



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:45 AM UTC

PDB ID : 3AB1 / pdb_00003ab1
Title : Crystal Structure of Ferredoxin NADP+ Oxidoreductase
Authors : Muraki, N.; Seo, D.; Kurisu, G.
Deposited on : 2009-11-30
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

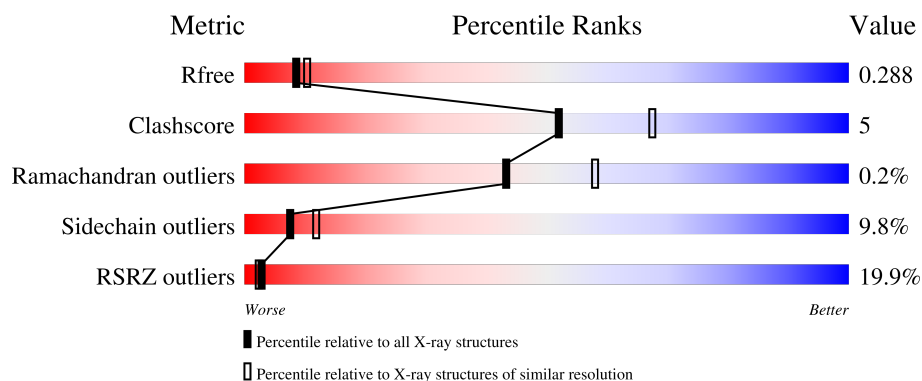
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	360	 16% 72% 15% • 12%
1	B	360	 20% 78% 13% • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5216 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 Ferredoxin–NADP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2438	1543	422	466	7			
1	B	336	Total	C	N	O	S	0	0	0
			2575	1629	447	491	8			

- 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
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		

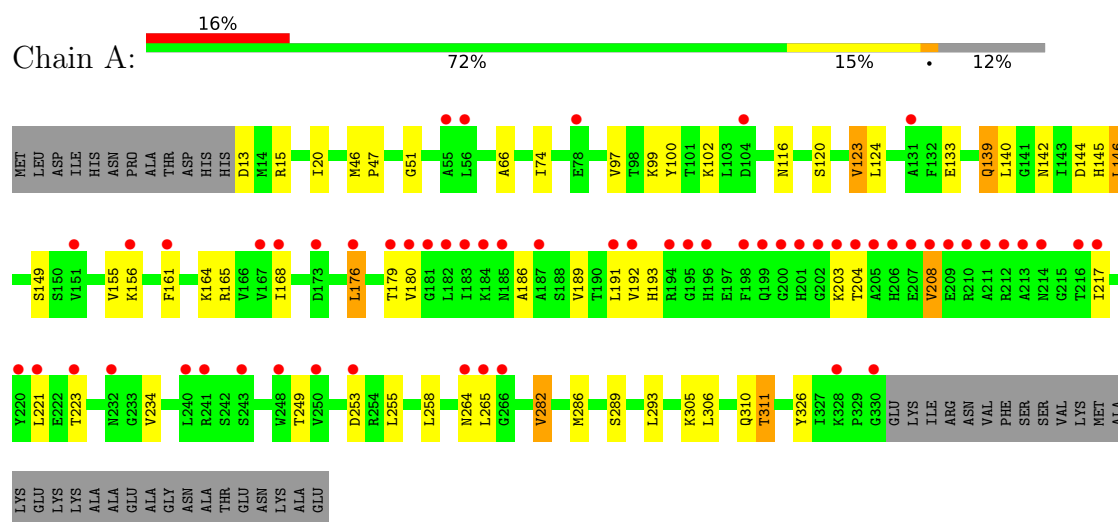
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total 48	O 48	0	0
3	B	49	Total 49	O 49	0	0

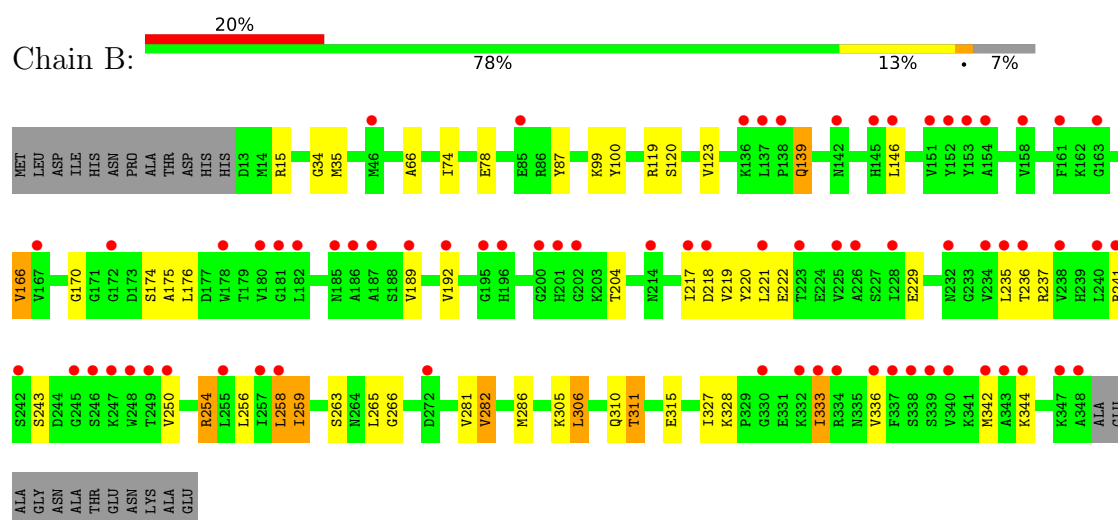
3 Residue-property plots [i](#)

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: Ferredoxin–NADP reductase



• Molecule 1: Ferredoxin–NADP reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.51Å 127.97Å 128.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 2.39 39.57 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.57-2.39) 99.6 (39.57-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.289 0.238 , 0.288	Depositor DCC
R_{free} test set	1668 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: 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	0.54	0/2486	0.79	0/3374
1	B	0.54	0/2624	0.83	0/3557
All	All	0.54	0/5110	0.81	0/6931

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	2438	0	2426	29	0
1	B	2575	0	2567	23	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	48	0	0	0	0
3	B	49	0	0	0	0
All	All	5216	0	5055	52	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 5.

All (52) 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:66:ALA:H	1:B:310:GLN:HE22	1.21	0.87
1:B:139:GLN:HE21	1:B:139:GLN:H	1.27	0.78
1:A:139:GLN:HE21	1:A:139:GLN:H	1.30	0.77
1:A:123:VAL:HG22	1:A:293:LEU:HD12	1.68	0.73
1:A:306:LEU:O	1:A:311:THR:HG21	1.90	0.71
1:A:66:ALA:H	1:A:310:GLN:HE22	1.40	0.70
1:A:123:VAL:HG22	1:A:293:LEU:CD1	2.30	0.61
1:B:66:ALA:H	1:B:310:GLN:NE2	1.95	0.60
1:A:15:ARG:O	1:A:120:SER:HA	2.02	0.58
1:A:264:ASN:OD1	1:A:265:LEU:N	2.39	0.56
1:A:176:LEU:HG	1:A:208:VAL:HG11	1.88	0.56
1:B:222:GLU:HB3	1:B:243:SER:HB2	1.91	0.53
1:A:142:ASN:C	1:A:142:ASN:HD22	2.16	0.53
1:B:333:ILE:HD13	1:B:333:ILE:H	1.74	0.51
1:A:168:ILE:HD12	1:A:179:THR:HG22	1.92	0.50
1:B:306:LEU:O	1:B:311:THR:HG21	2.11	0.50
1:A:142:ASN:C	1:A:142:ASN:ND2	2.71	0.49
1:B:34:GLY:HA3	1:B:87:TYR:CD2	2.47	0.48
1:B:218:ASP:HB3	1:B:220:TYR:CE1	2.49	0.48
1:B:305:LYS:NZ	1:B:311:THR:HG22	2.29	0.47
1:B:175:ALA:HA	1:B:258:LEU:HD23	1.95	0.46
1:A:179:THR:HG21	1:A:191:LEU:HB2	1.98	0.46
1:A:155:VAL:HG13	1:A:161:PHE:CE2	2.51	0.45
1:A:102:LYS:HE3	1:A:326:TYR:OH	2.17	0.44
1:B:256:LEU:HG	1:B:258:LEU:HD22	1.98	0.44
1:A:99:LYS:HG2	1:A:100:TYR:H	1.83	0.44
1:B:229:GLU:HB2	1:B:237:ARG:HB2	2.00	0.44
1:B:282:VAL:HG13	1:B:286:MET:HA	2.00	0.44
1:A:176:LEU:O	1:A:179:THR:OG1	2.35	0.43
1:A:204:THR:O	1:A:208:VAL:HG13	2.18	0.43
1:B:99:LYS:HD2	1:B:100:TYR:H	1.83	0.43
1:A:99:LYS:HG2	1:A:100:TYR:N	2.34	0.43
1:A:142:ASN:ND2	1:A:144:ASP:H	2.16	0.43
1:B:229:GLU:C	1:B:236:THR:HG22	2.44	0.43
1:A:51:GLY:HA2	2:A:361:FAD:O3B	2.19	0.42
1:A:282:VAL:HG22	1:A:286:MET:C	2.44	0.42
1:B:189:VAL:HB	1:B:217:ILE:HG22	2.01	0.42
1:A:145:HIS:CD2	1:A:146:LEU:HD13	2.55	0.42
1:B:35:MET:HE1	1:B:342:MET:SD	2.59	0.42
1:A:165:ARG:O	1:A:253:ASP:N	2.44	0.42
1:B:15:ARG:O	1:B:120:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:THR:HG23	1:B:315:GLU:OE1	2.19	0.42
1:A:46:MET:HB3	1:A:47:PRO:CD	2.50	0.42
1:A:203:LYS:H	1:A:203:LYS:HG2	1.65	0.41
1:B:170:GLY:HA2	1:B:259:ILE:HG22	2.02	0.41
1:A:20:ILE:HG12	1:A:97:VAL:HG21	2.01	0.41
1:A:193:HIS:HB3	1:A:221:LEU:HD23	2.03	0.41
1:A:164:LYS:O	1:A:186:ALA:HB1	2.21	0.41
1:B:327:ILE:HG22	1:B:328:LYS:HG3	2.02	0.41
1:A:189:VAL:HB	1:A:217:ILE:HG22	2.03	0.41
1:B:218:ASP:HB3	1:B:220:TYR:HE1	1.86	0.40
1:B:166:VAL:HB	1:B:254:ARG:HB3	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	316/360 (88%)	306 (97%)	10 (3%)	0	100	100
1	B	334/360 (93%)	321 (96%)	12 (4%)	1 (0%)	36	50
All	All	650/720 (90%)	627 (96%)	22 (3%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	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	258/292 (88%)	234 (91%)	24 (9%)	8	14
1	B	272/292 (93%)	244 (90%)	28 (10%)	7	11
All	All	530/584 (91%)	478 (90%)	52 (10%)	7	12

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	74	ILE
1	A	116	ASN
1	A	123	VAL
1	A	124	LEU
1	A	133	GLU
1	A	139	GLN
1	A	140	LEU
1	A	146	LEU
1	A	149	SER
1	A	156	LYS
1	A	176	LEU
1	A	180	VAL
1	A	192	VAL
1	A	208	VAL
1	A	223	THR
1	A	234	VAL
1	A	249	THR
1	A	255	LEU
1	A	258	LEU
1	A	282	VAL
1	A	289	SER
1	A	305	LYS
1	A	311	THR
1	B	74	ILE
1	B	78	GLU
1	B	119	ARG
1	B	123	VAL
1	B	139	GLN
1	B	146	LEU
1	B	166	VAL
1	B	174	SER
1	B	176	LEU

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Mol	Chain	Res	Type
1	B	192	VAL
1	B	204	THR
1	B	219	VAL
1	B	221	LEU
1	B	235	LEU
1	B	241	ARG
1	B	250	VAL
1	B	254	ARG
1	B	258	LEU
1	B	259	ILE
1	B	263	SER
1	B	265	LEU
1	B	281	VAL
1	B	282	VAL
1	B	306	LEU
1	B	311	THR
1	B	333	ILE
1	B	336	VAL
1	B	344	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	116	ASN
1	A	139	GLN
1	A	142	ASN
1	A	193	HIS
1	A	199	GLN
1	A	239	HIS
1	A	310	GLN
1	B	32	GLN
1	B	37	ASN
1	B	116	ASN
1	B	139	GLN
1	B	142	ASN
1	B	193	HIS
1	B	199	GLN
1	B	201	HIS
1	B	264	ASN
1	B	310	GLN
1	B	335	ASN

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](#)

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
2	FAD	B	361	-	58,58,58	1.14	5 (8%)	85,89,89	1.59	17 (20%)
2	FAD	A	361	-	58,58,58	1.11	7 (12%)	85,89,89	1.64	15 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	361	-	-	0/34/50/50	0/6/6/6
2	FAD	A	361	-	-	1/34/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	361	FAD	C4X-N5	3.71	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	FAD	C4X-N5	3.54	1.38	1.30
2	B	361	FAD	C2A-N3A	3.12	1.39	1.33
2	B	361	FAD	C2A-N1A	3.00	1.39	1.33
2	B	361	FAD	C10-N1	2.76	1.38	1.33
2	A	361	FAD	C2A-N1A	2.66	1.38	1.33
2	A	361	FAD	P-O3P	2.54	1.62	1.59
2	A	361	FAD	C10-N1	2.50	1.38	1.33
2	B	361	FAD	C5A-N7A	-2.42	1.34	1.39
2	A	361	FAD	C2A-N3A	2.42	1.38	1.33
2	A	361	FAD	PA-O3P	2.21	1.61	1.59
2	A	361	FAD	C8A-N7A	2.20	1.35	1.31

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	FAD	N3A-C2A-N1A	-6.21	119.18	128.58
2	B	361	FAD	N3A-C2A-N1A	-5.94	119.60	128.58
2	A	361	FAD	C5A-C4A-N3A	-4.54	120.46	126.72
2	B	361	FAD	C5A-C4A-N3A	-4.45	120.59	126.72
2	A	361	FAD	N9A-C8A-N7A	-4.20	107.97	113.94
2	B	361	FAD	N9A-C8A-N7A	-4.08	108.14	113.94
2	A	361	FAD	C5A-N7A-C8A	3.97	109.69	103.45
2	A	361	FAD	C2A-N3A-C4A	3.71	120.88	111.83
2	B	361	FAD	C5A-N7A-C8A	3.56	109.05	103.45
2	B	361	FAD	C2A-N3A-C4A	3.40	120.13	111.83
2	B	361	FAD	N3A-C4A-N9A	3.29	132.77	127.17
2	B	361	FAD	C4-N3-C2	-3.27	119.83	125.64
2	A	361	FAD	C4-N3-C2	-3.18	119.99	125.64
2	A	361	FAD	C4A-C5A-N7A	-3.13	107.01	110.58
2	B	361	FAD	C4X-C4-N3	2.78	120.33	113.25
2	A	361	FAD	N3A-C4A-N9A	2.76	131.86	127.17
2	A	361	FAD	C4X-C10-N10	2.74	120.41	116.48
2	B	361	FAD	C4X-C10-N10	2.57	120.17	116.48
2	A	361	FAD	C10-C4X-N5	-2.55	119.59	124.81
2	A	361	FAD	C4X-C4-N3	2.47	119.54	113.25
2	B	361	FAD	O4-C4-C4X	-2.43	120.12	126.53
2	B	361	FAD	C5X-C9A-N10	2.40	120.14	117.97
2	A	361	FAD	C4X-C10-N1	-2.36	118.80	124.59
2	A	361	FAD	O4-C4-C4X	-2.25	120.60	126.53
2	B	361	FAD	C4X-C10-N1	-2.22	119.15	124.59
2	B	361	FAD	C6A-C5A-C4A	2.17	120.14	117.18
2	B	361	FAD	C4A-N9A-C8A	2.17	108.02	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	FAD	C10-C4X-N5	-2.13	120.45	124.81
2	B	361	FAD	C4A-C5A-N7A	-2.13	108.15	110.58
2	B	361	FAD	C9A-C5X-N5	-2.12	120.21	122.45
2	A	361	FAD	C4-C4X-C10	2.05	120.44	116.93
2	A	361	FAD	O3B-C3B-C4B	-2.03	105.25	111.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	361	FAD	O4B-C4B-C5B-O5B

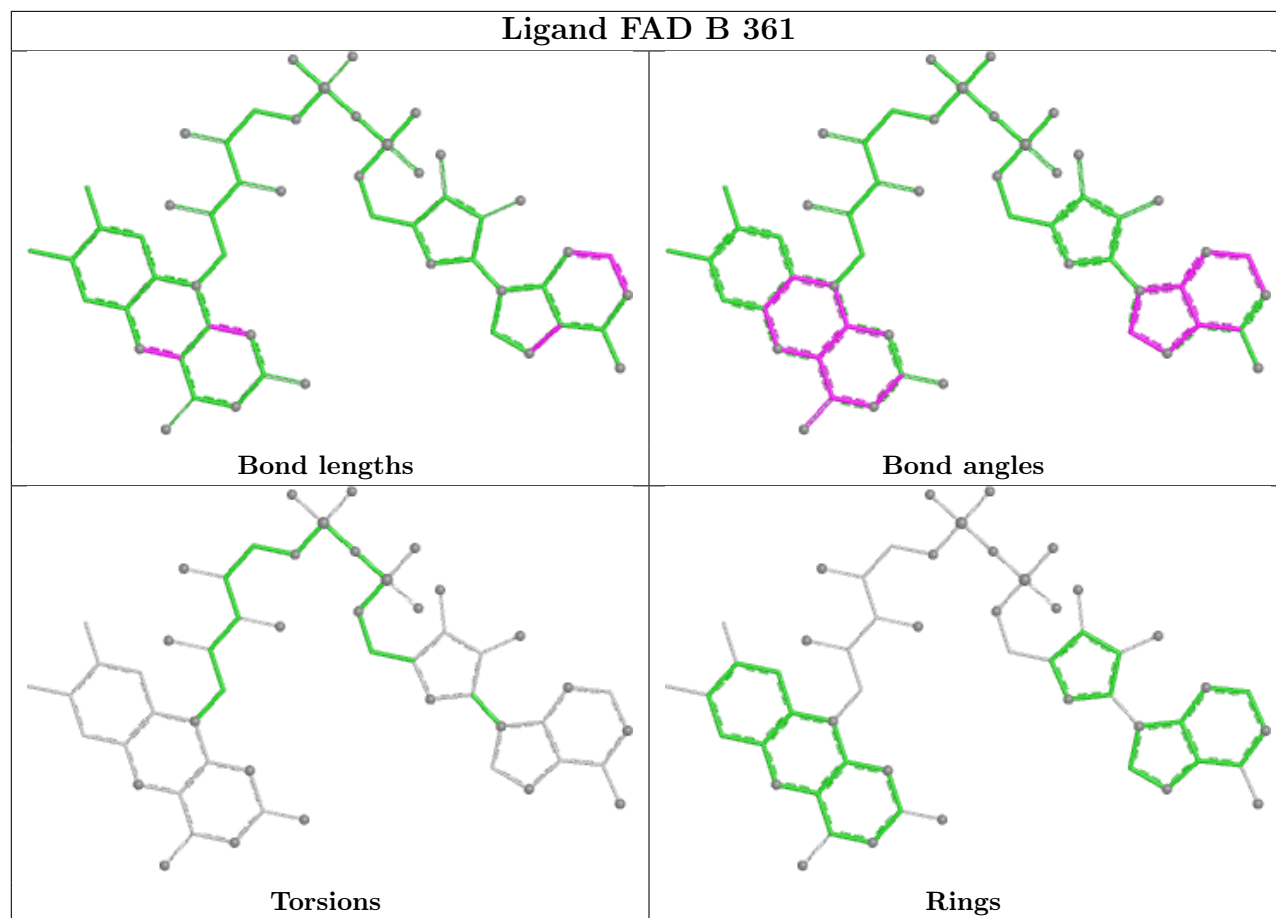
There are no ring outliers.

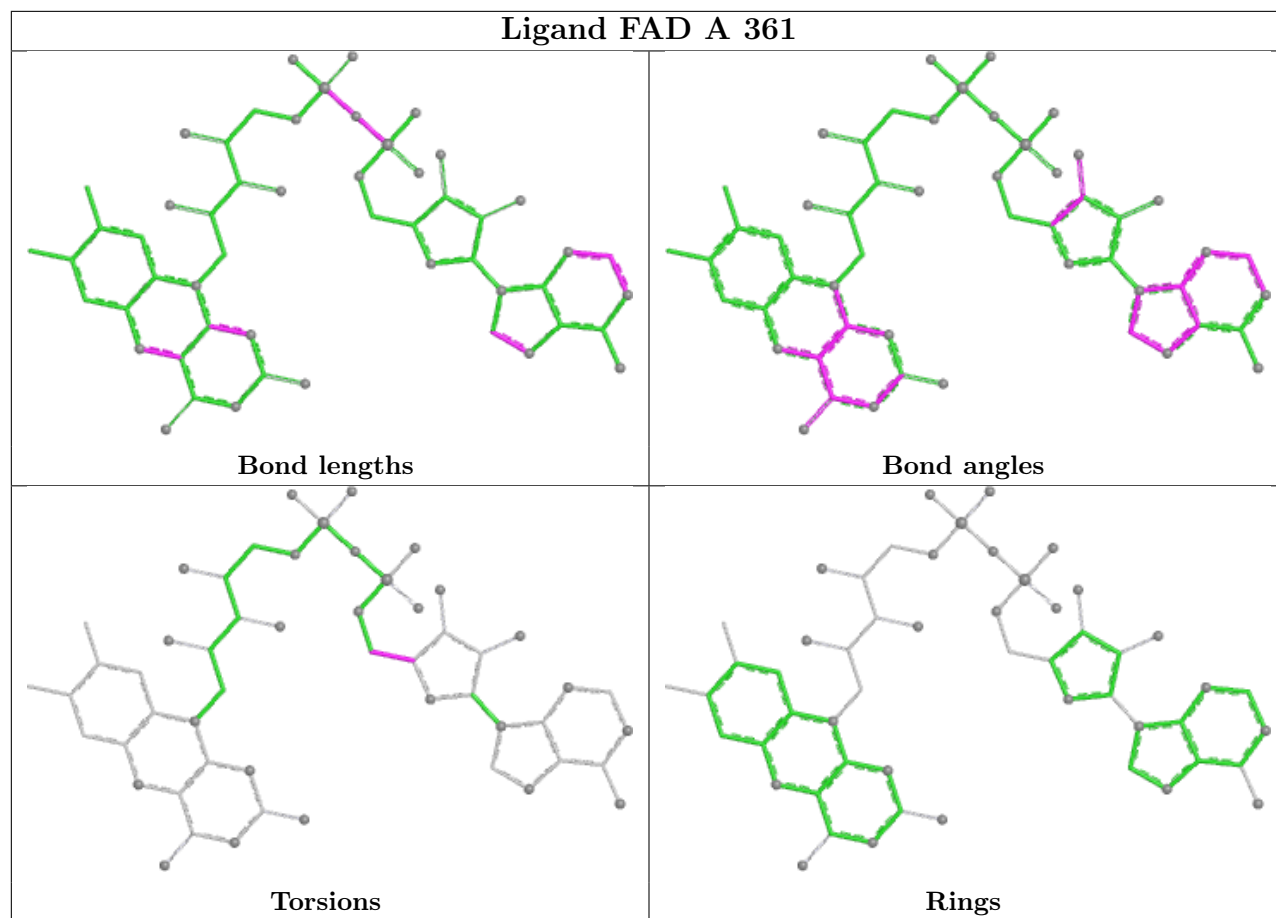
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	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 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 361





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	318/360 (88%)	1.12	59 (18%) 3 3	14, 42, 70, 86	2 (0%)
1	B	336/360 (93%)	1.05	71 (21%) 2 2	15, 43, 69, 86	1 (0%)
All	All	654/720 (90%)	1.08	130 (19%) 3 2	14, 43, 70, 86	3 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ARG	11.7
1	A	78	GLU	7.7
1	A	205	ALA	7.4
1	B	46	MET	7.1
1	A	200	GLY	6.3
1	B	200	GLY	5.7
1	B	333	ILE	5.2
1	A	208	VAL	5.1
1	B	348	ALA	5.0
1	B	246	SER	5.0
1	A	213	ALA	5.0
1	A	182	LEU	4.6
1	A	204	THR	4.3
1	B	245	GLY	4.3
1	B	347	LYS	4.2
1	A	198	PHE	4.2
1	B	338	SER	4.2
1	A	330	GLY	4.1
1	B	272	ASP	4.0
1	B	201	HIS	4.0
1	B	234	VAL	4.0
1	B	336	VAL	3.8
1	A	223	THR	3.7
1	B	235	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	202	GLY	3.6
1	A	180	VAL	3.6
1	B	343	ALA	3.5
1	A	183	ILE	3.5
1	A	264	ASN	3.5
1	A	187	ALA	3.5
1	B	202	GLY	3.5
1	B	240	LEU	3.4
1	B	238	VAL	3.3
1	B	334	ARG	3.3
1	A	181	GLY	3.2
1	A	203	LYS	3.2
1	B	178	TRP	3.2
1	B	151	VAL	3.2
1	B	250	VAL	3.2
1	A	201	HIS	3.2
1	A	206	HIS	3.1
1	B	218	ASP	3.1
1	B	236	THR	3.1
1	B	247	LYS	3.1
1	A	196	HIS	3.1
1	A	232	ASN	3.1
1	A	176	LEU	3.1
1	A	179	THR	3.0
1	A	253	ASP	3.0
1	B	163	GLY	3.0
1	A	191	LEU	2.9
1	A	221	LEU	2.9
1	B	226	ALA	2.9
1	A	216	THR	2.9
1	A	207	GLU	2.9
1	B	340	VAL	2.9
1	A	195	GLY	2.9
1	A	156	LYS	2.8
1	B	138	PRO	2.8
1	B	223	THR	2.8
1	B	182	LEU	2.8
1	A	241	ARG	2.8
1	B	232	ASN	2.8
1	B	241	ARG	2.8
1	B	225	VAL	2.8
1	B	255	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	266	GLY	2.7
1	A	161	PHE	2.6
1	B	342	MET	2.6
1	B	248	TRP	2.6
1	B	339	SER	2.6
1	A	192	VAL	2.5
1	B	186	ALA	2.5
1	B	249	THR	2.5
1	A	250	VAL	2.5
1	B	152	TYR	2.5
1	A	167	VAL	2.5
1	A	265	LEU	2.5
1	B	154	ALA	2.5
1	A	220	TYR	2.4
1	B	153	TYR	2.4
1	A	214	ASN	2.4
1	B	145	HIS	2.4
1	B	181	GLY	2.4
1	B	146	LEU	2.4
1	A	199	GLN	2.4
1	B	185	ASN	2.4
1	B	161	PHE	2.4
1	B	257	ILE	2.4
1	A	185	ASN	2.4
1	B	85	GLU	2.4
1	B	187	ALA	2.4
1	B	192	VAL	2.4
1	A	173	ASP	2.3
1	B	258	LEU	2.3
1	B	344	LYS	2.3
1	A	209	GLU	2.3
1	B	332	LYS	2.3
1	A	211	ALA	2.3
1	A	184	LYS	2.3
1	B	136	LYS	2.3
1	A	104	ASP	2.3
1	B	189	VAL	2.3
1	B	337	PHE	2.2
1	B	242	SER	2.2
1	A	240	LEU	2.2
1	B	137	LEU	2.2
1	A	151	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	172	GLY	2.2
1	B	195	GLY	2.2
1	A	243	SER	2.2
1	B	228	ILE	2.2
1	B	158	VAL	2.2
1	A	248	TRP	2.1
1	B	142	ASN	2.1
1	A	131	ALA	2.1
1	B	180	VAL	2.1
1	B	217	ILE	2.1
1	B	221	LEU	2.1
1	A	212	ARG	2.1
1	A	55	ALA	2.1
1	A	56	LEU	2.1
1	B	196	HIS	2.1
1	B	214	ASN	2.1
1	B	167	VAL	2.1
1	B	330	GLY	2.1
1	A	210	ARG	2.1
1	A	217	ILE	2.0
1	A	168	ILE	2.0
1	A	328	LYS	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.

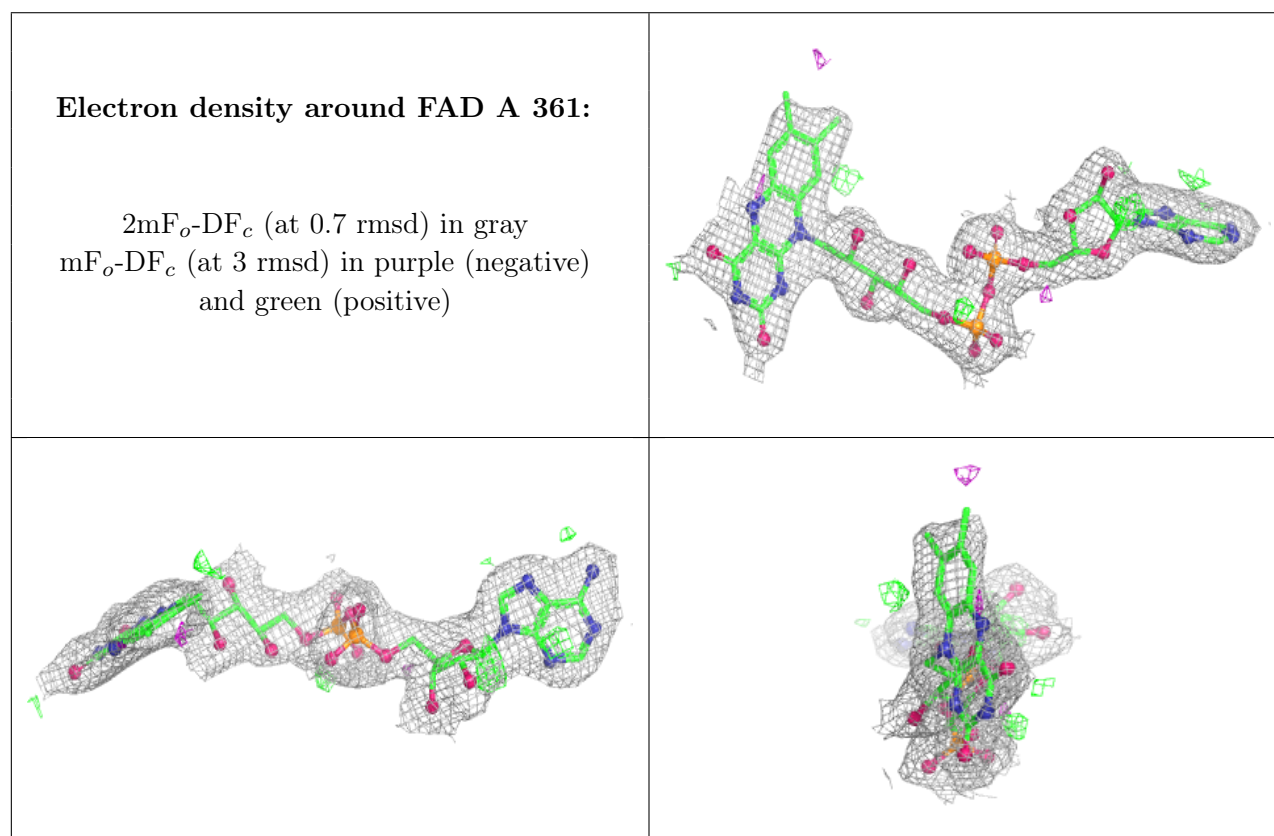
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	361	53/53	0.95	0.09	27,30,39,39	0

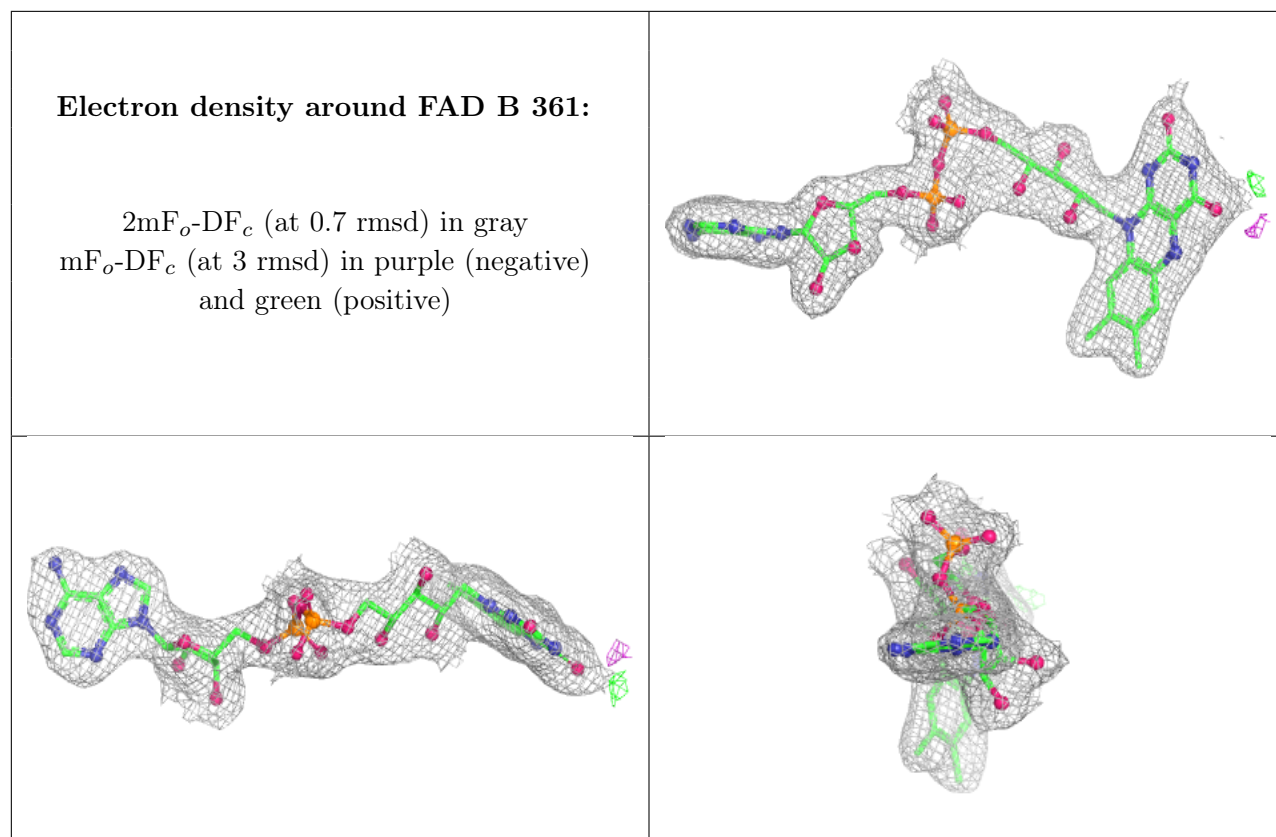
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	361	53/53	0.97	0.06	18,25,26,26	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.