Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 01:54 PM EST

PDB ID	:	4NMC
Title	:	Crystal structure of oxidized proline utilization A (PutA) from Geobacter sulfurreducens PCA complexed with Zwittergent 3-12
Authors	:	Singh, H.; Tanner, J.J.
Deposited on	:	2013-11-14
Resolution	:	1.90 Å(reported)

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

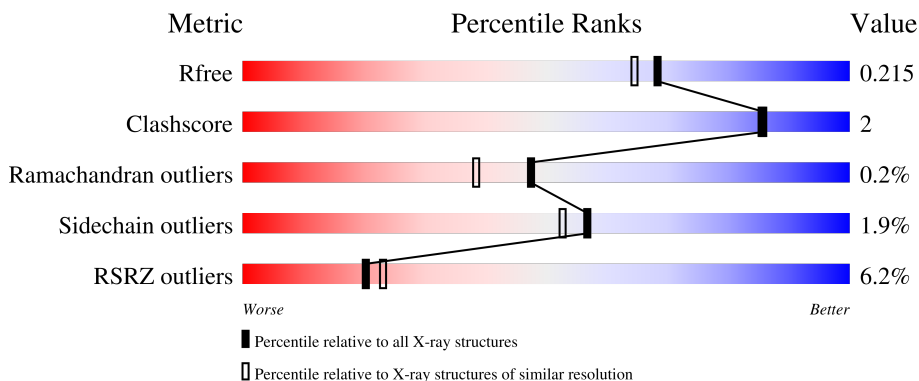|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	Percentile Ranks	Value
Rfree		0.215
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		1.9%
RSRZ outliers		6.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	1005	8% / 86% / 7% / 6%
1	B	1005	3% / 91% / 5% / •

2   Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15901 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 Proline dehydrogenase and Delta-1-pyrroline-5-carboxylate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	941	Total	C	N	O	S	0	1	0
			7149	4552	1230	1332	35			
1	B	969	Total	C	N	O	S	0	1	0
			7473	4764	1289	1384	36			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q746X3
B	0	SER	-	expression tag	UNP Q746X3

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

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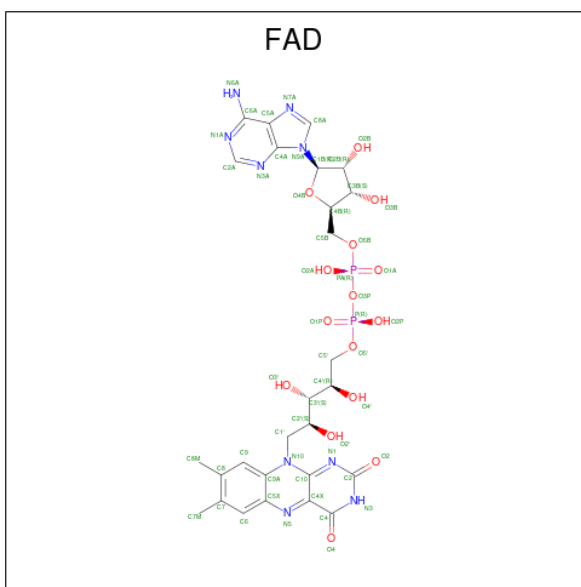
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
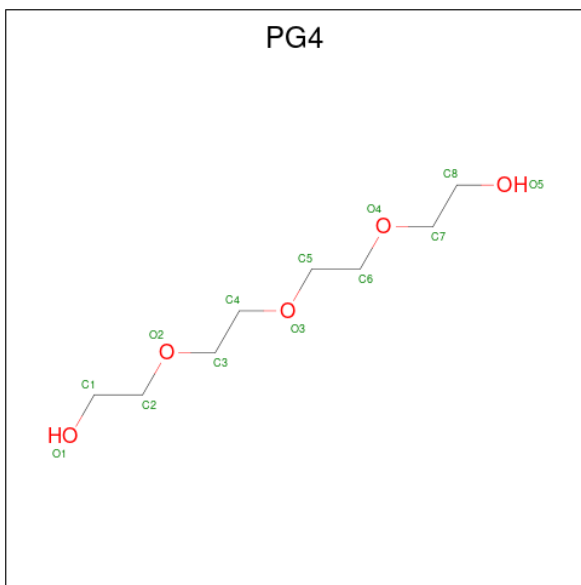
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 8	O 5	0	0
3	B	1	Total 10	C 6	O 4	0	0
3	B	1	Total 11	C 7	O 4	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0

- Molecule 5 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (three-letter code: C15) (formula: $C_{17}H_{38}NO_3S$).
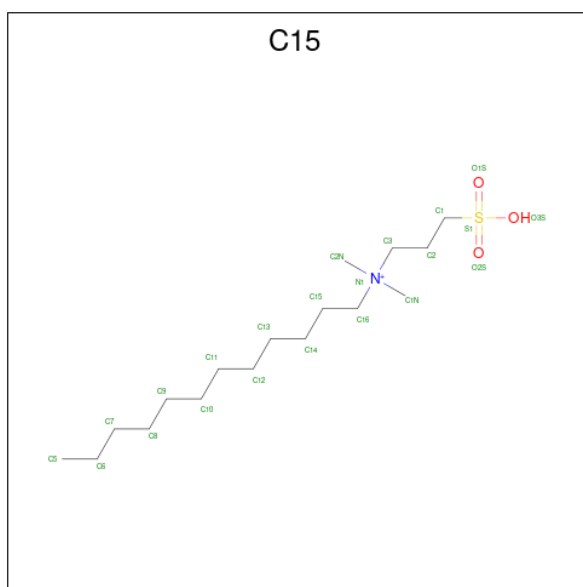
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 9	C 9	0	0

- Molecule 6 is (2S)-2-HYDROXYPROPANOIC ACID (three-letter code: 2OP) (formula: $C_3H_6O_3$).
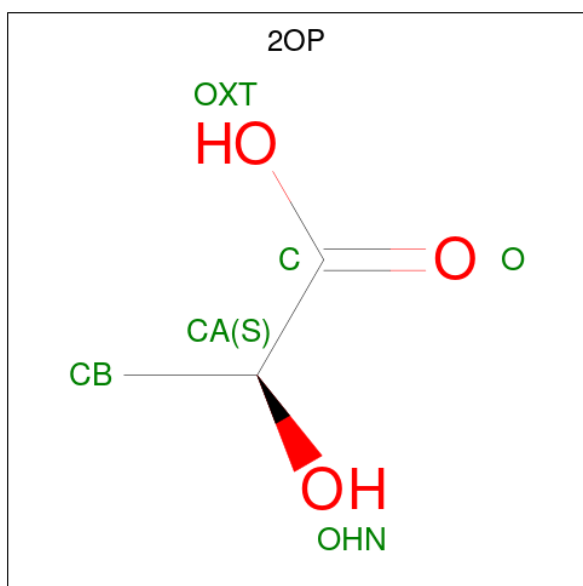
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 6	C 3	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	492	Total O 492 492	0	0
7	B	630	Total O 630 630	0	0

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: Proline dehydrogenase and Delta-1-pyrroline-5-carboxylate dehydrogenase
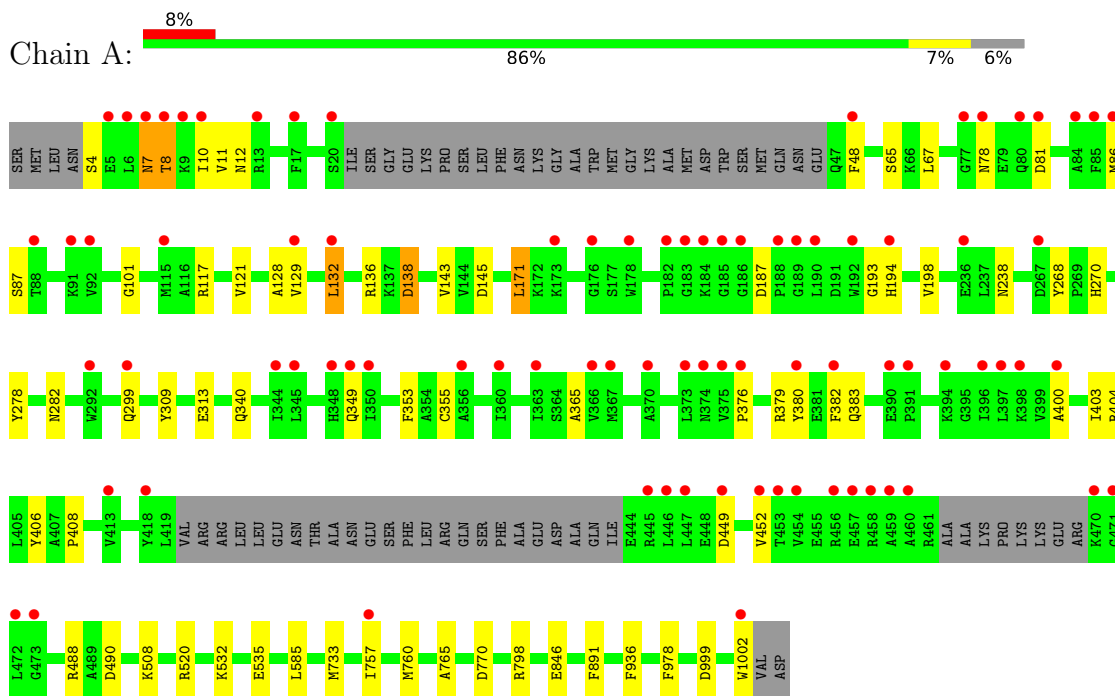
Chain A:

• Molecule 1: Proline dehydrogenase and Delta-1-pyrroline-5-carboxylate dehydrogenase

Chain B:
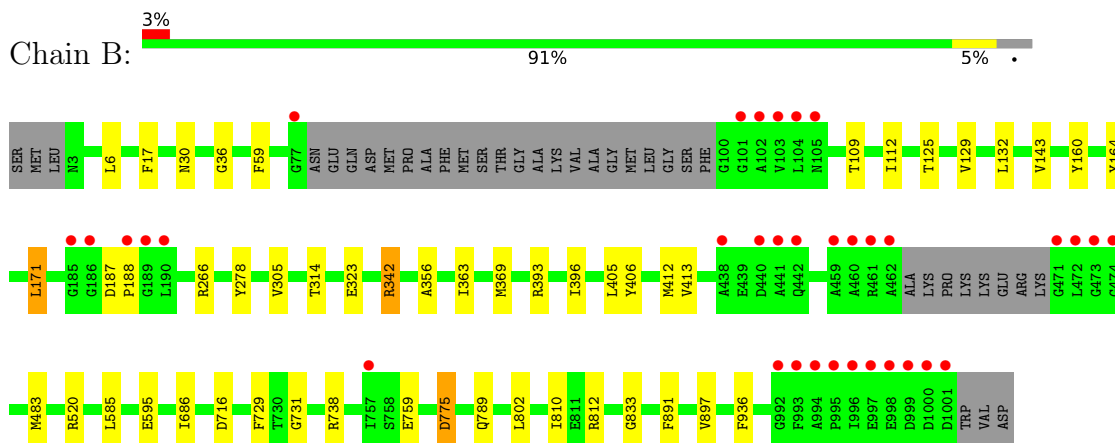
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.08Å 157.21Å 190.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 1.90 47.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.04-1.90) 99.2 (47.04-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.180 , 0.213 0.182 , 0.215	Depositor DCC
R_{free} test set	11085 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å²)	25.0	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 50.7	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15901	wwPDB-VP
Average B, all atoms (Å²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: K, PG4, C15, FAD, 2OP

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	0.33	0/7312	0.50	0/9936
1	B	0.35	0/7642	0.51	0/10363
All	All	0.34	0/14954	0.50	0/20299

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 (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	7149	0	6839	40	0
1	B	7473	0	7270	25	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
3	A	13	0	18	0	0
3	B	21	0	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	9	0	14	0	0
6	B	6	0	5	0	0
7	A	492	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	630	0	0	2	0
All	All	15901	0	14234	65	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 (65) 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:8:THR:O	1:A:12:ASN:ND2	2.31	0.62
1:B:810:ILE:HD11	1:B:897:VAL:HG11	1.81	0.61
1:A:406:TYR:HB2	2:A:2001:FAD:HM72	1.84	0.60
1:B:393:ARG:HD2	1:B:405:LEU:HD21	1.82	0.59
1:A:383:GLN:HG2	1:A:404:ARG:HB3	1.84	0.59
1:A:187:ASP:O	1:A:193:GLY:HA2	2.03	0.58
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.37	0.58
1:A:299:GLN:NE2	1:A:349:GLN:O	2.36	0.58
1:A:508:LYS:NZ	7:A:2588:HOH:O	2.38	0.56
1:B:143:VAL:HG13	1:B:406:TYR:HA	1.89	0.54
1:B:716:ASP:OD1	1:B:738:ARG:NH1	2.30	0.53
1:B:363:ILE:HD13	1:B:396:ILE:HD11	1.91	0.53
1:A:171:LEU:HD23	1:A:198:VAL:HG13	1.91	0.53
1:B:775:ASP:CG	1:B:812:ARG:HH12	2.13	0.52
1:A:10:ILE:HG12	1:A:365:ALA:HA	1.91	0.51
1:B:406:TYR:HB2	2:B:2001:FAD:HM72	1.93	0.50
1:A:1002:TRP:HH2	1:B:314:THR:HG1	1.59	0.49
1:A:65:SER:HB3	1:A:101:GLY:HA3	1.94	0.49
1:A:355:CYS:HB3	1:A:382:PHE:HD1	1.77	0.49
1:B:595:GLU:OE1	1:B:686:ILE:HG12	2.14	0.48
1:A:48:PHE:HE1	1:A:86:MET:HG3	1.80	0.47
1:B:160:TYR:CZ	1:B:164:TYR:HE2	2.33	0.47
1:A:355:CYS:HB3	1:A:382:PHE:CD1	2.50	0.47
1:A:48:PHE:CE1	1:A:86:MET:HG3	2.50	0.47
1:B:342:ARG:HB2	1:B:369:MET:SD	2.55	0.46
1:B:112:ILE:HG22	1:B:412:MET:HE3	1.97	0.46
1:A:143:VAL:HG13	1:A:406:TYR:HA	1.96	0.46
1:A:145:ASP:OD2	1:A:406:TYR:OH	2.22	0.46
1:A:282:ASN:ND2	1:A:340:GLN:OE1	2.46	0.45
1:A:488:ARG:HB3	1:A:490:ASP:OD1	2.17	0.45
1:A:7:ASN:O	1:A:11:VAL:HG23	2.16	0.45
1:A:7:ASN:OD1	1:A:449:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LYS:HD2	1:A:535:GLU:HB2	1.98	0.45
1:B:125:THR:O	1:B:129:VAL:HG23	2.16	0.45
1:A:382:PHE:CD2	1:A:400:ALA:HB1	2.52	0.45
1:A:733:MET:HA	1:A:760:MET:HB3	1.98	0.45
1:B:59:PHE:CZ	1:B:109:THR:HA	2.51	0.45
1:B:759:GLU:HG3	7:B:2213:HOH:O	2.17	0.44
1:B:6:LEU:HD21	1:B:369:MET:HG2	2.00	0.44
1:A:765:ALA:HA	1:A:798:ARG:O	2.18	0.43
1:A:400:ALA:HB3	1:A:403:ILE:HD11	2.01	0.43
1:A:309:TYR:O	1:A:313:GLU:HG2	2.19	0.42
1:A:449:ASP:HB3	1:A:452:VAL:HG23	2.00	0.42
1:A:757:ILE:HD13	1:A:978:PHE:CZ	2.54	0.42
1:B:789:GLN:HG2	1:B:833:GLY:O	2.20	0.42
2:B:2001:FAD:H4'	2:B:2001:FAD:H1'1	1.84	0.42
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.90	0.42
1:B:305:VAL:HG12	1:B:356:ALA:HB3	2.02	0.42
1:B:729:PHE:CZ	1:B:731:GLY:HA3	2.54	0.42
1:A:376:PRO:HG2	1:A:379:ARG:HG2	2.01	0.42
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.87	0.41
1:A:4:SER:O	1:A:8:THR:OG1	2.35	0.41
1:A:136:ARG:C	1:A:138:ASP:H	2.24	0.41
1:A:353:PHE:O	1:A:380:TYR:HA	2.21	0.41
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.92	0.41
1:A:67:LEU:HD21	1:A:770:ASP:OD1	2.21	0.41
1:A:238:ASN:ND2	7:A:2478:HOH:O	2.52	0.41
1:B:59:PHE:HZ	1:B:109:THR:HA	1.86	0.41
1:B:810:ILE:HD13	1:B:810:ILE:HA	1.85	0.41
1:A:846:GLU:HG2	7:A:2444:HOH:O	2.21	0.40
1:B:187:ASP:HA	1:B:188:PRO:HD2	1.98	0.40
1:B:483:MET:SD	7:B:2538:HOH:O	2.62	0.40
1:A:121:VAL:HG22	1:A:408:PRO:O	2.20	0.40
1:B:30:ASN:O	1:B:36:GLY:HA3	2.20	0.40
1:A:268:TYR:CE2	1:A:270:HIS:HB2	2.57	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	934/1005 (93%)	905 (97%)	26 (3%)	3 (0%)	41	31
1	B	964/1005 (96%)	945 (98%)	19 (2%)	0	100	100
All	All	1898/2010 (94%)	1850 (98%)	45 (2%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	HIS
1	A	128	ALA
1	A	129	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	705/821 (86%)	692 (98%)	13 (2%)	59	55
1	B	752/821 (92%)	738 (98%)	14 (2%)	57	53
All	All	1457/1642 (89%)	1430 (98%)	27 (2%)	57	53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	THR
1	A	87	SER

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Mol	Chain	Res	Type
1	A	117	ARG
1	A	132	LEU
1	A	138	ASP
1	A	171	LEU
1	A	278	TYR
1	A	520	ARG
1	A	585	LEU
1	A	891	PHE
1	A	936	PHE
1	A	999	ASP
1	B	17	PHE
1	B	132	LEU
1	B	171	LEU
1	B	266	ARG
1	B	278	TYR
1	B	323	GLU
1	B	342	ARG
1	B	413	VAL
1	B	520	ARG
1	B	585	LEU
1	B	775	ASP
1	B	802	LEU
1	B	891	PHE
1	B	936	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	PG4	B	2002	-	9,9,12	0.59	0	8,8,11	0.77	0
5	C15	B	2005	-	8,8,21	0.33	0	7,7,26	0.62	0
6	2OP	B	2006	-	5,5,5	0.82	0	4,6,6	0.92	0
3	PG4	B	2003	-	10,10,12	0.61	0	9,9,11	0.87	0
2	FAD	B	2001	-	53,58,58	1.99	15 (28%)	68,89,89	1.48	12 (17%)
2	FAD	A	2001	-	53,58,58	2.17	18 (33%)	68,89,89	1.49	13 (19%)
3	PG4	A	2002	-	12,12,12	0.64	0	11,11,11	0.84	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
3	PG4	B	2002	-	-	1/7/7/10	-
5	C15	B	2005	-	-	4/6/6/21	-
6	2OP	B	2006	-	-	0/4/4/4	-
3	PG4	B	2003	-	-	4/8/8/10	-
2	FAD	B	2001	-	-	6/30/50/50	0/6/6/6
2	FAD	A	2001	-	-	15/30/50/50	0/6/6/6
3	PG4	A	2002	-	-	5/10/10/10	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	O4-C4	7.51	1.37	1.23
2	B	2001	FAD	O4-C4	6.96	1.36	1.23
2	A	2001	FAD	O2-C2	6.61	1.36	1.24
2	B	2001	FAD	O2-C2	5.94	1.35	1.24
2	A	2001	FAD	C4X-N5	4.73	1.39	1.30
2	B	2001	FAD	C4X-N5	4.59	1.39	1.30
2	A	2001	FAD	C2-N1	3.43	1.44	1.36
2	B	2001	FAD	C2B-C1B	-3.22	1.48	1.53
2	A	2001	FAD	C2B-C1B	-3.21	1.48	1.53
2	A	2001	FAD	C10-N1	3.12	1.39	1.33
2	B	2001	FAD	C6A-N6A	2.97	1.44	1.34
2	A	2001	FAD	C6A-N6A	2.94	1.44	1.34
2	A	2001	FAD	O2'-C2'	-2.91	1.37	1.43
2	A	2001	FAD	PA-O5B	-2.77	1.48	1.59
2	B	2001	FAD	C2A-N3A	2.62	1.36	1.32
2	A	2001	FAD	O4'-C4'	-2.60	1.37	1.43
2	B	2001	FAD	C2-N1	2.50	1.42	1.36
2	B	2001	FAD	PA-O5B	-2.49	1.49	1.59
2	A	2001	FAD	C2A-N3A	2.44	1.36	1.32
2	B	2001	FAD	C10-N1	2.43	1.38	1.33
2	B	2001	FAD	O4B-C4B	-2.42	1.39	1.45
2	B	2001	FAD	O2'-C2'	-2.37	1.38	1.43
2	A	2001	FAD	PA-O2A	-2.28	1.44	1.55
2	B	2001	FAD	PA-O2A	-2.24	1.44	1.55
2	B	2001	FAD	O2B-C2B	-2.23	1.37	1.43
2	A	2001	FAD	O4B-C4B	-2.21	1.40	1.45
2	A	2001	FAD	O3'-C3'	-2.19	1.37	1.43
2	A	2001	FAD	O2B-C2B	-2.15	1.37	1.43
2	B	2001	FAD	O4'-C4'	-2.14	1.38	1.43
2	A	2001	FAD	O3B-C3B	-2.12	1.38	1.43
2	B	2001	FAD	P-O1P	2.09	1.58	1.50
2	A	2001	FAD	P-O1P	2.05	1.58	1.50
2	A	2001	FAD	C10-N10	2.03	1.41	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	FAD	N3A-C2A-N1A	-5.65	119.85	128.68
2	B	2001	FAD	N3A-C2A-N1A	-5.65	119.85	128.68
2	B	2001	FAD	C4-C4X-N5	3.38	123.05	118.23
2	B	2001	FAD	C4-N3-C2	-3.31	119.53	125.64
2	A	2001	FAD	O2P-P-O5'	-3.11	93.28	107.75
2	B	2001	FAD	C4X-C4-N3	3.10	121.06	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	FAD	O5'-P-O1P	3.06	121.04	109.07
2	A	2001	FAD	C4-C4X-N5	2.89	122.34	118.23
2	A	2001	FAD	C4-N3-C2	-2.77	120.53	125.64
2	A	2001	FAD	C4X-C4-N3	2.76	120.20	113.19
2	B	2001	FAD	O2-C2-N1	-2.67	117.40	121.83
2	B	2001	FAD	O4-C4-C4X	-2.59	119.72	126.60
2	B	2001	FAD	O5'-P-O1P	2.53	118.96	109.07
2	A	2001	FAD	C4X-C10-N1	-2.45	119.05	124.73
2	A	2001	FAD	O5B-PA-O1A	2.44	118.60	109.07
2	A	2001	FAD	C5'-C4'-C3'	-2.40	107.58	112.20
2	A	2001	FAD	O2A-PA-O5B	-2.32	96.97	107.75
2	A	2001	FAD	O4-C4-C4X	-2.30	120.49	126.60
2	B	2001	FAD	O2P-P-O5'	-2.27	97.20	107.75
2	B	2001	FAD	C4X-C10-N10	2.23	119.74	116.48
2	B	2001	FAD	C4A-C5A-N7A	-2.23	107.08	109.40
2	A	2001	FAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	A	2001	FAD	C10-C4X-N5	-2.16	120.28	124.86
2	B	2001	FAD	C10-C4X-N5	-2.13	120.33	124.86
2	B	2001	FAD	C10-N1-C2	2.00	120.91	116.90

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	C5B-O5B-PA-O1A
2	A	2001	FAD	C2'-C3'-C4'-O4'
2	A	2001	FAD	O3'-C3'-C4'-O4'
2	A	2001	FAD	C5'-O5'-P-O1P
2	B	2001	FAD	P-O3P-PA-O5B
2	B	2001	FAD	N10-C1'-C2'-O2'
2	B	2001	FAD	N10-C1'-C2'-C3'
2	B	2001	FAD	C1'-C2'-C3'-C4'
2	A	2001	FAD	C3B-C4B-C5B-O5B
2	A	2001	FAD	O3'-C3'-C4'-C5'
2	A	2001	FAD	C2'-C3'-C4'-C5'
3	B	2003	PG4	O3-C5-C6-O4
3	A	2002	PG4	O3-C5-C6-O4
3	B	2003	PG4	O2-C3-C4-O3
5	B	2005	C15	C7-C8-C9-C10
3	A	2002	PG4	O2-C3-C4-O3
2	A	2001	FAD	O4B-C4B-C5B-O5B
5	B	2005	C15	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	B	2001	FAD	C3B-C4B-C5B-O5B
5	B	2005	C15	C6-C7-C8-C9
3	A	2002	PG4	O4-C7-C8-O5
3	A	2002	PG4	O1-C1-C2-O2
2	A	2001	FAD	P-O3P-PA-O5B
3	B	2003	PG4	C3-C4-O3-C5
3	A	2002	PG4	C1-C2-O2-C3
3	B	2003	PG4	C5-C6-O4-C7
2	B	2001	FAD	C5B-O5B-PA-O3P
2	A	2001	FAD	C5'-O5'-P-O2P
3	B	2002	PG4	O2-C3-C4-O3
5	B	2005	C15	C11-C10-C9-C8
2	A	2001	FAD	O2'-C2'-C3'-C4'
2	A	2001	FAD	C5B-O5B-PA-O3P
2	A	2001	FAD	C5'-O5'-P-O3P
2	A	2001	FAD	O2'-C2'-C3'-O3'
2	A	2001	FAD	C5B-O5B-PA-O2A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	FAD	2	0
2	A	2001	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 C15 B 2005

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 2001

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 2001

Bond lengths

Bond angles

Torsions

Rings
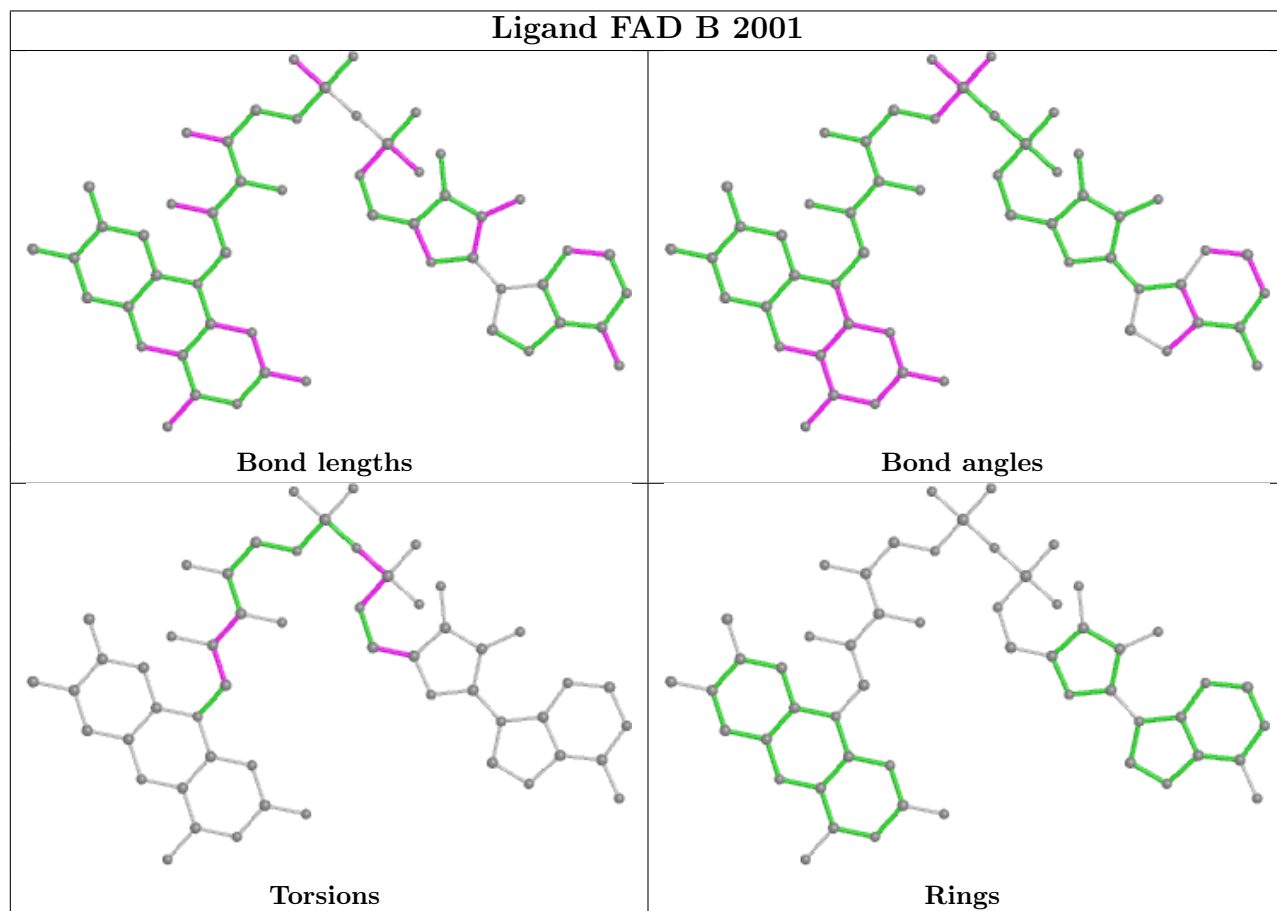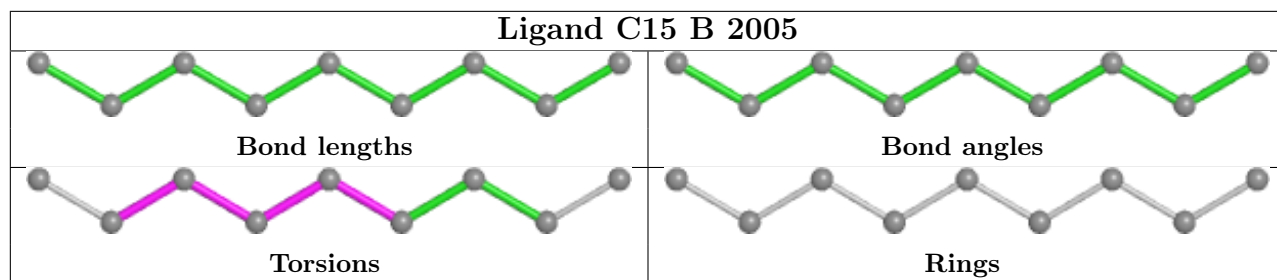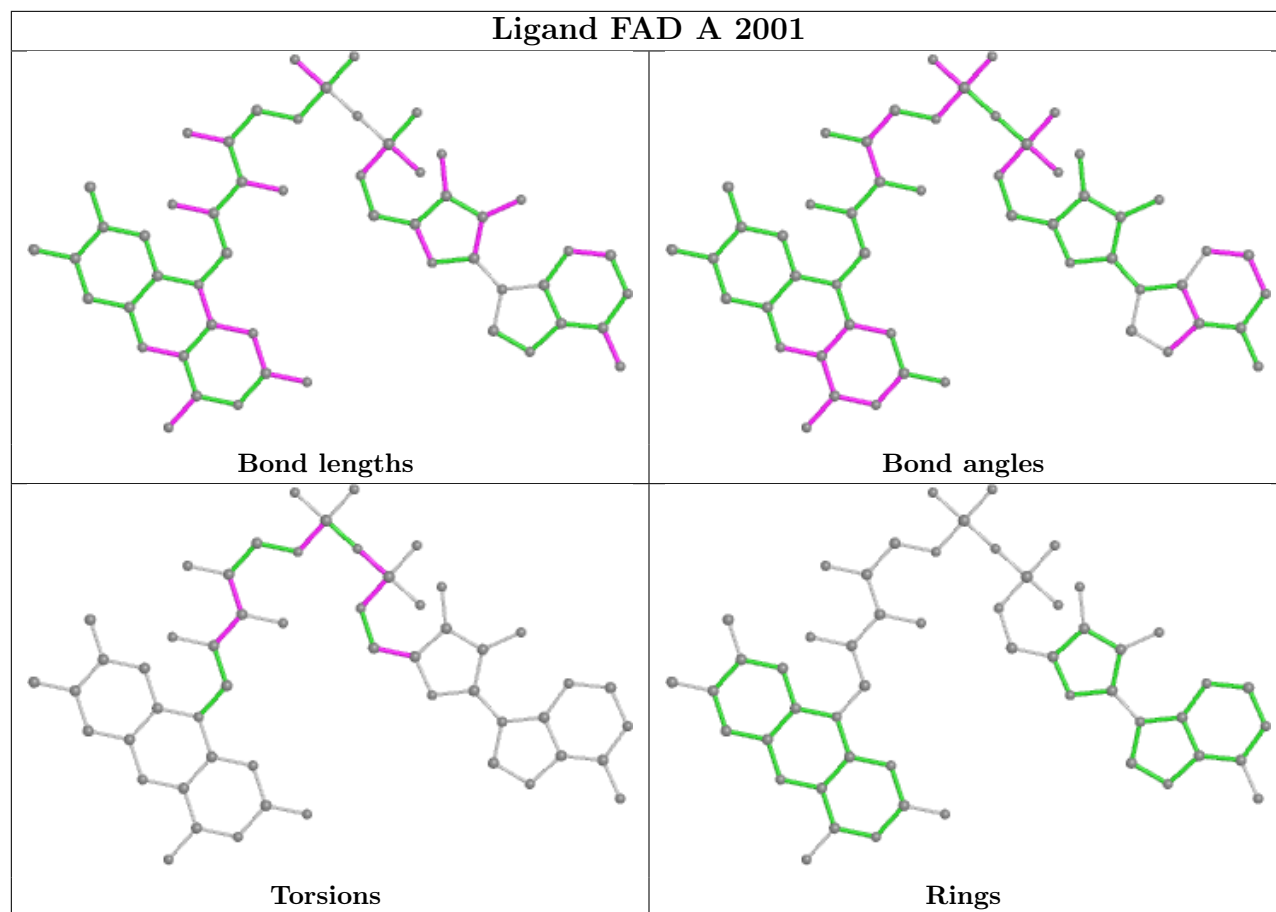
5.7 Other polymers ⓘ

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 ⓘ

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	941/1005 (93%)	0.29	84 (8%)	9	11	10, 27, 81, 104	0
1	B	969/1005 (96%)	-0.03	34 (3%)	44	47	11, 24, 48, 67	0
All	All	1910/2010 (95%)	0.13	118 (6%)	20	23	10, 25, 71, 104	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	ALA	8.0
1	B	994	ALA	6.9
1	A	350	ILE	6.5
1	B	996	ILE	6.3
1	A	459	ALA	5.8
1	A	472	LEU	5.8
1	A	471	GLY	5.7
1	A	185	GLY	5.2
1	A	10	ILE	5.2
1	A	188	PRO	5.2
1	B	995	PRO	5.0
1	A	460	ALA	5.0
1	A	375	VAL	5.0
1	B	473	GLY	4.9
1	A	6	LEU	4.7
1	A	473	GLY	4.7
1	A	183	GLY	4.6
1	A	363	ILE	4.5
1	A	454	VAL	4.3
1	A	447	LEU	4.2
1	A	452	VAL	4.1
1	B	997	GLU	4.0
1	A	366	VAL	4.0
1	A	370	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	472	LEU	3.9
1	A	186	GLY	3.9
1	A	189	GLY	3.8
1	A	360	ILE	3.8
1	B	471	GLY	3.7
1	A	190	LEU	3.7
1	B	186	GLY	3.7
1	A	7	ASN	3.7
1	B	992	GLY	3.7
1	A	453	THR	3.7
1	A	394	LYS	3.7
1	A	458	ARG	3.7
1	A	367	MET	3.6
1	A	80	GLN	3.5
1	B	103	VAL	3.5
1	A	194	HIS	3.5
1	B	104	LEU	3.4
1	B	999	ASP	3.4
1	B	101	GLY	3.3
1	A	20	SER	3.3
1	A	376	PRO	3.3
1	A	178	TRP	3.2
1	B	459	ALA	3.2
1	B	189	GLY	3.2
1	A	81	ASP	3.2
1	A	1002	TRP	3.2
1	B	462	ALA	3.2
1	B	998	GLU	3.2
1	B	441	ALA	3.2
1	B	440	ASP	3.1
1	A	374	ASN	3.1
1	A	397	LEU	3.0
1	A	344	ILE	3.0
1	B	188	PRO	3.0
1	B	1001	ASP	3.0
1	A	396	ILE	2.9
1	A	184	LYS	2.9
1	A	456	ARG	2.9
1	A	380	TYR	2.9
1	A	470	LYS	2.9
1	A	9	LYS	2.9
1	A	398	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	192	TRP	2.8
1	A	8	THR	2.8
1	A	48	PHE	2.8
1	A	92	VAL	2.8
1	A	457	GLU	2.8
1	A	88	THR	2.7
1	A	85	PHE	2.7
1	B	461	ARG	2.7
1	A	86	MET	2.7
1	A	176	GLY	2.7
1	A	345	LEU	2.6
1	A	299	GLN	2.6
1	A	349	GLN	2.6
1	A	17	PHE	2.6
1	A	78	ASN	2.6
1	B	185	GLY	2.5
1	B	190	LEU	2.5
1	A	267	ASP	2.5
1	B	1000	ASP	2.5
1	B	993	PHE	2.4
1	A	390	GLU	2.4
1	A	115	MET	2.3
1	A	356	ALA	2.3
1	A	182	PRO	2.3
1	A	382	PHE	2.3
1	A	413	VAL	2.3
1	B	77	GLY	2.3
1	A	129	VAL	2.3
1	A	292	TRP	2.3
1	A	391	PRO	2.3
1	B	757	ILE	2.2
1	A	449	ASP	2.2
1	B	442	GLN	2.2
1	A	5	GLU	2.2
1	A	373	LEU	2.2
1	B	105	ASN	2.2
1	A	77	GLY	2.2
1	A	132	LEU	2.2
1	A	400	ALA	2.2
1	A	173	LYS	2.2
1	A	418	TYR	2.2
1	A	446	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	91	LYS	2.1
1	B	102	ALA	2.1
1	B	438	ALA	2.1
1	A	84	ALA	2.1
1	A	236	GLU	2.1
1	A	757	ILE	2.1
1	A	348	HIS	2.0
1	A	13	ARG	2.0
1	A	445	ARG	2.0
1	B	474	GLY	2.0

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

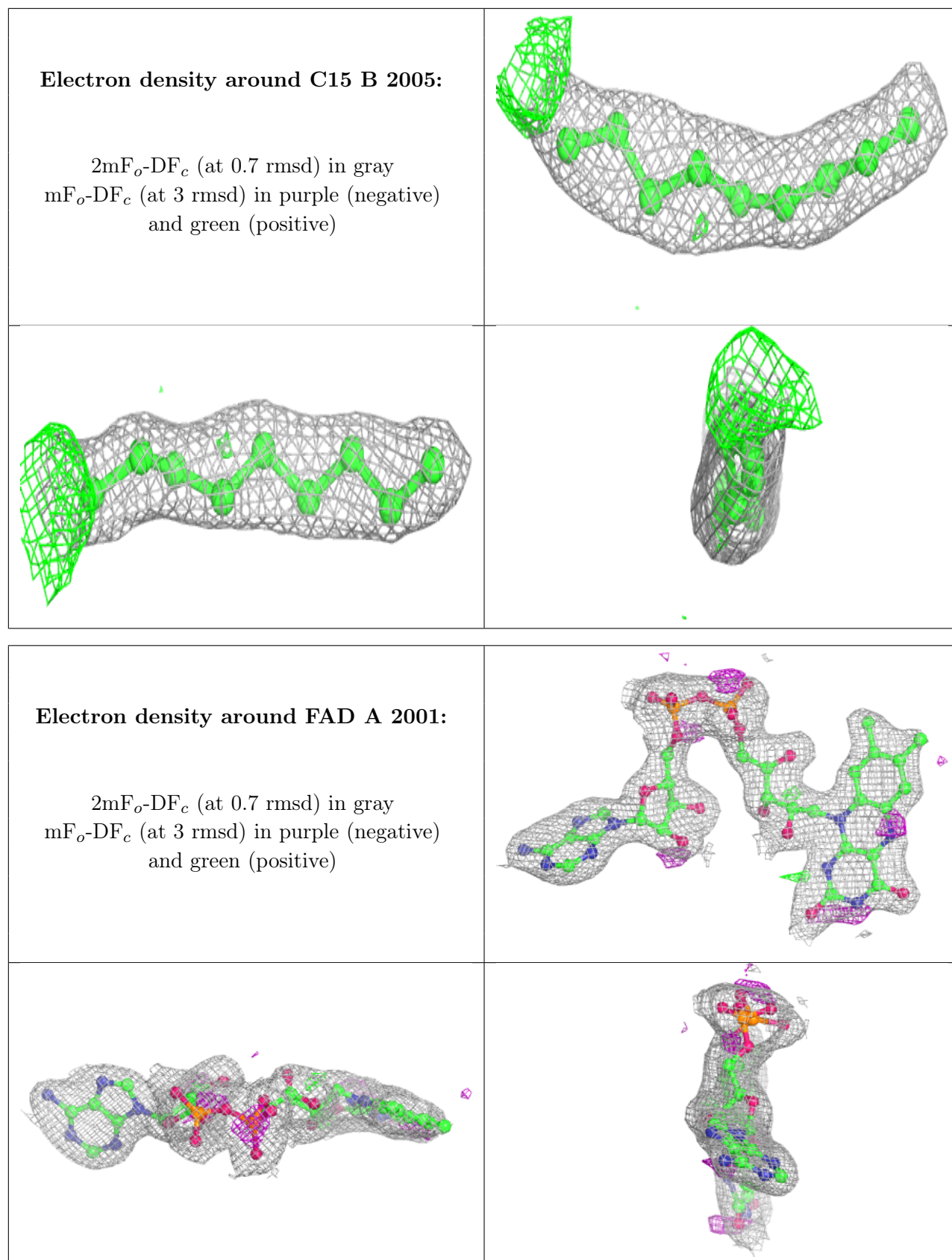There are no non-standard protein/DNA/RNA residues in this entry.

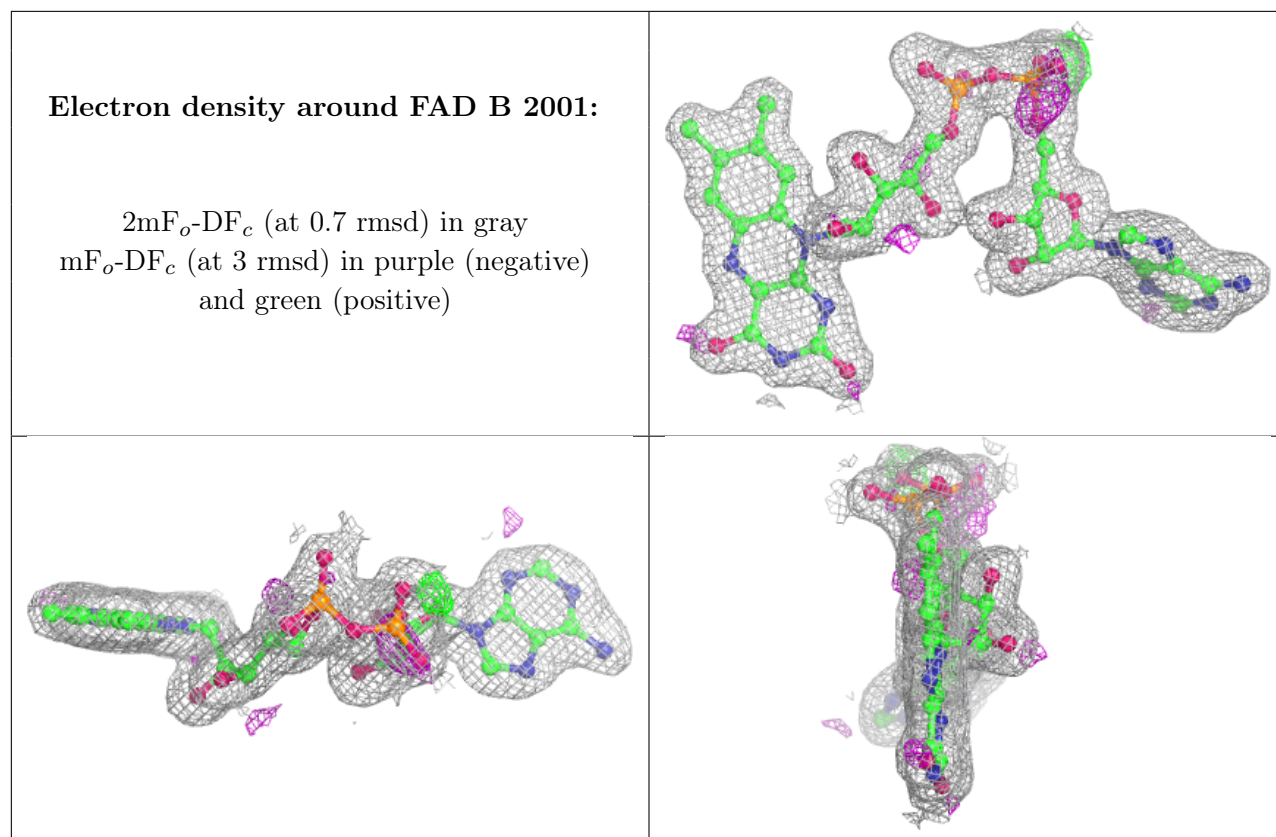## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
3	PG4	B	2003	11/13	0.81	0.17	47,50,61,63	0
3	PG4	A	2002	13/13	0.88	0.14	47,50,55,57	0
3	PG4	B	2002	10/13	0.91	0.18	28,32,36,36	0
5	C15	B	2005	9/22	0.91	0.14	38,43,49,49	0
2	FAD	A	2001	53/53	0.93	0.12	31,36,50,55	0
6	2OP	B	2006	6/6	0.96	0.13	22,28,37,41	0
2	FAD	B	2001	53/53	0.97	0.10	11,17,22,23	0
4	K	A	2003	1/1	0.99	0.06	18,18,18,18	0
4	K	B	2004	1/1	0.99	0.09	17,17,17,17	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 C15 B 2005:

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

Electron density around FAD A 2001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)

6.5 Other polymers ⓘ

There are no such residues in this entry.