



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:30 pm BST

PDB ID : 6C76
Title : Structure of Iron containing alcohol dehydrogenase from *Thermococcus thioreducens* in an orthorhombic crystal form
Authors : Larson, S.B.; McPherson, A.
Deposited on : 2018-01-20
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

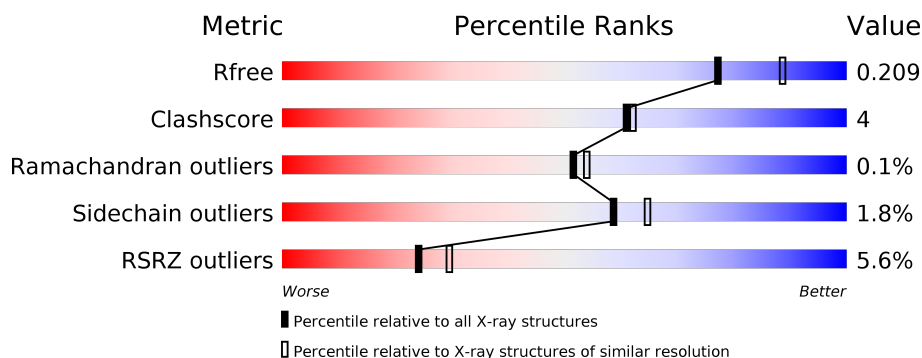
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	378	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 93% 7% </div> </div>
1	B	378	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 11%, orange 1%, yellow 1%, green 87%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 11% 84% 15% </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12595 atoms, of which 6245 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.

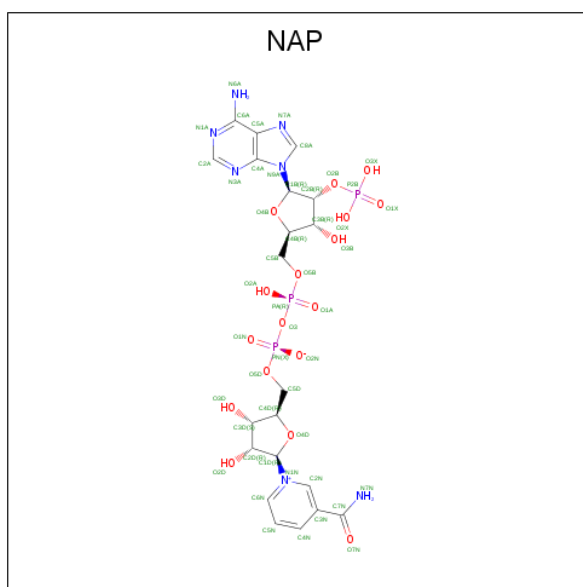
- Molecule 1 is a protein called Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	378	Total	C	H	N	O	S	0	11	0
			6055	1912	3079	507	544	13			
1	B	378	Total	C	H	N	O	S	0	18	0
			6142	1938	3124	515	553	12			

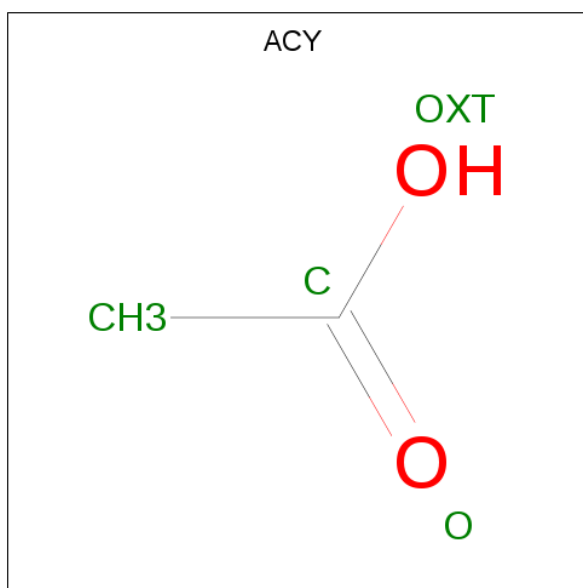
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).

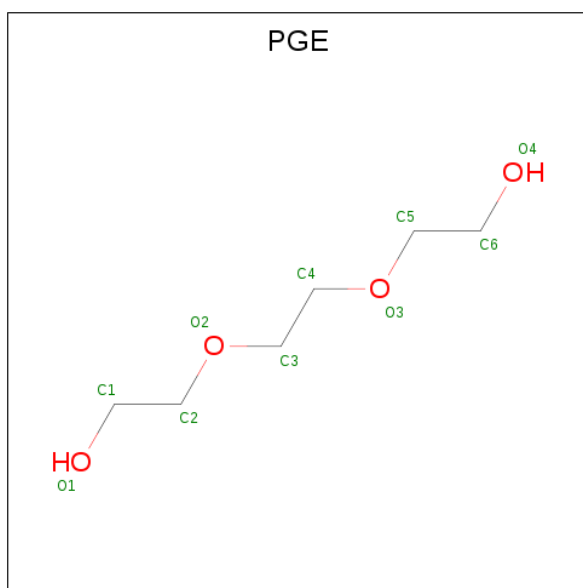


- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			24	6	14	4		

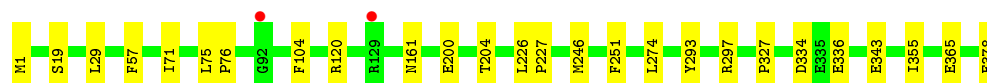
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total 167	O 167	0	7
6	B	126	Total 126	O 126	0	7

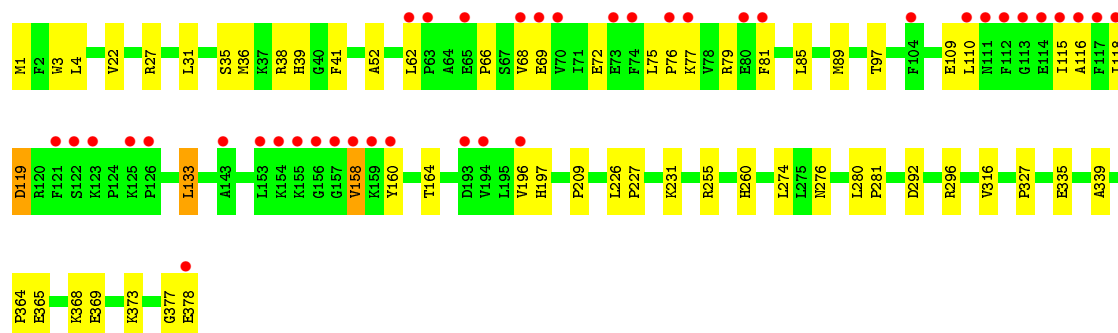
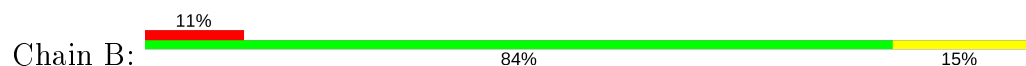
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Alcohol dehydrogenase



• Molecule 1: Alcohol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.92Å 111.98Å 142.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.04 – 2.10 33.04 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.8 (33.04-2.10) 89.9 (33.04-2.10)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.154 , 0.204 0.165 , 0.209	Depositor DCC
R_{free} test set	2018 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12595	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: ACY, PGE, NAP, FE

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	0/3090	0.49	0/4173
1	B	0.33	0/3162	0.48	0/4267
All	All	0.33	0/6252	0.49	0/8440

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ASN	Peptide
1	B	115	ILE	Mainchain

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	2976	3079	3058	14	1
1	B	3018	3124	3100	42	1
2	A	1	0	0	0	0
3	A	48	25	25	0	0
4	B	4	3	3	0	0
5	B	10	14	14	0	0
6	A	167	0	0	2	0
6	B	126	0	0	1	0
All	All	6350	6245	6200	55	1

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 4.

All (55) 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:197:HIS:CD2	1:B:260[A]:HIS:NE2	2.48	0.81
1:B:197:HIS:HD2	1:B:260[A]:HIS:CE1	2.00	0.80
1:B:197:HIS:HD2	1:B:260[A]:HIS:NE2	1.85	0.74
1:B:196:VAL:HG12	1:B:260[A]:HIS:CE1	2.26	0.71
1:B:85:LEU:HD13	1:B:133:LEU:HB3	1.76	0.66
1:B:68:VAL:O	1:B:72:GLU:HG2	1.98	0.64
1:A:29:LEU:HD12	1:A:57:PHE:O	2.00	0.62
1:B:27:ARG:HD2	1:B:81:PHE:O	2.04	0.58
1:B:75:LEU:O	1:B:79:ARG:HB2	2.05	0.55
1:B:116:ALA:HB1	1:B:160:TYR:HB3	1.89	0.54
1:B:377:GLY:O	1:B:378:GLU:O	2.26	0.53
1:B:196:VAL:HG12	1:B:260[A]:HIS:HE1	1.74	0.52
1:B:335:GLU:OE1	1:B:339:ALA:HB2	2.09	0.52
1:B:369[A]:GLU:HG3	1:B:373[A]:LYS:HE2	1.92	0.51
1:B:66:PRO:HB3	1:B:97:THR:OG1	2.12	0.50
1:A:274:LEU:HD11	1:A:327:PRO:HD2	1.93	0.50
1:B:274:LEU:HD11	1:B:327:PRO:HD2	1.94	0.49
1:B:41:PHE:HB3	1:B:89[B]:MET:CE	2.42	0.49
1:A:246:MET:CE	1:B:209:PRO:HB2	2.43	0.49
1:B:196:VAL:HG21	1:B:276:ASN:HB3	1.95	0.49
1:A:334:ASP:OD2	1:A:336:GLU:HG2	2.12	0.49
1:B:35:SER:HA	1:B:38:ARG:HG3	1.95	0.49
1:A:120:ARG:CZ	1:A:355:ILE:HD11	2.43	0.48
1:B:69:GLU:O	1:B:72:GLU:HB2	2.13	0.48
1:B:35:SER:HA	1:B:38:ARG:CG	2.44	0.48
1:B:75:LEU:N	1:B:76:PRO:CD	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:O	1:B:110:LEU:C	2.52	0.47
1:A:365:GLU:HG3	6:A:639:HOH:O	2.14	0.47
1:B:197:HIS:CD2	1:B:260[A]:HIS:CE1	2.89	0.47
1:B:77:LYS:H	1:B:77:LYS:HG2	1.48	0.46
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.98	0.46
1:A:120:ARG:NH2	1:A:355:ILE:HD11	2.30	0.46
1:B:36:MET:HG3	1:B:89[A]:MET:HG2	1.97	0.45
1:B:280:LEU:HB3	1:B:281:PRO:HD3	1.99	0.44
1:B:31:LEU:HD12	1:B:31:LEU:N	2.32	0.44
1:B:109:GLU:HG2	1:B:110:LEU:N	2.33	0.44
1:A:75:LEU:N	1:A:76:PRO:CD	2.81	0.43
1:B:118:ILE:HG23	1:B:119:ASP:N	2.33	0.42
1:B:72:GLU:HA	1:B:72:GLU:OE1	2.19	0.42
1:A:1[A]:MET:HE3	1:A:1[A]:MET:HB2	1.72	0.42
1:B:196:VAL:HG22	1:B:280:LEU:HD22	2.02	0.42
1:A:293:TYR:O	1:A:297:ARG:HG2	2.20	0.42
1:B:3:TRP:HE3	1:B:4:LEU:N	2.18	0.42
1:A:200:GLU:O	1:A:204:THR:HG23	2.20	0.42
1:B:364:PRO:O	1:B:368[B]:LYS:HG3	2.20	0.42
1:B:22:VAL:HG23	1:B:52:ALA:CB	2.51	0.41
1:A:226:LEU:N	1:A:227:PRO:CD	2.84	0.41
1:A:19:SER:HB2	6:A:614:HOH:O	2.20	0.41
1:B:231[B]:LYS:NZ	6:B:506[B]:HOH:O	2.54	0.41
1:B:35:SER:O	1:B:39:HIS:HD2	2.05	0.41
1:B:292:ASP:O	1:B:296[B]:ARG:HG3	2.20	0.40
1:A:71:ILE:HD13	1:A:104:PHE:CE2	2.56	0.40
1:B:280:LEU:N	1:B:281:PRO:HD2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:OE2	1:B:39:HIS:HE2[2_565]	1.53	0.07

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	386/378 (102%)	381 (99%)	5 (1%)	0	100	100
1	B	394/378 (104%)	371 (94%)	22 (6%)	1 (0%)	41	41
All	All	780/756 (103%)	752 (96%)	27 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	LEU

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	319/308 (104%)	316 (99%)	3 (1%)	78	84
1	B	326/308 (106%)	318 (98%)	8 (2%)	47	52
All	All	645/616 (105%)	634 (98%)	11 (2%)	59	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	PHE
1	A	343	GLU
1	A	378	GLU
1	B	1	MET
1	B	119	ASP
1	B	133	LEU
1	B	158	VAL
1	B	164	THR
1	B	255	ARG
1	B	316	VAL
1	B	365	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS
1	B	197	HIS
1	B	351	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	NAP	A	402	-	45,52,52	0.82	1 (2%)	56,80,80	1.12	5 (8%)
4	ACY	B	401	-	1,3,3	1.53	0	0,3,3	0.00	-
5	PGE	B	402	-	9,9,9	0.47	0	8,8,8	0.22	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	PGE	B	402	-	-	2/7/7/7	-
3	NAP	A	402	-	-	5/31/67/67	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAP	C5A-C4A	2.38	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAP	N3A-C2A-N1A	-3.78	122.77	128.68
3	A	402	NAP	C2B-C3B-C4B	2.20	106.78	101.99
3	A	402	NAP	C3N-C7N-N7N	2.11	120.28	117.75
3	A	402	NAP	C2A-N1A-C6A	2.10	122.35	118.75
3	A	402	NAP	C4A-C5A-N7A	-2.08	107.24	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

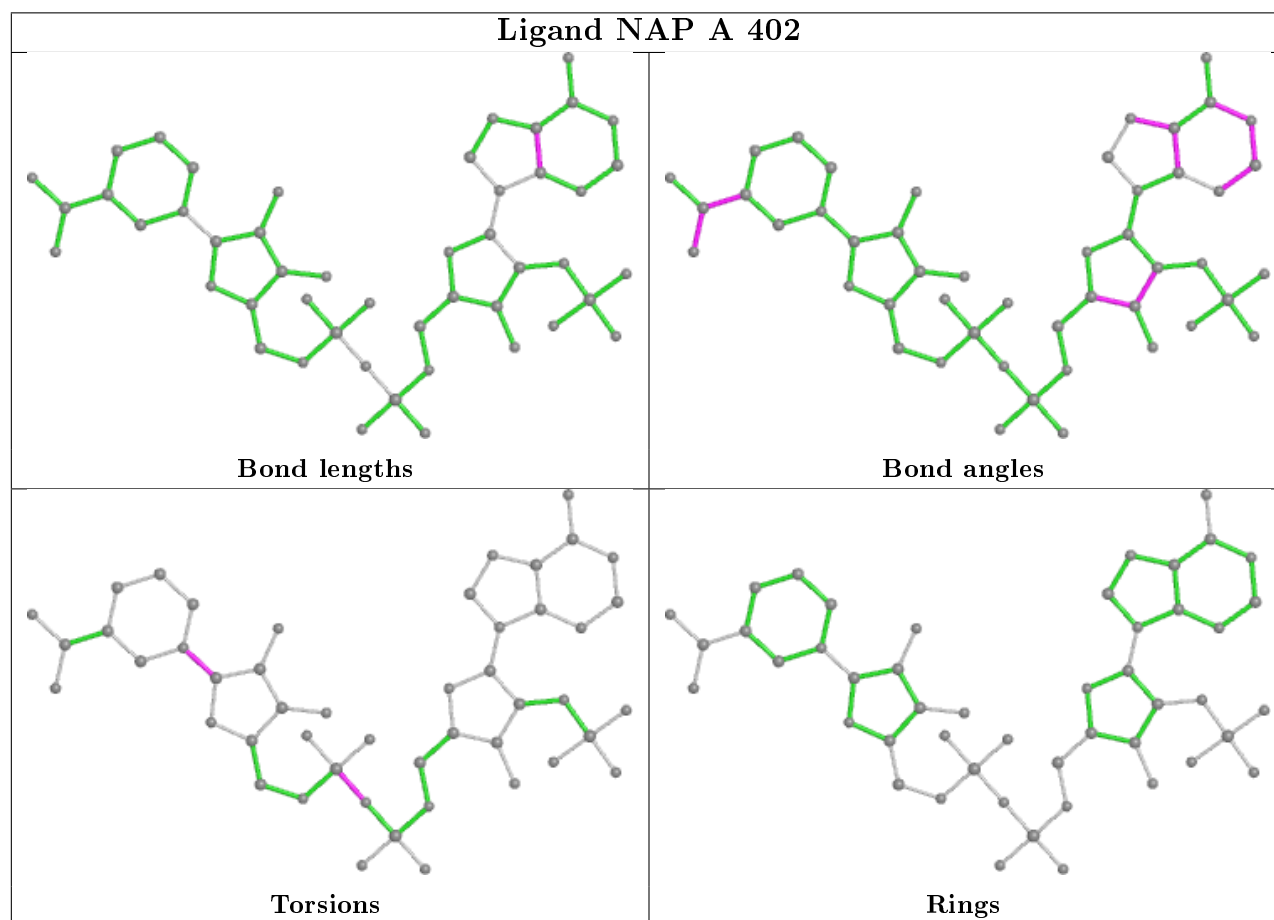
Mol	Chain	Res	Type	Atoms
3	A	402	NAP	O4D-C1D-N1N-C2N
3	A	402	NAP	O4D-C1D-N1N-C6N
3	A	402	NAP	C2D-C1D-N1N-C2N
3	A	402	NAP	C2D-C1D-N1N-C6N
5	B	402	PGE	O2-C3-C4-O3
3	A	402	NAP	PA-O3-PN-O5D
5	B	402	PGE	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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	378/378 (100%)	-0.24	2 (0%) 91 92	19, 35, 61, 95	0
1	B	378/378 (100%)	0.35	40 (10%) 6 7	21, 46, 104, 126	0
All	All	756/756 (100%)	0.06	42 (5%) 24 29	19, 39, 89, 126	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	TYR	7.3
1	B	115	ILE	5.1
1	B	158	VAL	5.0
1	B	114	GLU	4.6
1	B	110	LEU	4.4
1	B	117	PHE	4.3
1	B	121	PHE	4.2
1	B	111	ASN	4.2
1	B	80	GLU	4.1
1	B	113	GLY	4.0
1	B	125	LYS	3.9
1	B	157	GLY	3.8
1	B	156	GLY	3.4
1	A	129[A]	ARG	3.3
1	B	118	ILE	3.2
1	B	126	PRO	3.0
1	B	153	LEU	3.0
1	B	123	LYS	3.0
1	B	155[A]	LYS	2.9
1	B	63	PRO	2.7
1	B	77	LYS	2.7
1	B	112	PHE	2.7
1	B	74	PHE	2.6
1	B	68	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	143	ALA	2.5
1	B	122	SER	2.5
1	B	378	GLU	2.5
1	B	116	ALA	2.5
1	B	196	VAL	2.4
1	B	154[A]	LYS	2.4
1	B	194	VAL	2.3
1	B	193	ASP	2.3
1	B	104	PHE	2.3
1	B	73	GLU	2.3
1	A	92	GLY	2.2
1	B	65[A]	GLU	2.2
1	B	62	LEU	2.1
1	B	159	LYS	2.1
1	B	69	GLU	2.1
1	B	76	PRO	2.1
1	B	81	PHE	2.0
1	B	70	VAL	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](#)

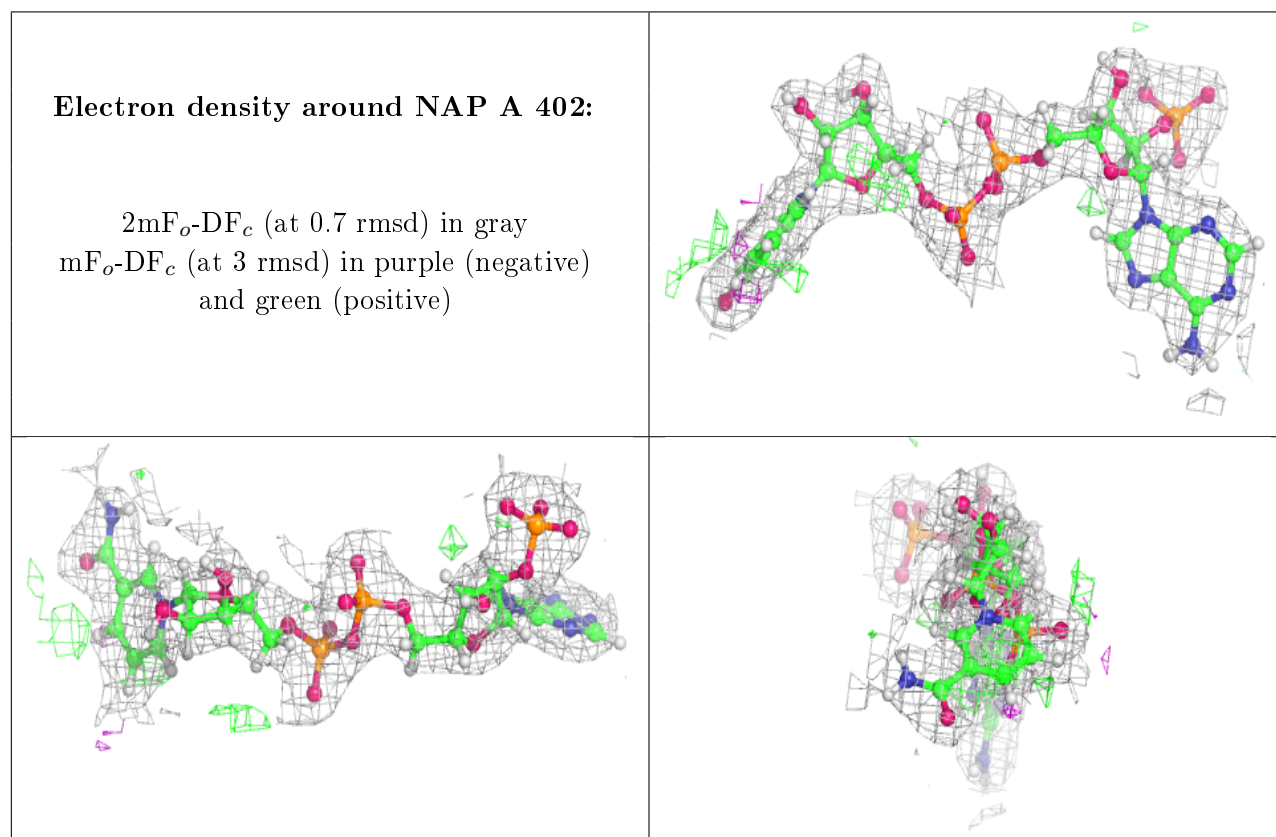
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
5	PGE	B	402	10/10	0.76	0.32	71,82,85,87	0
4	ACY	B	401	4/4	0.94	0.33	43,49,53,57	0
2	FE	A	401	1/1	0.98	0.07	65,65,65,65	0
3	NAP	A	402	48/48	0.98	0.19	23,31,35,44	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.