



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 06:10 PM EDT

PDB ID : 9BBO / pdb_00009bbo
Title : Proline utilization A complexed with the product L-glutamate in the aldehyde dehydrogenase active site
Authors : Tanner, J.J.
Deposited on : 2024-04-06
Resolution : 1.50 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

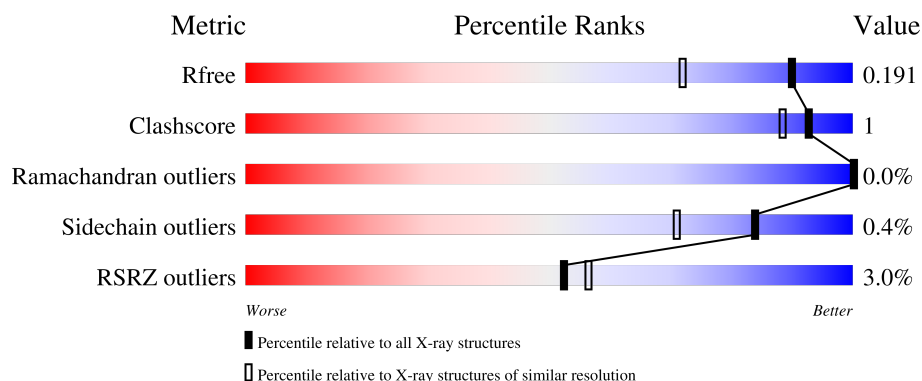
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	2% 94% 5%
1	B	1235	3% 95% • •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 20529 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.

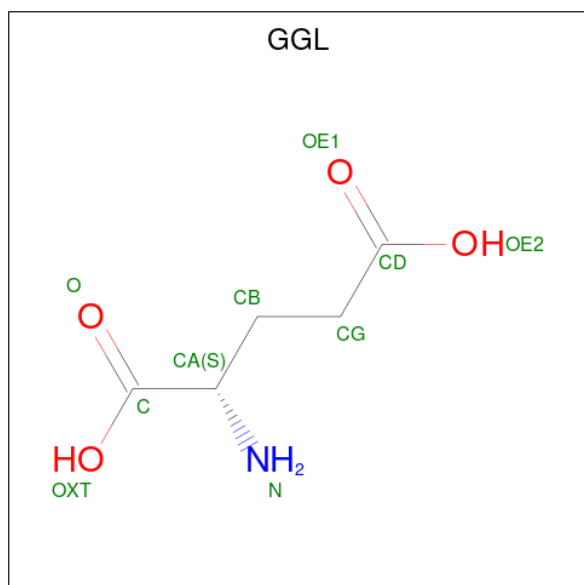
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1219	Total	C	N	O	S	0	23	0
			9203	5799	1651	1718	35			
1	B	1218	Total	C	N	O	S	0	15	0
			9146	5764	1643	1705	34			

There are 4 discrepancies between the modelled and reference sequences:

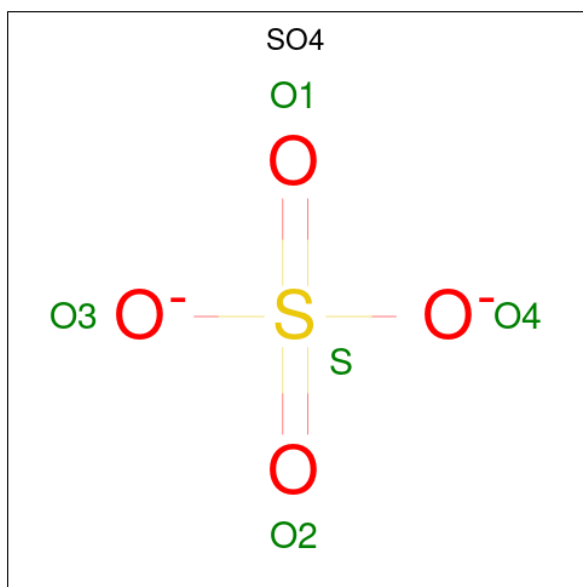
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is GAMMA-L-GLUTAMIC ACID (CCD ID: GGL) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



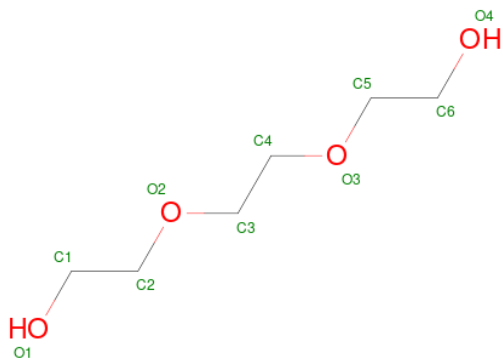
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



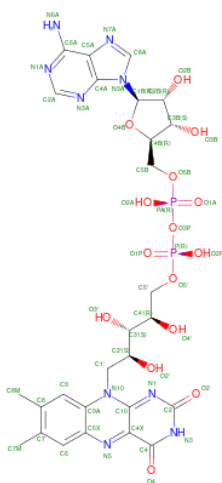
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



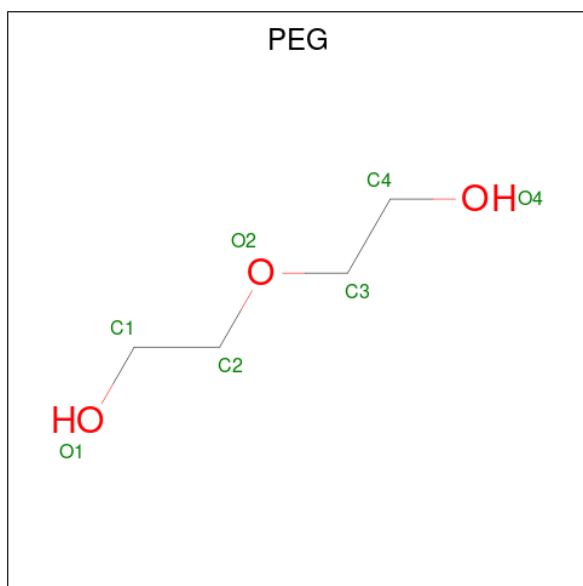
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

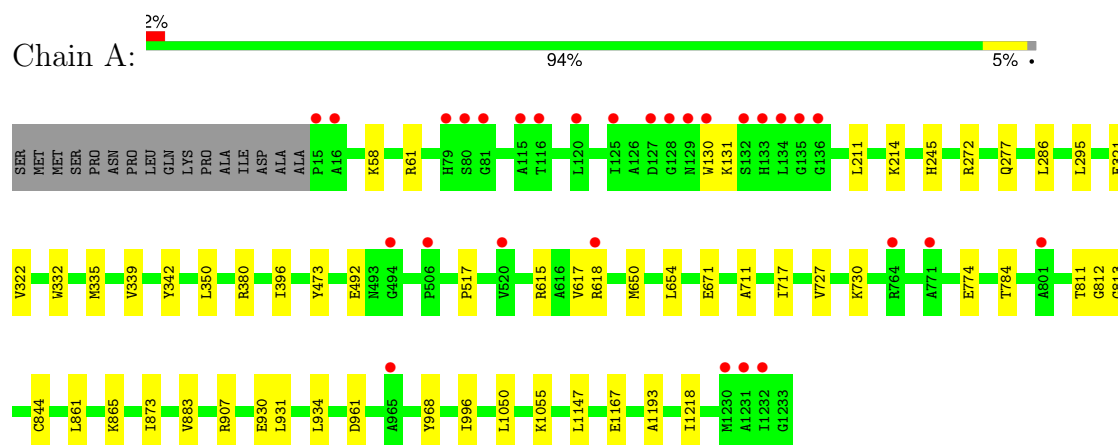
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	995	Total	O	0	0
			995	995		
7	B	987	Total	O	0	0
			987	987		

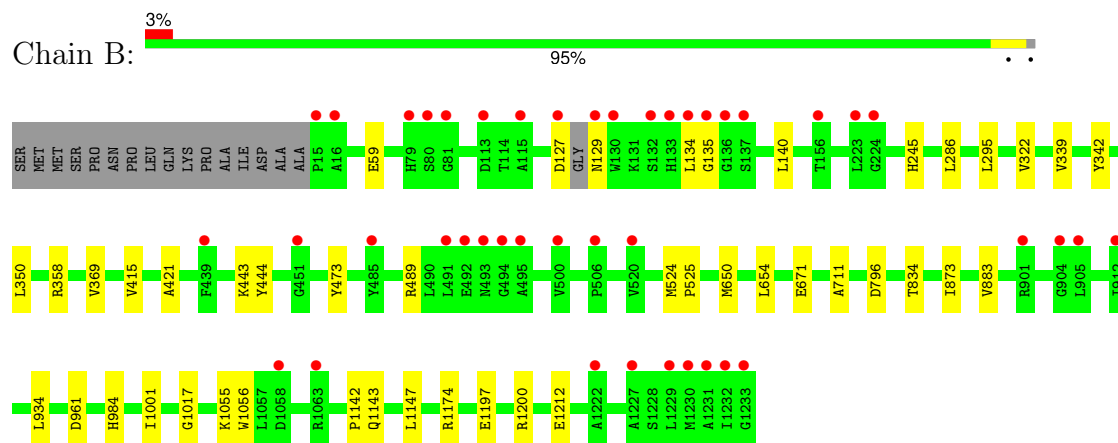
3 Residue-property plots

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	101.38Å 102.44Å 127.60Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	51.77 – 1.50 51.77 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (51.77-1.50) 97.0 (51.77-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.50Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5156: ???)	Depositor
R, R_{free}	0.169 , 0.191 0.169 , 0.191	Depositor DCC
R_{free} test set	19611 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20529	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 3.07% 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: SO4, PGE, PEG, FAD, GGL

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	0.25	0/9427	0.46	0/12815
1	B	0.25	0/9354	0.46	0/12718
All	All	0.25	0/18781	0.46	0/25533

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	9203	0	9340	32	0
1	B	9146	0	9271	25	0
2	A	10	0	7	0	0
2	B	10	0	7	0	0
3	A	25	0	0	0	0
3	B	20	0	0	0	0
4	A	10	0	14	0	0
4	B	10	0	14	0	0
5	A	53	0	31	2	0
5	B	53	0	31	1	0
6	B	7	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	995	0	0	0	0
7	B	987	0	0	2	0
All	All	20529	0	18725	54	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 1.

All (54) 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:961:ASP:OD2	1:B:1055:LYS:NZ	2.22	0.72
1:B:127:ASP:O	1:B:129:ASN:N	2.29	0.66
1:B:339[B]:VAL:HG21	1:B:350:LEU:HD21	1.78	0.65
1:B:134:LEU:HB3	1:B:140[A]:LEU:HD21	1.80	0.63
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.83	0.60
1:A:1147:LEU:HD22	1:B:1147:LEU:HD13	1.85	0.58
1:B:834[A]:THR:HG22	1:B:1001:ILE:HD11	1.87	0.56
1:A:473:TYR:HB2	5:A:1308:FAD:HM71	1.88	0.56
1:B:873:ILE:HG13	1:B:883:VAL:HB	1.88	0.56
1:A:907:ARG:HD2	1:A:931:LEU:HD23	1.89	0.55
1:A:339[B]:VAL:HG21	1:A:350:LEU:HD21	1.88	0.55
1:B:443:LYS:HD2	1:B:444:TYR:HD2	1.72	0.55
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.89	0.55
1:B:796:ASP:OD1	1:B:1174[A]:ARG:NH2	2.41	0.54
1:A:245:HIS:CE1	1:A:295[B]:LEU:HD21	2.43	0.53
1:A:1055:LYS:NZ	1:B:961:ASP:OD2	2.36	0.53
1:B:650:MET:O	1:B:654:LEU:HG	2.10	0.50
1:A:861:LEU:HG	1:A:865:LYS:HE3	1.92	0.50
1:A:650:MET:O	1:A:654:LEU:HG	2.11	0.50
1:A:671:GLU:HG3	1:A:711:ALA:HB2	1.95	0.49
1:B:524[A]:MET:HE3	1:B:525:PRO:HD2	1.94	0.49
1:B:1143:GLN:O	1:B:1147:LEU:HG	2.13	0.49
1:A:813[A]:GLY:HA2	1:A:968:TYR:CD1	2.48	0.48
1:A:615:ARG:HG2	1:A:618:ARG:NH2	2.28	0.48
1:B:473:TYR:HE2	1:B:489:ARG:HH12	1.61	0.48
1:B:473:TYR:HB2	5:B:1308:FAD:HM72	1.95	0.48
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.50	0.47
1:B:1017:GLY:HA2	7:B:1486:HOH:O	2.15	0.45
1:A:492:GLU:HB3	5:A:1308:FAD:H4'	1.99	0.45
1:A:130:TRP:CZ2	1:A:131:LYS:HE2	2.51	0.45
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.98	0.44
1:A:396:ILE:HG13	1:A:517:PRO:HB3	1.99	0.44
1:A:784[B]:THR:HA	1:A:811[B]:THR:HG21	2.00	0.43
1:A:996[A]:ILE:HD12	1:A:1218:ILE:HG12	2.00	0.43
1:A:784[A]:THR:HG22	1:A:811[A]:THR:HB	2.00	0.43
1:A:812[A]:GLY:HA2	1:A:844:CYS:HB3	2.00	0.43
1:A:861:LEU:HD21	1:A:930:GLU:CD	2.44	0.43
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.43	0.43
1:B:245:HIS:CE1	1:B:295[A]:LEU:HD11	2.54	0.43
1:A:332:TRP:HZ3	1:A:335[A]:MET:HE2	1.83	0.42
1:A:717:ILE:HG12	1:A:727:VAL:HG11	2.02	0.42
1:B:1197:GLU:HA	1:B:1200:ARG:HG2	2.01	0.42
1:A:211:LEU:HD23	1:A:214:LYS:HD2	2.01	0.42
1:B:1212:GLU:OE2	7:B:1401:HOH:O	2.22	0.42
1:A:617:VAL:HG12	1:A:774:GLU:HB2	2.01	0.41
1:A:1167:GLU:HA	1:A:1193:ALA:O	2.20	0.41
1:B:369:VAL:HG12	1:B:421:ALA:HB3	2.01	0.41
1:B:984:HIS:C	1:B:984:HIS:CD2	2.98	0.41
1:A:380[A]:ARG:HE	1:A:380[A]:ARG:HB2	1.65	0.41
1:A:58:LYS:HD3	1:A:61:ARG:NH2	2.36	0.41
1:A:618:ARG:HG2	1:A:774:GLU:OE2	2.21	0.40
1:B:671:GLU:HG3	1:B:711:ALA:HB2	2.03	0.40
1:B:358:ARG:HG2	1:B:415:VAL:HG11	2.04	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	1241/1235 (100%)	1220 (98%)	21 (2%)	0	100 100
1	B	1230/1235 (100%)	1205 (98%)	24 (2%)	1 (0%)	48 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2471/2470 (100%)	2425 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	GLY

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	940/951 (99%)	936 (100%)	4 (0%)	84	71
1	B	931/951 (98%)	928 (100%)	3 (0%)	86	75
All	All	1871/1902 (98%)	1864 (100%)	7 (0%)	84	71

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	GLU
1	A	342	TYR
1	A	730	LYS
1	A	934	LEU
1	B	59	GLU
1	B	342	TYR
1	B	934	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	419	GLN
1	A	501	HIS
1	A	872	HIS
1	A	894	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1140	ASN
1	A	1143	GLN
1	B	501	HIS
1	B	667	ASN
1	B	1115	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](#)

16 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	SO4	A	1303	-	4,4,4	0.65	0	6,6,6	0.40	0
3	SO4	B	1303	-	4,4,4	0.68	0	6,6,6	0.08	0
5	FAD	B	1308	-	58,58,58	2.56	16 (27%)	85,89,89	1.76	19 (22%)
3	SO4	A	1305	-	4,4,4	0.70	0	6,6,6	0.25	0
3	SO4	A	1302	-	4,4,4	0.56	0	6,6,6	0.30	0
2	GGL	B	1301	-	8,9,9	1.10	0	8,11,11	1.27	2 (25%)
3	SO4	A	1304	-	4,4,4	0.69	0	6,6,6	0.13	0
3	SO4	B	1302	-	4,4,4	0.58	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	B	1307	-	9,9,9	0.52	0	8,8,8	0.19	0
2	GGL	A	1301	-	8,9,9	1.13	0	8,11,11	1.37	1 (12%)
3	SO4	A	1306	-	4,4,4	0.67	0	6,6,6	0.14	0
3	SO4	B	1305	-	4,4,4	0.69	0	6,6,6	0.15	0
4	PGE	A	1307	-	9,9,9	0.51	0	8,8,8	0.21	0
5	FAD	A	1308	-	58,58,58	2.59	19 (32%)	85,89,89	1.65	15 (17%)
3	SO4	B	1304	-	4,4,4	0.68	0	6,6,6	0.22	0
6	PEG	B	1306	-	6,6,6	0.51	0	5,5,5	0.33	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	FAD	B	1308	-	-	5/34/50/50	0/6/6/6
4	PGE	B	1307	-	-	0/7/7/7	-
2	GGL	B	1301	-	-	2/9/9/9	-
2	GGL	A	1301	-	-	0/9/9/9	-
4	PGE	A	1307	-	-	1/7/7/7	-
5	FAD	A	1308	-	-	6/34/50/50	0/6/6/6
6	PEG	B	1306	-	-	1/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1308	FAD	PA-O3P	-8.87	1.49	1.59
5	B	1308	FAD	PA-O3P	-8.83	1.50	1.59
5	A	1308	FAD	O4-C4	6.73	1.36	1.23
5	B	1308	FAD	O4-C4	6.47	1.35	1.23
5	B	1308	FAD	C4X-N5	6.22	1.44	1.30
5	A	1308	FAD	C4X-N5	6.08	1.43	1.30
5	B	1308	FAD	O2-C2	5.54	1.35	1.24
5	B	1308	FAD	C6-C5X	5.37	1.48	1.40
5	A	1308	FAD	P-O3P	5.30	1.65	1.59
5	B	1308	FAD	C10-N1	5.14	1.43	1.33
5	A	1308	FAD	C10-N1	5.10	1.43	1.33
5	A	1308	FAD	C6-C5X	4.82	1.47	1.40
5	A	1308	FAD	C9-C9A	4.59	1.47	1.39
5	A	1308	FAD	O2-C2	4.44	1.33	1.24
5	B	1308	FAD	C9-C9A	4.09	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1308	FAD	C6A-N6A	3.75	1.43	1.34
5	A	1308	FAD	C6A-N6A	3.66	1.43	1.34
5	B	1308	FAD	C9A-C5X	-3.39	1.35	1.41
5	A	1308	FAD	C9A-C5X	-2.98	1.36	1.41
5	A	1308	FAD	C5X-N5	2.87	1.44	1.39
5	A	1308	FAD	PA-O5B	-2.76	1.48	1.59
5	A	1308	FAD	O2'-C2'	-2.73	1.37	1.43
5	B	1308	FAD	C5X-N5	2.70	1.44	1.39
5	B	1308	FAD	C2-N1	2.65	1.42	1.36
5	B	1308	FAD	PA-O2A	-2.57	1.43	1.55
5	A	1308	FAD	C2-N1	2.42	1.42	1.36
5	A	1308	FAD	C4X-C10	-2.38	1.37	1.44
5	B	1308	FAD	C10-N10	2.34	1.42	1.37
5	A	1308	FAD	C5A-C4A	2.21	1.43	1.39
5	A	1308	FAD	C10-N10	2.10	1.41	1.37
5	B	1308	FAD	C4X-C10	-2.10	1.38	1.44
5	B	1308	FAD	C2A-N3A	2.10	1.37	1.33
5	A	1308	FAD	PA-O2A	-2.06	1.45	1.55
5	A	1308	FAD	O4B-C4B	-2.04	1.40	1.45
5	B	1308	FAD	O2'-C2'	-2.01	1.39	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1308	FAD	N3A-C2A-N1A	-5.86	119.71	128.58
5	A	1308	FAD	N3A-C2A-N1A	-4.89	121.18	128.58
5	A	1308	FAD	C5A-C4A-N3A	-4.84	120.05	126.72
5	B	1308	FAD	C5A-C4A-N3A	-4.41	120.65	126.72
5	B	1308	FAD	N3A-C4A-N9A	4.02	134.01	127.17
5	A	1308	FAD	N3A-C4A-N9A	3.93	133.86	127.17
5	A	1308	FAD	C5A-N7A-C8A	3.82	109.46	103.45
5	B	1308	FAD	C4X-C10-N10	3.67	121.74	116.48
5	A	1308	FAD	O2A-PA-O3P	-3.58	97.59	107.27
5	B	1308	FAD	C9-C9A-N10	-3.57	117.05	121.85
5	B	1308	FAD	C5A-N7A-C8A	3.35	108.72	103.45
5	B	1308	FAD	C2A-N3A-C4A	3.35	120.02	111.83
5	A	1308	FAD	N9A-C8A-N7A	-3.25	109.32	113.94
5	A	1308	FAD	C2A-N3A-C4A	3.19	119.63	111.83
5	B	1308	FAD	N9A-C8A-N7A	-3.12	109.52	113.94
5	A	1308	FAD	C4A-C5A-N7A	-3.10	107.03	110.58
5	B	1308	FAD	C4'-C3'-C2'	2.83	118.28	113.57
5	A	1308	FAD	C4X-C10-N10	2.79	120.48	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1308	FAD	C4-N3-C2	-2.72	120.81	125.64
5	A	1308	FAD	C4X-C4-N3	2.68	120.09	113.25
5	B	1308	FAD	O3P-PA-O1A	2.65	118.69	110.70
5	B	1308	FAD	C9A-N10-C10	-2.65	116.71	120.75
5	B	1308	FAD	C4A-N9A-C8A	2.65	108.52	105.74
5	B	1308	FAD	O2A-PA-O3P	-2.57	100.33	107.27
5	B	1308	FAD	C4-N3-C2	-2.56	121.10	125.64
5	A	1308	FAD	O4-C4-C4X	-2.52	119.89	126.53
5	B	1308	FAD	C5X-C9A-N10	2.45	120.18	117.97
5	B	1308	FAD	O5'-C5'-C4'	2.41	115.79	109.36
5	B	1308	FAD	C4A-C5A-N7A	-2.35	107.89	110.58
5	A	1308	FAD	C9-C9A-N10	-2.28	118.79	121.85
5	A	1308	FAD	C4A-N9A-C8A	2.25	108.10	105.74
5	B	1308	FAD	C4-C4X-C10	2.23	120.76	116.93
5	B	1308	FAD	C2A-N1A-C6A	2.18	122.31	118.73
2	A	1301	GGL	OE2-CD-CG	2.10	120.64	114.00
2	B	1301	GGL	OXT-C-O	-2.10	119.32	124.08
5	A	1308	FAD	C9A-N10-C10	-2.09	117.56	120.75
2	B	1301	GGL	OE2-CD-CG	2.01	120.34	114.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

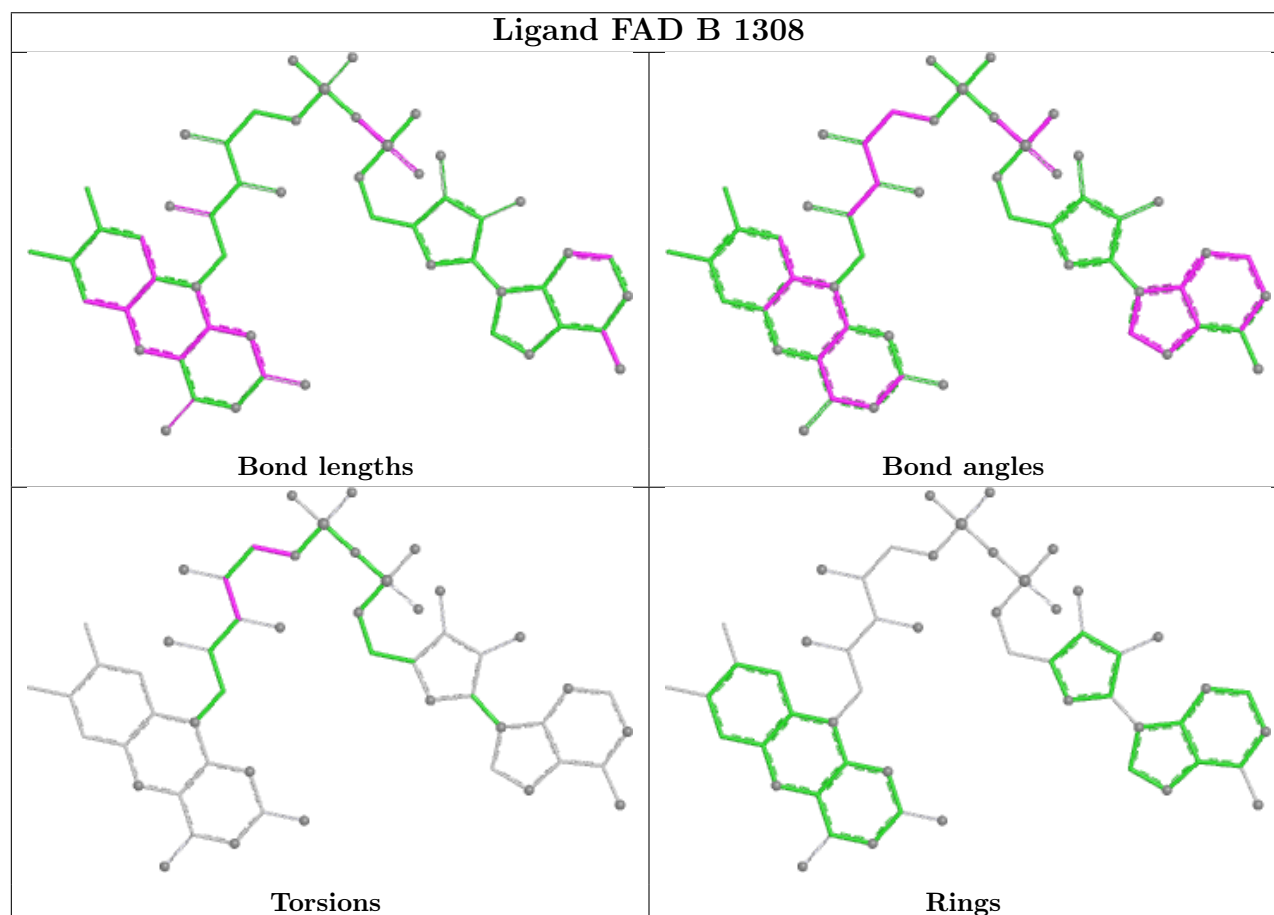
Mol	Chain	Res	Type	Atoms
5	A	1308	FAD	P-O3P-PA-O5B
5	A	1308	FAD	C2'-C3'-C4'-O4'
5	B	1308	FAD	C2'-C3'-C4'-O4'
5	B	1308	FAD	O3'-C3'-C4'-O4'
5	B	1308	FAD	O3'-C3'-C4'-C5'
5	A	1308	FAD	C2'-C3'-C4'-C5'
5	B	1308	FAD	C2'-C3'-C4'-C5'
5	A	1308	FAD	O3'-C3'-C4'-O4'
4	A	1307	PGE	O3-C5-C6-O4
5	A	1308	FAD	O3'-C3'-C4'-C5'
6	B	1306	PEG	O1-C1-C2-O2
5	A	1308	FAD	C4'-C5'-O5'-P
2	B	1301	GGL	OE1-CD-CG-CB
5	B	1308	FAD	C4'-C5'-O5'-P
2	B	1301	GGL	OE2-CD-CG-CB

There are no ring outliers.

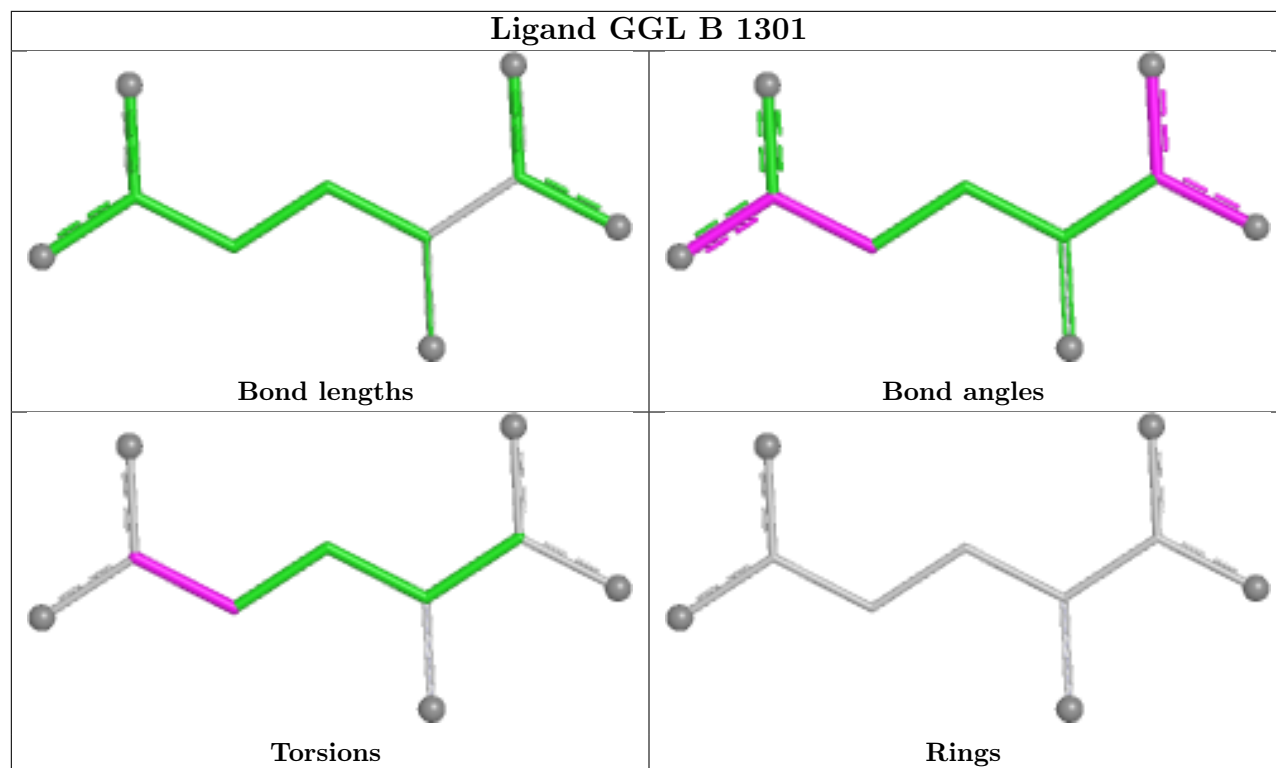
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1308	FAD	1	0
5	A	1308	FAD	2	0

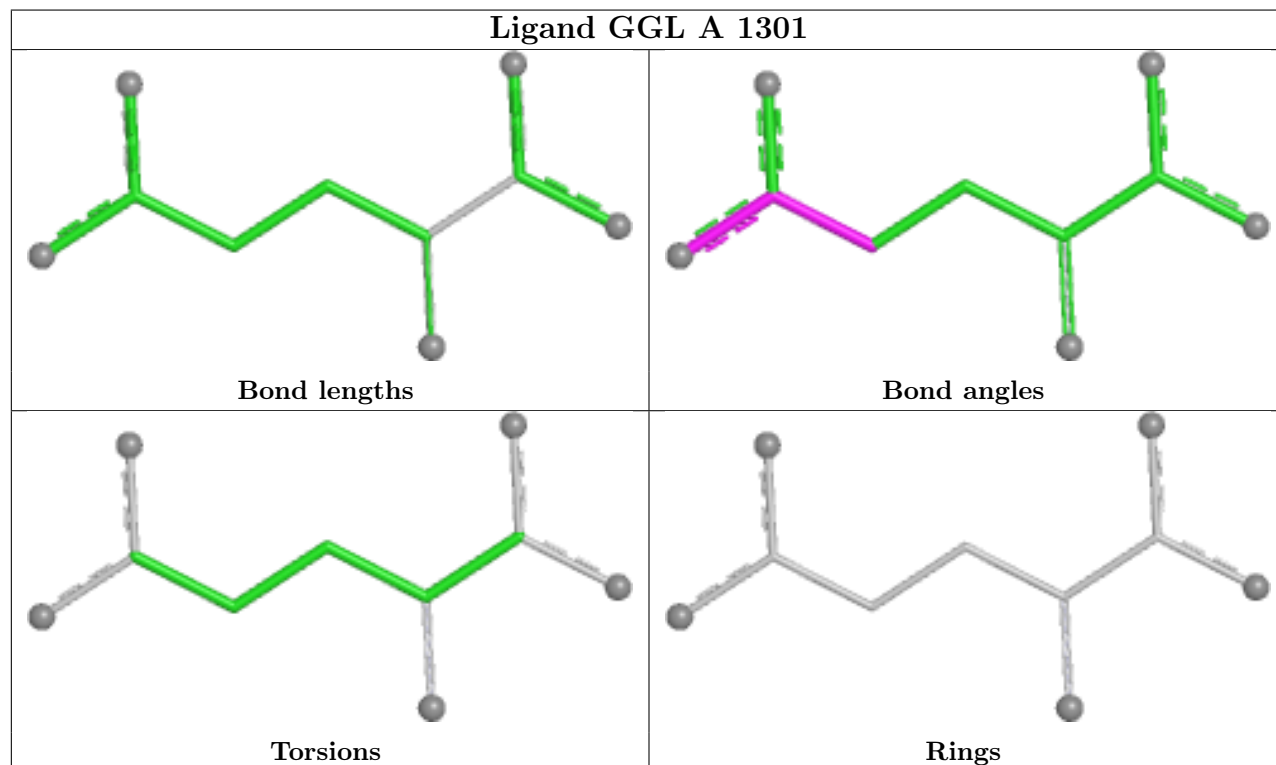
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

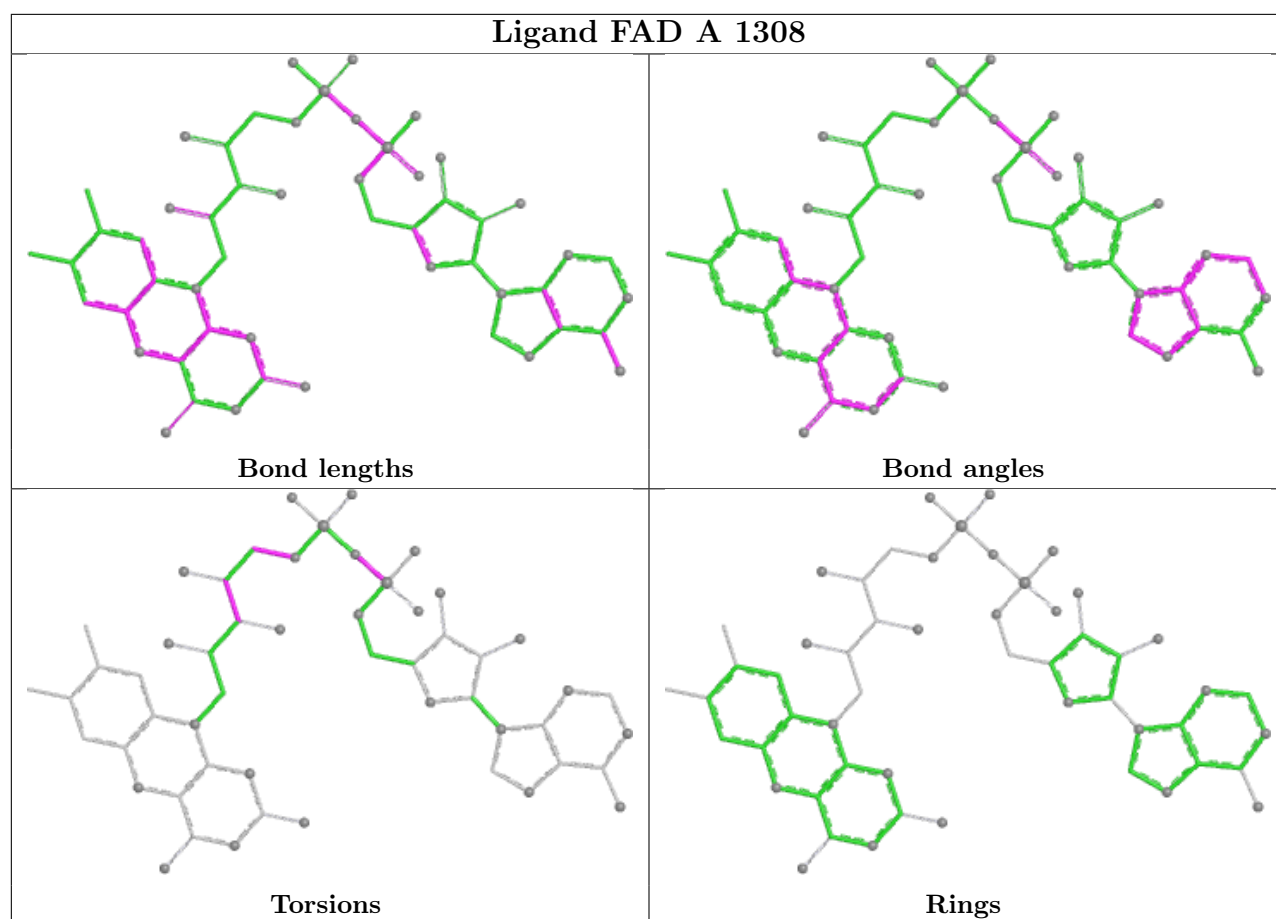


Ligand GGL B 1301



Ligand GGL A 1301





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	1219/1235 (98%)	0.06	29 (2%) 59 63	7, 20, 36, 66	23 (1%)
1	B	1218/1235 (98%)	0.14	43 (3%) 47 51	7, 20, 38, 63	15 (1%)
All	All	2437/2470 (98%)	0.10	72 (2%) 52 56	7, 20, 36, 66	38 (1%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	5.5
1	B	136	GLY	4.9
1	B	129	ASN	4.1
1	B	1233	GLY	4.0
1	A	80	SER	3.8
1	B	223	LEU	3.8
1	A	134	LEU	3.7
1	A	127	ASP	3.7
1	A	136	GLY	3.7
1	B	1232	ILE	3.5
1	B	491	LEU	3.4
1	B	1231	ALA	3.4
1	B	134	LEU	3.3
1	B	1230	MET	3.3
1	A	79	HIS	3.2
1	B	137	SER	3.2
1	A	132	SER	3.2
1	B	493	ASN	3.2
1	A	128	GLY	3.1
1	B	133	HIS	3.0
1	B	16	ALA	3.0
1	A	506	PRO	3.0
1	B	905	LEU	3.0
1	A	130	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	135	GLY	2.8
1	A	1231	ALA	2.8
1	B	904	GLY	2.8
1	A	129	ASN	2.8
1	B	1229	LEU	2.8
1	A	115	ALA	2.7
1	B	130	TRP	2.7
1	B	492	GLU	2.7
1	B	485	TYR	2.6
1	B	132	SER	2.6
1	B	494	GLY	2.6
1	B	912	ILE	2.6
1	A	1230	MET	2.6
1	B	15	PRO	2.5
1	B	224	GLY	2.4
1	A	125	ILE	2.4
1	A	1232	ILE	2.4
1	B	500	VAL	2.4
1	B	495	ALA	2.4
1	B	901	ARG	2.4
1	A	801	ALA	2.3
1	B	439	PHE	2.3
1	A	15	PRO	2.3
1	A	764	ARG	2.3
1	B	79	HIS	2.3
1	A	771	ALA	2.3
1	B	506	PRO	2.3
1	B	81	GLY	2.3
1	B	1222	ALA	2.2
1	B	1227	ALA	2.2
1	A	16	ALA	2.2
1	A	965	ALA	2.2
1	A	494	GLY	2.2
1	B	451	GLY	2.2
1	A	116	THR	2.1
1	B	156	THR	2.1
1	B	80	SER	2.1
1	A	120	LEU	2.1
1	B	127	ASP	2.1
1	B	1063	ARG	2.1
1	A	81	GLY	2.1
1	B	113	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	520	VAL	2.0
1	A	618	ARG	2.0
1	A	133	HIS	2.0
1	B	115	ALA	2.0
1	B	520	VAL	2.0
1	B	1058	ASP	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](#)

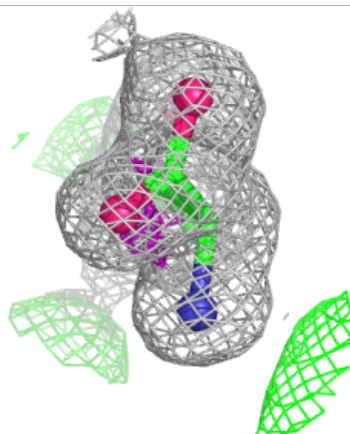
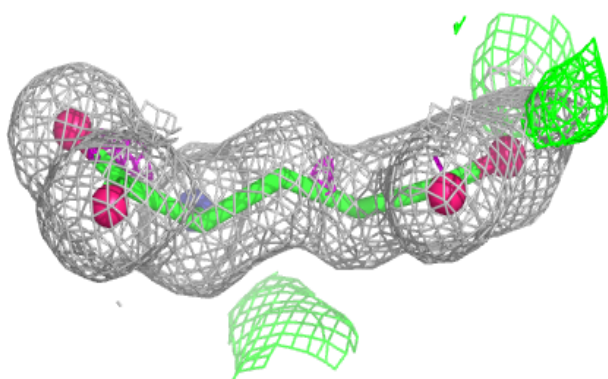
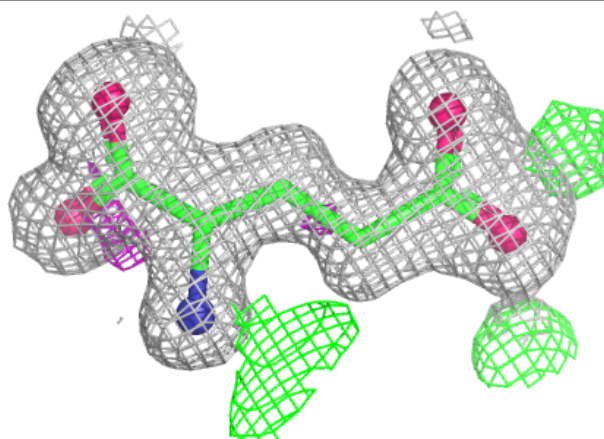
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	1306	5/5	0.81	0.13	43,47,48,50	5
6	PEG	B	1306	7/7	0.86	0.13	30,32,36,38	0
4	PGE	A	1307	10/10	0.89	0.12	22,29,40,41	0
3	SO4	B	1305	5/5	0.89	0.11	32,33,36,43	5
3	SO4	B	1304	5/5	0.90	0.13	20,25,35,37	5
3	SO4	A	1305	5/5	0.90	0.14	28,29,35,39	5
3	SO4	B	1303	5/5	0.91	0.12	26,28,30,31	5
4	PGE	B	1307	10/10	0.92	0.10	23,30,38,39	0
3	SO4	A	1304	5/5	0.93	0.11	20,25,28,32	5
2	GGL	A	1301	10/10	0.95	0.07	15,18,22,26	0
5	FAD	B	1308	53/53	0.96	0.07	13,16,27,32	0
2	GGL	B	1301	10/10	0.97	0.06	13,16,18,19	0
5	FAD	A	1308	53/53	0.97	0.07	11,15,21,32	0
3	SO4	A	1303	5/5	0.98	0.06	17,20,25,29	5
3	SO4	A	1302	5/5	0.99	0.04	14,15,18,18	0
3	SO4	B	1302	5/5	0.99	0.04	12,12,17,17	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.

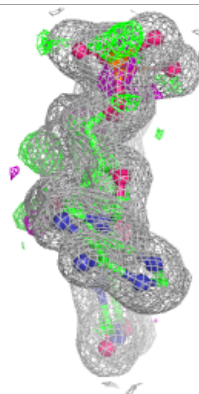
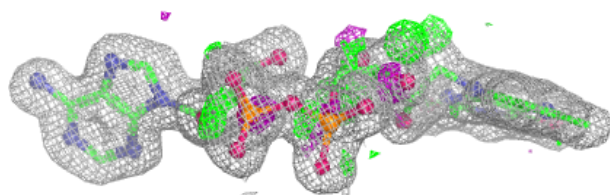
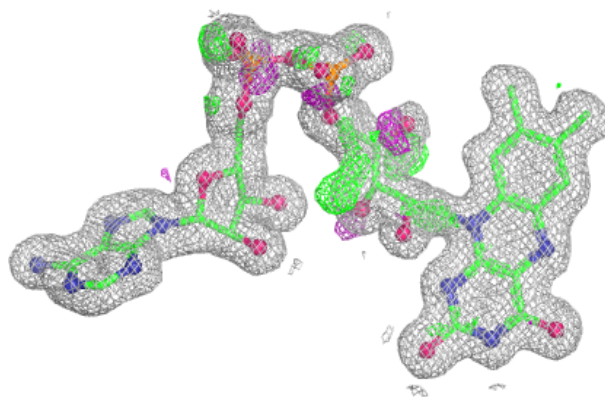
Electron density around GGL A 1301:

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



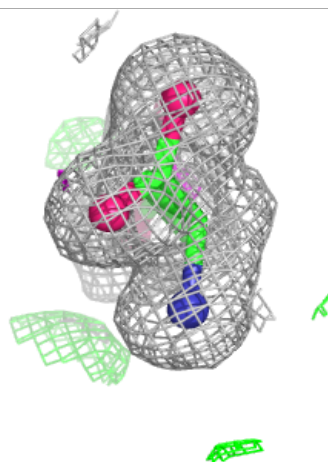
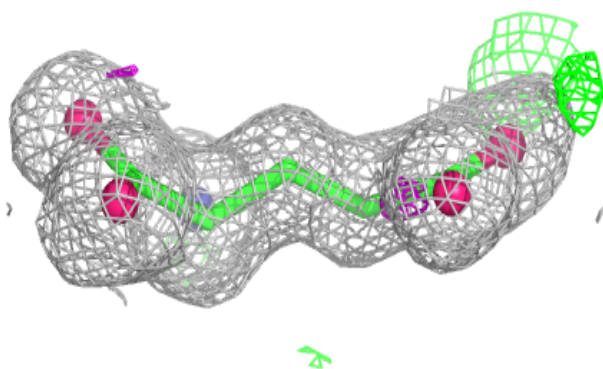
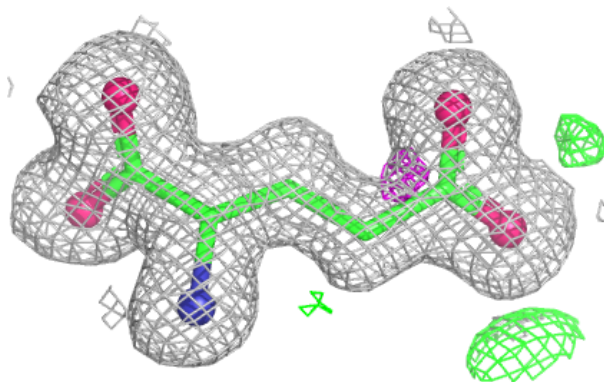
Electron density around FAD B 1308:

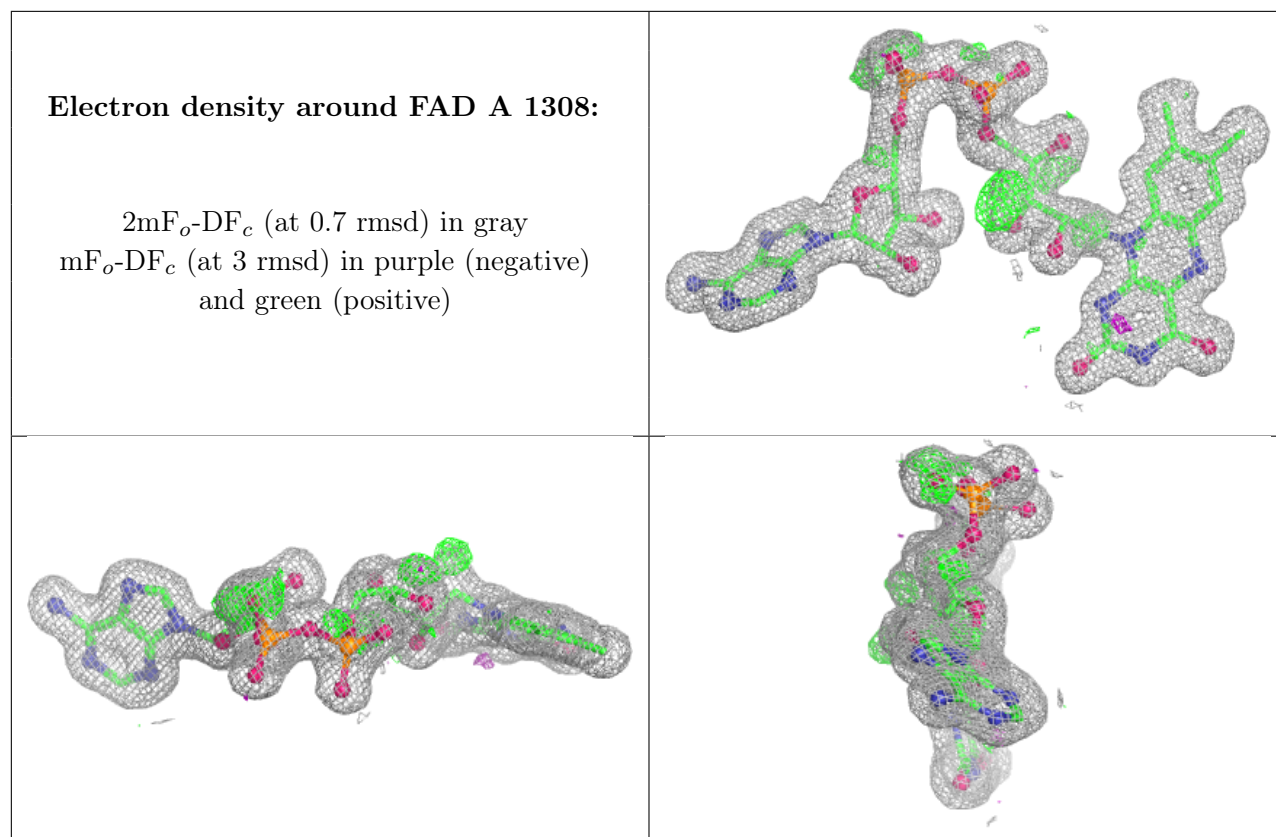
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GGL B 1301:

$2mF_o-DF_c$ (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.