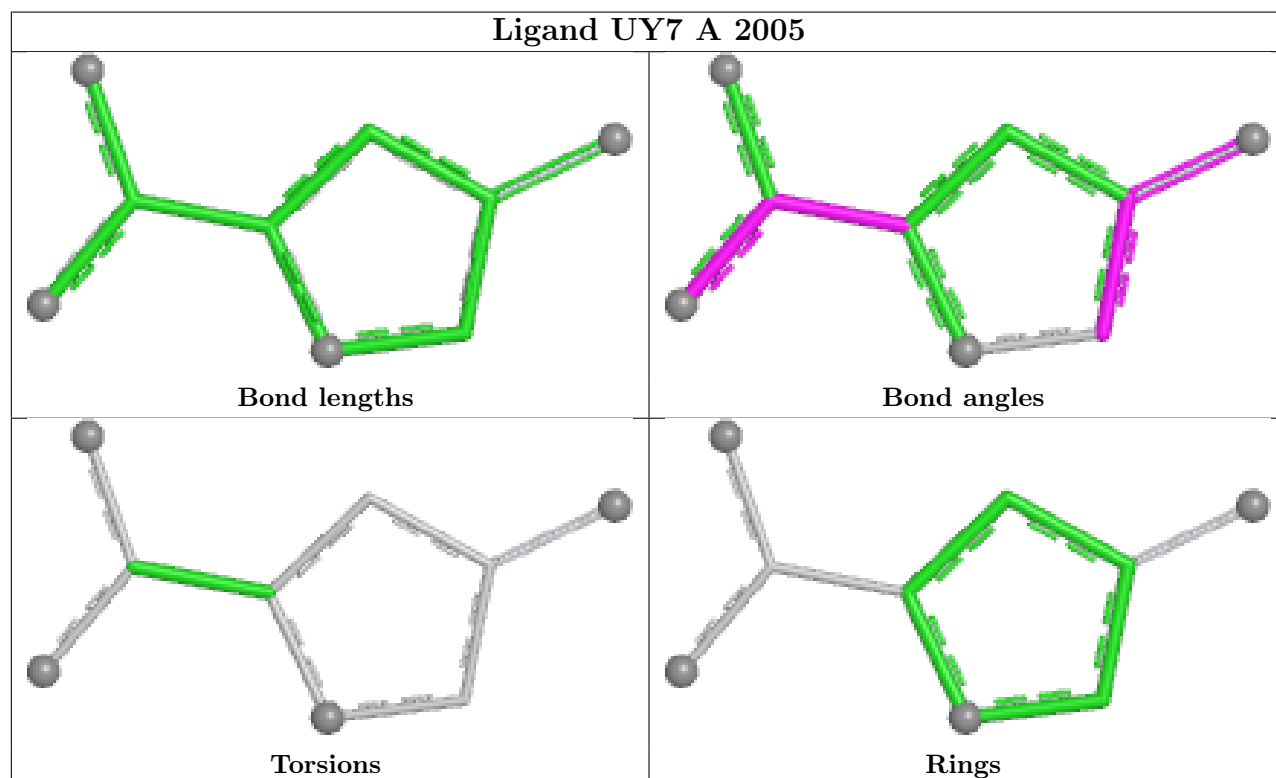
Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	C2'-C3'-C4'-O4'
2	A	2001	FAD	C2'-C3'-C4'-C5'
2	A	2001	FAD	O3'-C3'-C4'-O4'
2	B	2001	FAD	C2'-C3'-C4'-C5'
2	B	2001	FAD	O3'-C3'-C4'-C5'
2	B	2001	FAD	O3'-C3'-C4'-O4'
2	B	2001	FAD	C2'-C3'-C4'-O4'
2	A	2001	FAD	O3'-C3'-C4'-C5'
4	B	2003	PEG	O2-C3-C4-O4
4	A	2003	PEG	O2-C3-C4-O4
7	B	2002	PGE	O3-C5-C6-O4
2	A	2001	FAD	P-O3P-PA-O5B
2	B	2001	FAD	P-O3P-PA-O5B

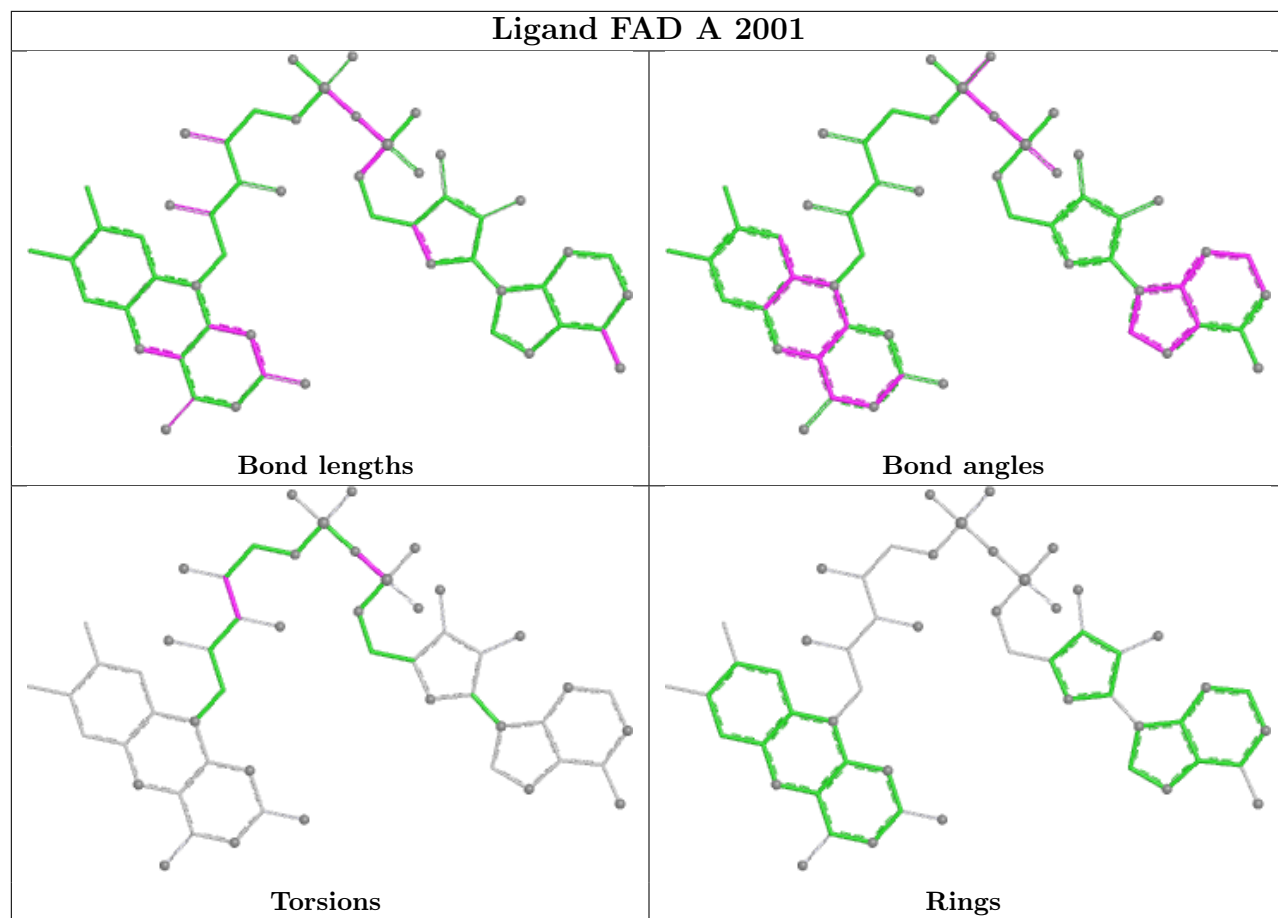
There are no ring outliers.

3 monomers are involved in 9 short contacts:

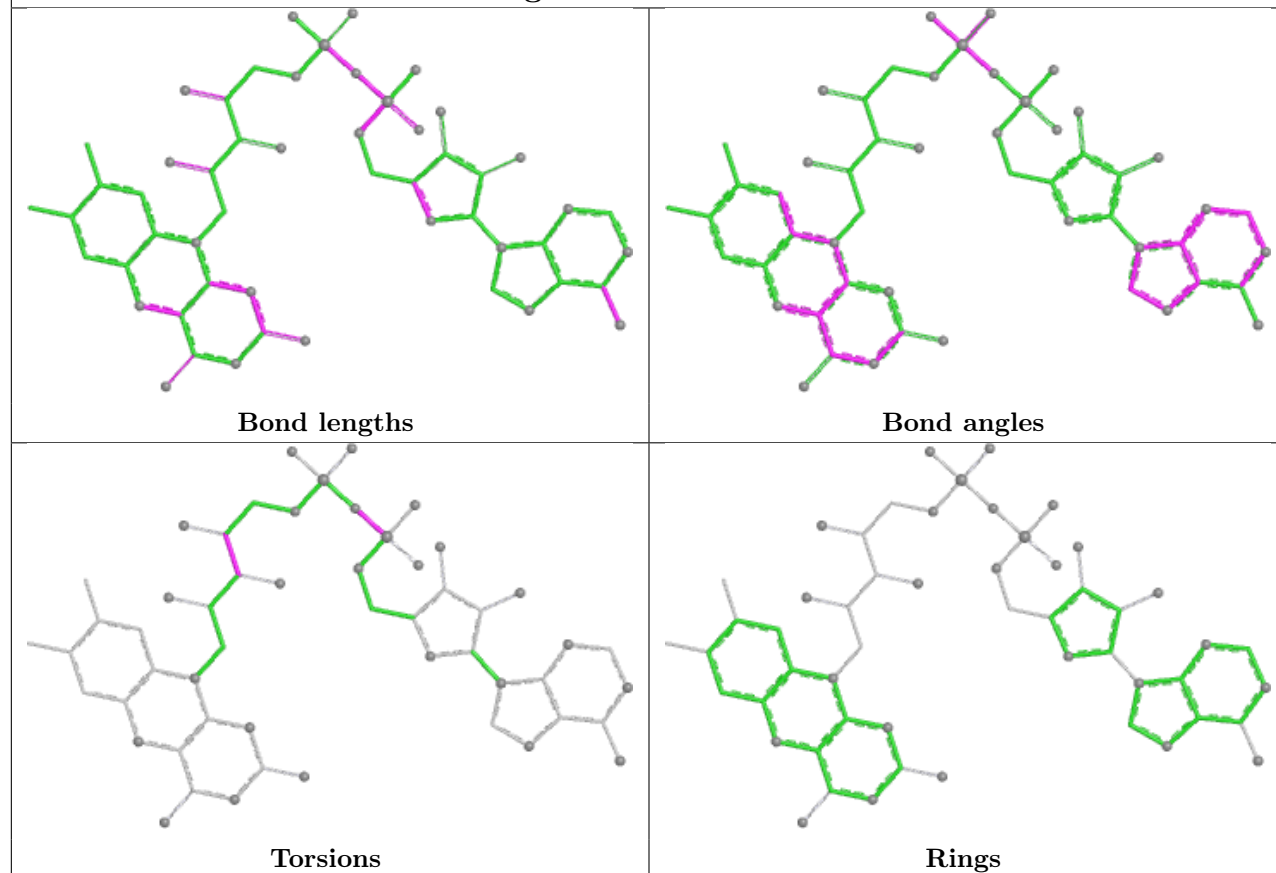
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2006	SO4	1	0
2	A	2001	FAD	4	0
2	B	2001	FAD	4	0

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.

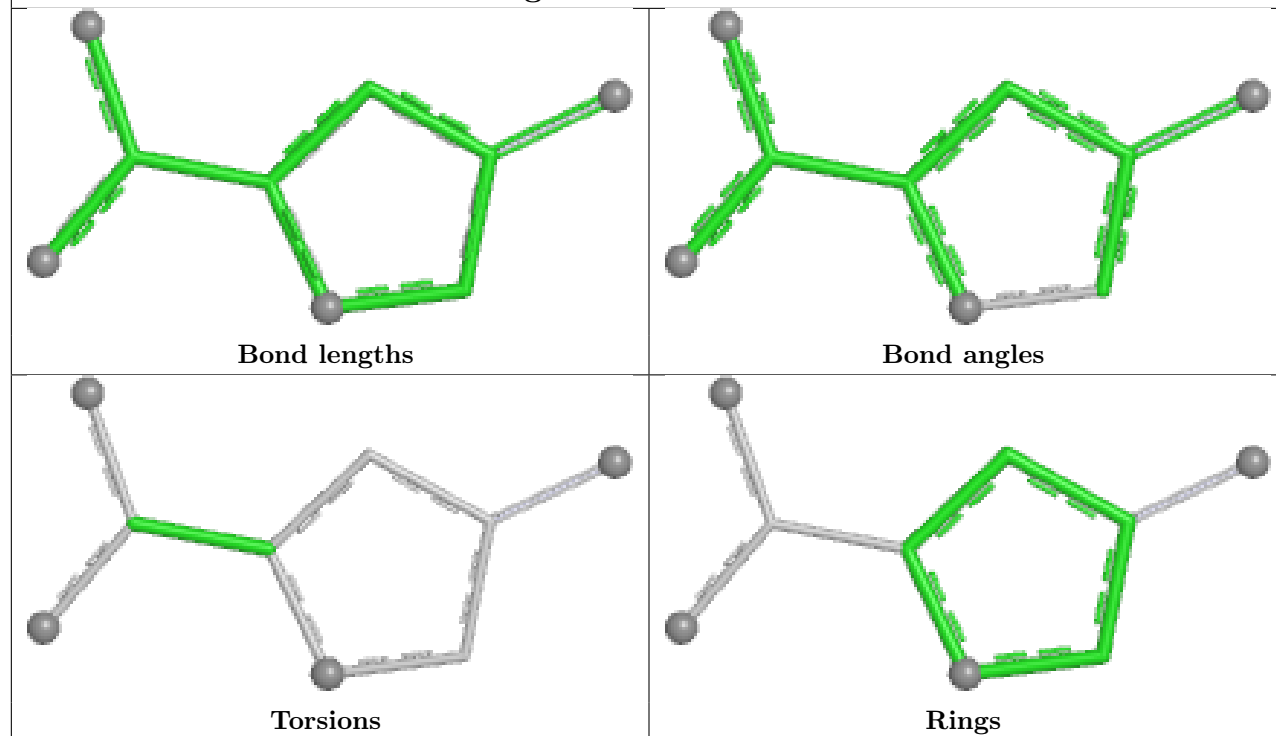


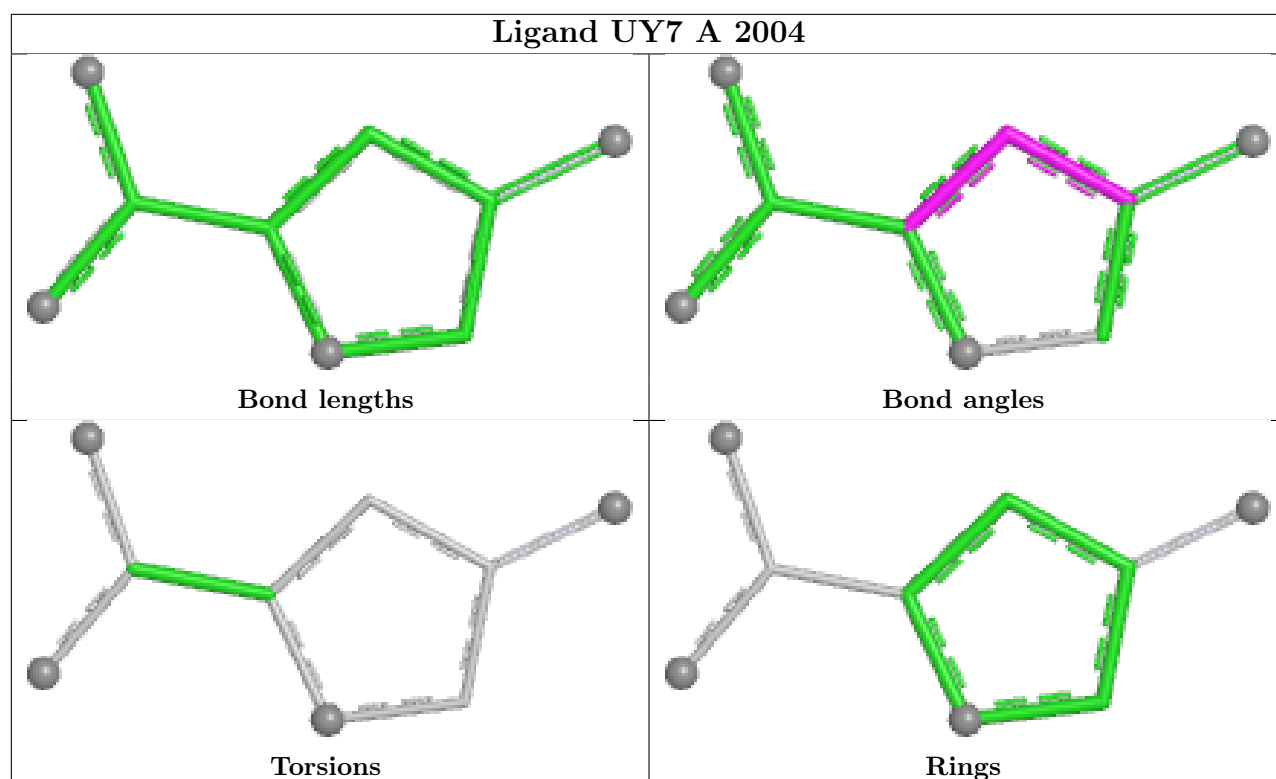


Ligand FAD B 2001



Ligand UY7 B 2004





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	1214/1235 (98%)	0.07	41 (3%)	48	51	8, 18, 35, 63	13 (1%)
1	B	1213/1235 (98%)	0.19	59 (4%)	35	37	8, 19, 37, 66	15 (1%)
All	All	2427/2470 (98%)	0.13	100 (4%)	41	44	8, 18, 37, 66	28 (1%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	PRO	5.3
1	B	905	LEU	5.0
1	B	906	GLY	4.9
1	B	495	ALA	4.4
1	B	912	ILE	4.3
1	A	127	ASP	4.2
1	A	14	ALA	4.1
1	B	14	ALA	4.1
1	B	485	TYR	4.0
1	B	138	ARG	3.9
1	B	1232	ILE	3.9
1	A	132	SER	3.9
1	B	129	ASN	3.8
1	B	492	GLU	3.7
1	A	1230	MET	3.7
1	B	1231	ALA	3.7
1	B	77	GLY	3.6
1	A	1232	ILE	3.6
1	B	1227	ALA	3.6
1	B	491	LEU	3.5
1	A	129	ASN	3.5
1	A	493	ASN	3.5
1	B	128	GLY	3.5
1	B	1230	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1231	ALA	3.5
1	B	493	ASN	3.5
1	B	494	GLY	3.4
1	A	763	GLY	3.4
1	B	156	THR	3.4
1	A	128	GLY	3.4
1	A	130	TRP	3.3
1	B	904	GLY	3.3
1	B	132	SER	3.3
1	B	223	LEU	3.2
1	B	74	ALA	3.2
1	B	1233	GLY	3.1
1	B	907	ARG	3.1
1	A	125	ILE	3.1
1	A	1229	LEU	3.1
1	A	1227	ALA	3.0
1	A	115	ALA	3.0
1	B	133	HIS	3.0
1	A	801	ALA	2.9
1	A	137	SER	2.9
1	B	503	ILE	2.9
1	A	495	ALA	2.9
1	A	485	TYR	2.9
1	B	928	ILE	2.7
1	B	115	ALA	2.7
1	B	134	LEU	2.7
1	A	111	ILE	2.7
1	A	494	GLY	2.6
1	A	492	GLU	2.6
1	A	134	LEU	2.6
1	B	909	VAL	2.6
1	B	497	SER	2.6
1	A	75	LEU	2.5
1	B	224	GLY	2.5
1	A	491	LEU	2.5
1	A	74	ALA	2.5
1	A	1228	SER	2.5
1	B	1147	LEU	2.5
1	A	800	PRO	2.4
1	B	1229	LEU	2.4
1	B	496	ASN	2.4
1	B	1140	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	112	PRO	2.4
1	A	965	ALA	2.4
1	B	131	LYS	2.4
1	B	150	VAL	2.3
1	A	119	ALA	2.3
1	B	508	VAL	2.3
1	B	1141	LEU	2.3
1	A	133	HIS	2.2
1	B	913	GLY	2.2
1	B	507	LYS	2.2
1	B	490	LEU	2.2
1	B	931	LEU	2.2
1	A	525	PRO	2.2
1	B	500	VAL	2.2
1	B	78	LYS	2.2
1	B	902	MET	2.1
1	B	112	PRO	2.1
1	B	506	PRO	2.1
1	B	812	GLY	2.1
1	A	116	THR	2.1
1	A	156	THR	2.1
1	A	939	ARG	2.1
1	B	113	ASP	2.1
1	B	1222	ALA	2.1
1	A	138	ARG	2.1
1	A	113	ASP	2.1
1	B	520	VAL	2.0
1	B	515	ALA	2.0
1	B	139	SER	2.0
1	B	1228	SER	2.0
1	A	131	LYS	2.0
1	B	124	LYS	2.0
1	B	914	LEU	2.0
1	A	796	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

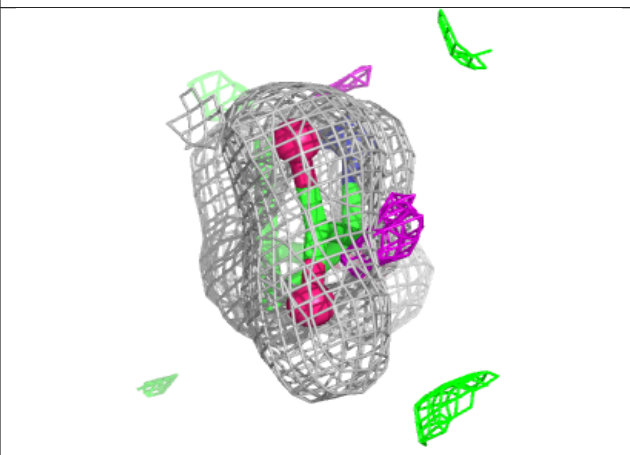
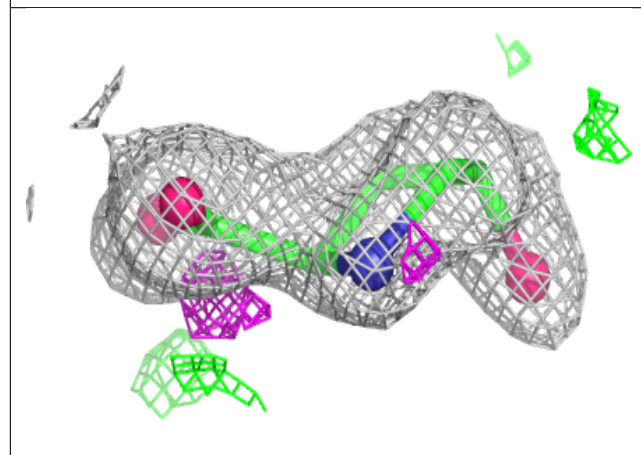
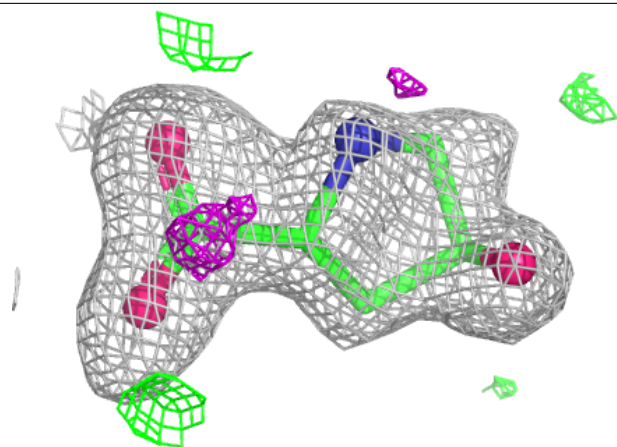
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	SO4	A	2011	5/5	0.78	0.20	70,72,73,74	5
6	SO4	B	2007	5/5	0.79	0.19	84,84,85,88	5
6	SO4	A	2009	5/5	0.81	0.16	56,56,62,66	5
6	SO4	B	2008	5/5	0.81	0.17	49,52,61,62	5
4	PEG	A	2003	7/7	0.84	0.16	49,52,54,54	0
4	PEG	B	2003	7/7	0.85	0.17	41,44,50,51	0
6	SO4	B	2006	5/5	0.88	0.12	54,56,58,59	5
6	SO4	A	2008	5/5	0.89	0.12	37,38,44,53	0
4	PEG	A	2006	7/7	0.90	0.10	28,29,38,38	0
5	UY7	A	2005	9/9	0.91	0.10	26,35,37,39	0
6	SO4	A	2010	5/5	0.92	0.11	29,32,43,44	5
7	PGE	B	2002	10/10	0.93	0.10	27,38,45,45	0
5	UY7	A	2004	9/9	0.94	0.08	17,18,19,24	0
2	FAD	B	2001	53/53	0.95	0.09	13,18,33,42	0
3	FMT	A	2002	3/3	0.95	0.12	21,21,29,29	0
2	FAD	A	2001	53/53	0.95	0.08	13,19,26,30	0
5	UY7	B	2004	9/9	0.96	0.06	15,16,21,24	0
6	SO4	A	2007	5/5	0.99	0.04	14,15,17,19	0
6	SO4	B	2005	5/5	0.99	0.03	14,14,18,18	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.

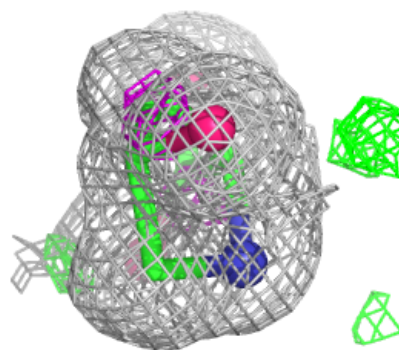
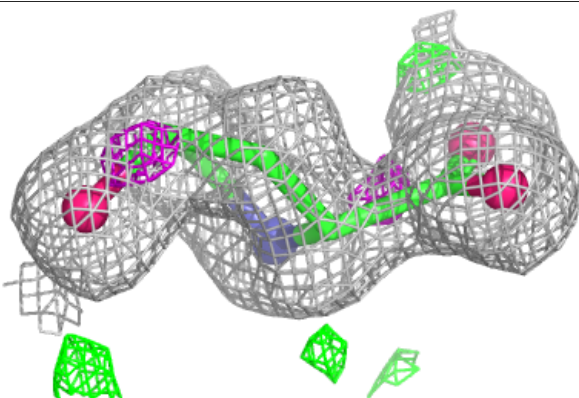
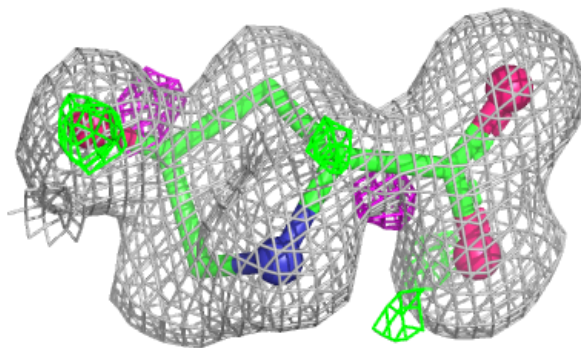
Electron density around UY7 A 2005:

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

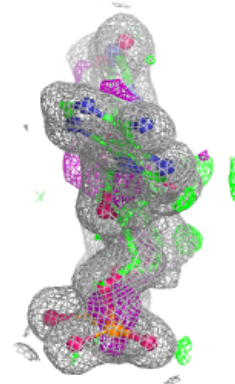
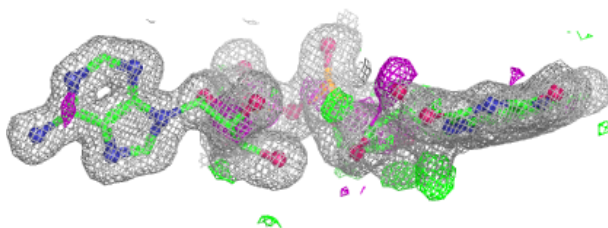
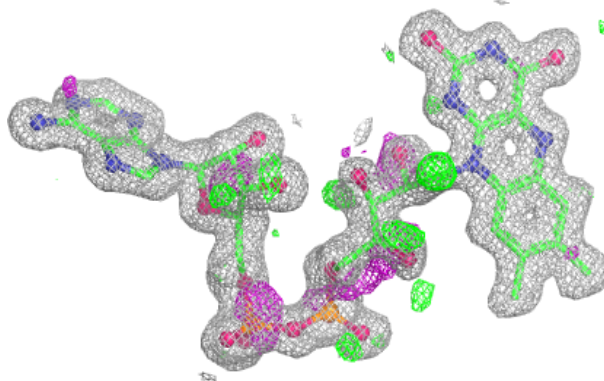


Electron density around UY7 A 2004:

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

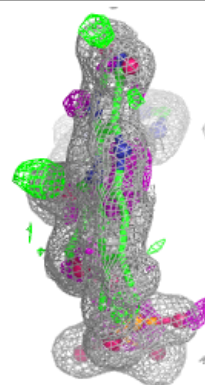
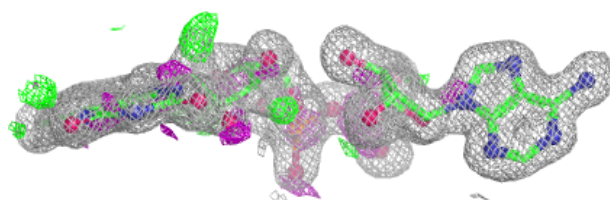
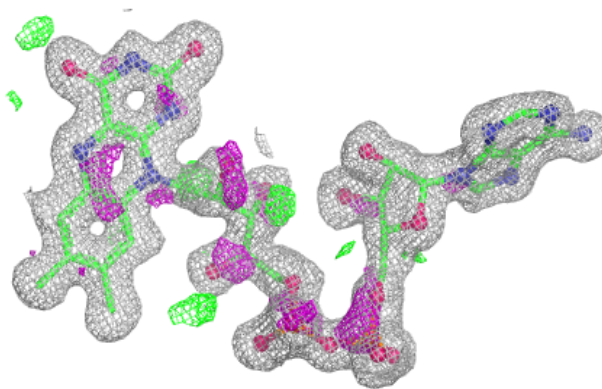
**Electron density around FAD B 2001:**

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

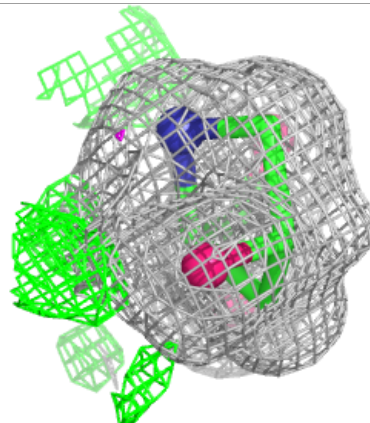
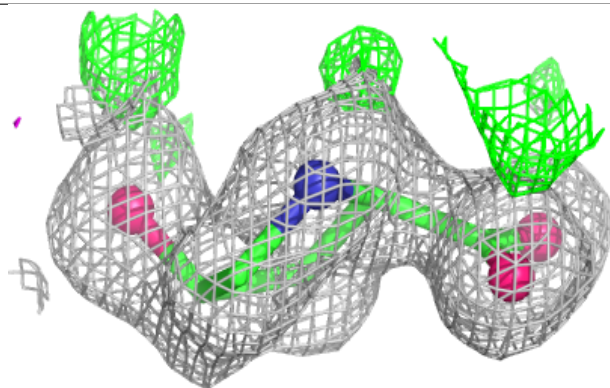
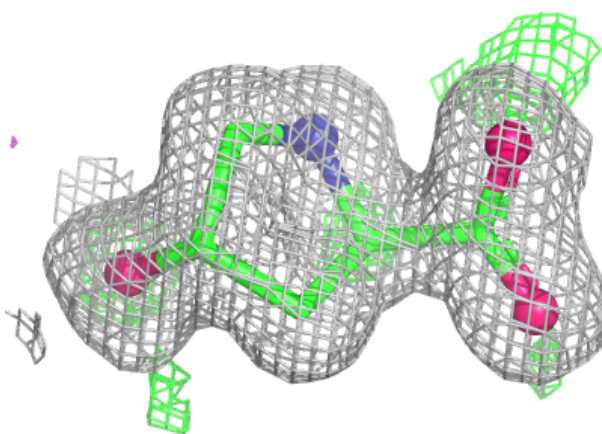


Electron density around FAD A 2001:

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

**Electron density around UY7 B 2004:**

$2mF_o-DF_c$ (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.